

Addressment of Uncertainty and Variability in  
Attributional Environmental Life Cycle Assessment

by

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## ABSTRACT

'Attributional' Life Cycle Assessment (LCA) quantitatively tracks the potential environmental impacts of international value chains, in retrospective, while ensuring that burden shifting is avoided. Despite the growing popularity of LCA as a decision-support tool, there are numerous concerns relating to uncertainty and variability in LCA that affects its reliability and credibility. It is pertinent that some part of future research in LCA be guided towards increasing reliability and credibility for decision-making, while utilizing the LCA framework established by ISO 14040.

In this dissertation, I have synthesized the present state of knowledge and application of uncertainty and variability in 'attributional' LCA, and contribute to its quantitative assessment.

Firstly, the present state of addressment of uncertainty and variability in LCA is consolidated and reviewed. It is evident that sources of uncertainty and variability exist in the following areas: ISO standards, supplementary guides, software tools, life cycle inventory (LCI) databases, all four methodological phases of LCA, and use of LCA information. One source of uncertainty and variability, each, is identified, selected, quantified, and its implications discussed.

The use of surrogate LCI data in lieu of missing dataset(s) or data-gaps is a source of uncertainty. Despite the widespread use of surrogate data, there has been no effort to (1) establish any form of guidance for the appropriate selection of surrogate data and, (2) estimate the uncertainty associated with the choice and use of surrogate data. A formal expert elicitation-based methodology to select the most appropriate surrogates and to quantify the associated uncertainty was proposed and implemented.

Product-evolution in a non-uniform manner is a source of temporal variability that is presently not considered in LCA modeling. The resulting use of outdated LCA

information will lead to misguided decisions affecting the issue at concern and eventually the environment. In order to demonstrate product-evolution within the scope of ISO 14044, and given that variability cannot be reduced, the sources of product-evolution were identified, generalized, analyzed and their implications (individual and coupled) on LCA results are quantified.

Finally, recommendations were provided for the advancement of robustness of 'attributional' LCA, with respect to uncertainty and variability.

## DEDICATION

I dedicate my academic endeavor to: (1) my dad and my mom, who put me on a path to curiosity, supported me, and continually encouraged me to be better, and (2) my advisor, Jay Golden, who taught me, guided me, pushed me and gave me opportunities to succeed.

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## CHAPTER 1

### INTRODUCTION

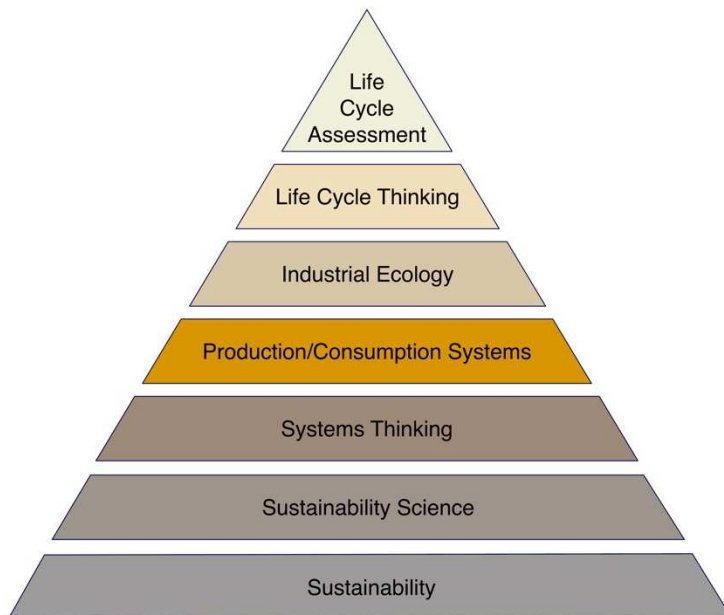
Sustainability is widely recognized as a key issue facing society in this century (Komiyama & Takeuchi, 2006). 'Sustainability' has become a popular word to highlight balanced responsibility across all aspects of a particular issue of concern. It is also widely used to redefine activities (e.g.: sustainable tourism, sustainable diet) and academic disciplines (e.g.: sustainable engineering, sustainable supply chain management). Lubin and Etsy (2010) refer to 'Sustainability' as an emerging business megatrend, in line with globalization, and information-based society. Given the widespread and profound embeddedness of sustainability in various fields and disciplines, the complexity of issues that fall within its purview can be confusing and overwhelming. Therefore, in the first sub-section (1.1), the author explores the concept of sustainability at the highest level and gradually brings focus to how this thesis fits within its purview, as shown in figure 1. This thesis lies at the intersection of sustainability and uncertainty, by focusing on the improvement of certainty in environmental life cycle assessment (LCA) of products. LCA is a methodology based on the life cycle thinking approach that is used to quantify the potential environmental impacts of products or process, while ensuring that burden shifting does not occur. LCA is being increasingly used to address sustainability goals as it relates to production and consumption, by providing quantification to environmental sustainability (O. Jolliet, Saadé-Sbeih, Shaked, Jolliet, & Crettaz, 2016).

'Uncertainty' is a consequence of the lack of certainty (Bedford and Cooke, 2001). Akin to sustainability, uncertainty also cuts across numerous issues and disciplines, but more importantly, the consideration of which is critical for decision making. Humans make decisions every day not just in their personal lives, but also to facilitate the economy and the society in a sustainable manner. The United

Nations Economic Commission for Europe (2005) implies that the lack of certainty causes political and economic instability, which is unsustainable for human civilization. On the importance of uncertainty, the second sub-section (1.2) of this chapter explores the notion of uncertainty, and how it applies to sustainability and life cycle assessment.

In the last section (1.3) of this chapter, the author delves into the need for this thesis research.

Figure 1: Hierarchical focus on the interlinkages between sustainability and life cycle assessment, in chapter 1



## **1.1 Sustainability: 10,000 Feet to 1 Foot**

The pressure on earth's natural resources, ecosystem services, and human health is increasing at a rapid pace (European Commission, 2010; Holmberg, 1998; Jolliet et al., 2015). Much of this pressure is attributed to the growing population and its burgeoning demand for energy and consumer goods & services (Hertwich, 2005), advancing technology, affluence growth, urbanization, and economic growth (Allenby, 2014).

### **1.1.1 What is Sustainability?**

Sustainability is considered to be a human-centered approach towards managing all vital resources in a balanced and responsible manner. Jackson (2010) offers a succinct definition of sustainability as "the art of living well, within the ecological limits of a finite planet". According to Kidd (1992), six, different but related, streams of thought served as drivers to the sustainability movement, in the 1950s, even before the word 'sustainability' was first used. These thought streams are: (1) ecological/carrying capacity, (2) resources/environment, (3) biosphere, (4) critique of technology, (5) "No growth - Slow growth", and (6) eco-development. Kidd (1992) cites the first use of the term 'sustainability' in the landmark article "A Blue Print for Survival" (Goldsmith, 1972), in the context of the future of humanity. It is understood that the term became popular after 1978 with its use extending to technology and policy discourses. Kidd (1992) states that the literature on sustainability is voluminous, and the search for a single definition of the term 'sustainability' is futile, due to its deep embeddedness in many fundamentally different concepts. He proposes that as long as the definitions are clearly communicated, then the existence of multiple meanings can be tolerated.



### **1.1.2 History of Sustainability and its Evolution**

Redman (1999) traces ancient history on the issue of sustainability to food shortages, biodiversity threats, and urban sprawl. Using archeological record, he demonstrates the constructive and destructive long-term relationships that various societies established with their environments. Examples of destructive relationships where environments degraded and threatened human survival include the clearing of Mayan forests, erosion of soil in ancient Greece and near total depletion of resources in Easter Island.

Kidd (1992) traces recent history on the issue of sustainability back to the end of World War II when there were doubts about resource availability for economic expansion in the industrialized nations. Later, there were a series of events such as the conservation movement (1960s and 1970s), publications of hard-hitting books and reports (Silent Spring, Limits to Growth, The Global 2000 Report, Resourceful Earth) and anthropogenic environmental disasters (industrial, nuclear, deforestation, mining) that served as drivers for a robust environmental movement. The economic deregulation in the 1990s led to globalization (Di Giovanni et al., 2008), which brought many issues relating to socio-economic exploitation (e.g.: child labor) under the scanner. The shoe company, Nike, became a poster-child for its use of exploitive contract labor in emerging economies for its sweatshop working conditions. Thereby the environmental/ecological movement transformed to include far-reaching socio-economic approaches.

Based on a literature review on sustainability, Giovannoni and Fabietti (2013) have identified three discourses (environmental, social and business) that have influenced the "evolving debate on sustainability." The three-pillar approach to sustainability that includes environmental, social and economics, also referred to as 3P's (People, Planet, Prosperity) or triple bottom line, has been used in sustainability

discourses in academic and public for a long time. The argument is that sustainability can be achieved only when there is an equal balance across the three pillars.

Komiyama and Takeuchi (2006) view sustainability as a problem with three fundamental interlinked levels of systems: global (climate, resources, ecosystem), social (politics, economy, industry, technology) and human (security, lifestyle, health, values, and norms). They demonstrate several sustainability problems that are an outcome of the inter-linkages between two systems. For example, global warming is a result of the interaction between social and world systems. Another example is the generation of waste, which is an outcome of the interaction between social and human systems.

To implement sustainability globally, the United Nations re-envisioned concept of development as one "to lead to self-fulfillment and creative partnership in the use of a nation's productive forces and its full human potential" (UN, 1980). The guiding principle for sustainable development (SD) was first framed in 1987 in the Brundtland Report, also known as "Our Common Future." The report envisioned the possibility of sustained human progress and survival provided that environmental resources be managed effectively (WCED, 1987). The concept of sustainable development involves the integration of environmental and physical constraints to all activities of life (Elkington, 1994; McCloskey, 1998). The 1992 Earth Summit adopted "Agenda 21", a global plan for sustainable development (United Nations, 1997). Despite the actionable goals of the 1992 Earth Summit, the tremendous economic growth, that promoted societal improvement, came with the price of climate change, biodiversity loss, land degradation, and other social and economic impacts and insecurities (UNFPA, 2011). At the Millennium Summit, in 2000, world leaders adopted eight time-bound goals (e.g.: eradicate extreme hunger and poverty), also referred to as the Millennium Development Goals (MDG), to be

accomplished before the end of the year 2015 (United Nations, 2006). The final recommendations were provided in 2005 in a document titled "Investing in Development: A Practical Plan to Achieve the Millennium Development Goals" (United Nations, 2006). In 2002, the World Summit on Sustainable Development (a.k.a. Johannesburg Summit) called for fundamental changes in the way that societies consume and produce, as indispensable for achieving sustainable development (United Nations, 2002). The United Nations suggested the use of 'Principle 7' of the Rio Declaration, which is "the principle of common but differentiated responsibilities." In other words, it stipulates that governments, relevant international organizations, the private sector and other major groups should actively work together in changing unsustainable consumption and production patterns. In over three decades, while progress has been made on many fronts, the United Nations has evidenced that progress has been unbalanced within and across countries. The United Nations has reported that only three of the eight MDG's has been achieved before the 2015 deadline (United Nations, 2016). The Post-2015 Agenda, which focused on what happens after the expiry of the MDG's, was discussed at the Rio+20 Summit. This discussion resulted in the establishment of 17 Sustainable Development Goals (SDG) and 169 targets, which has been published in the document titled "Transforming our World: The 2030 Agenda for Sustainable Development" (United Nations, 2015). Apart from the expansion of goals and targets, it is understood that the distinct evolution between the MDGs and SDGs is the inclusion of all stakeholders, especially since MDGs ignored migrants, refugees, and internally displaced people.

Research relating to sustainable development has been long pursued in disciplines such as geography, ecology, economics, but there is growing academic interest to promote a sustainability transition as a core research program – resulting in the evolution of the new field of science (Clark, 2007). At the same time, there

was growing concerns and discontent due to the influence of political agendas that were shaping sustainable development in the United Nations, in the late 1980s and early 1990s (Kates et al., 2001; Komiyama & Takeuchi, 2006). Calls for a science of sustainability, predicated on the understanding of the fundamental relationship between science and economy, that was free from political bias was made at the International Council for Science in the 1990s (Komiyama & Takeuchi, 2006). Clark (2007) differentiates the applications of sustainable development and sustainability science to clarify potential confusion in their scopes. He cites SD examples such as enabling access to clean and adequate water supplies, advancing cleaner energy, alleviating poverty, et cetera, and sustainability science examples such as mitigating climate change, adaptation strategies for climate change, biodiversity protection, et cetera.

### **1.1.3 Sustainability Science**

The seminal paper on sustainability science by Kates et al. (2001) defines the field as one that seeks to comprehend the characteristics of interactions (geographic scale, intensity scale, time scale, functional complexity, outlook range) between nature and society, and enable society to guide the interactions along sustainable trajectories. Miller (2012) views sustainability science as an emerging interdisciplinary field that aspires to transform knowledge into social actions that seek the well-being of nature and society. Wiek et al. (2012) refers to sustainability science as the “research that generates knowledge that matters to people’s decisions and engages in arenas where power dominates knowledge; and education that enables students to be visionary, creative, and rigorous in developing solutions and that leaves the protected space of the classroom to confront the dynamics and contradictions of the real world”. These different views of sustainability science together offer a somewhat holistic view of the academic discipline.

Kates et al. (2001) argue that sustainability science is considerably different from the general sciences based on the inclusion of the following four distinct aspects: (1) range of geographical scales, (2) range of temporal scales, (3) functional complexity, and (4) range of outlooks.

To address this new science, Komiyama & Takeuchi (2006) argue that novel methods and techniques need to be “used, extended or invented.” At the same time, multi-stakeholder participatory procedures should be utilized to prevent unintended consequences from scientific progress – checks and balances (Komiyama & Takeuchi, 2006). According to Clark (2007), sustainability science is neither “basic” research nor is it “applied” research, but it is both and referred to as “use-inspired basic research”. In other words, it advances useful knowledge (basic research) and informed action (applied research) by building a bridge in between the two.

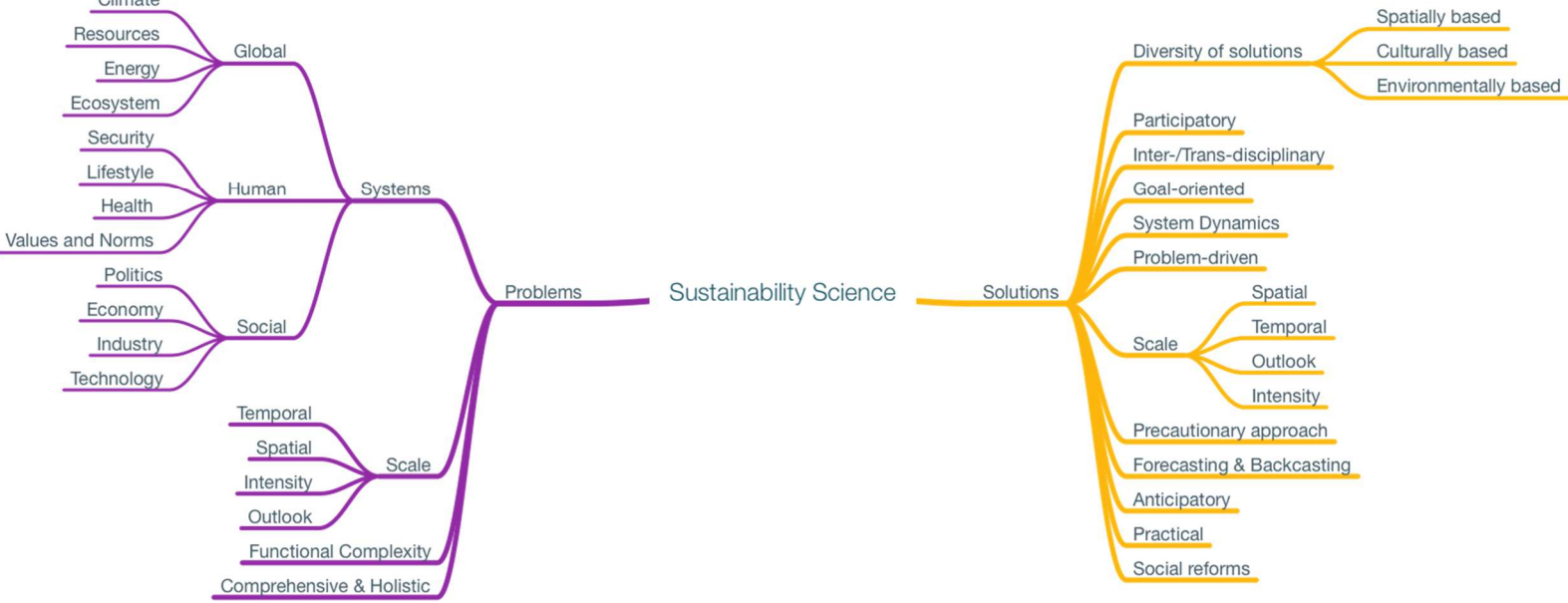
#### **1.1.3.1 Sustainability Science Problems**

Given the complexity of sustainability problems, Komiyama and Takeuchi (2006) recommend that sustainability science adopts a “comprehensive and holistic approach to identification of problems and perspectives.” At the same time, given the numerous systems and elements involved in sustainability, specialization is necessary to comprehend these complex issues. Komiyama and Takeuchi (2006) also recommend the transdisciplinary research where individual disciplines can provide quantitative criteria, and indicators pertinent to and grasp of sustainability issues. To solve highly complex problems in the coupled human-environmental systems, sustainability science is tapping into areas such as complex systems theory, cultural and political ecology, system dynamics, and uncertainty theory, that which is uncommon for other disciplines (Clark, 2007). We will explore system dynamics in the next subsection (1.1.4) and uncertainty theory in the section (1.2).

### **1.1.3.2 Sustainability Science Solutions**

When implementing solutions for sustainability problems Komiyama and Takeuchi (2006) argue for a diversity of solutions that are spatially, culturally and environmentally based, because a 'one-size fits all' solution cannot be expected to work. They recognize the need to anticipate problems, and, create and implement solutions for scenarios yet to occur. Even if the models used to anticipate problems cannot be verified, it is recommended that a precautionary approach is taken, and the search for solutions be continued (Komiyama & Takeuchi, 2006). Clark (2007) highlights the application of sustainability science to practical protections to earth systems, such as climate change, water scarcity management, adaptation to climate change, et cetera. While it is expected of sustainability science to build sound models to evaluate existing processes and predict for future scenarios, it also pertinent that sustainability science ensures the uptake of research outputs by society through social reforms and other measures to ensure global sustainability (Komiyama & Takeuchi, 2006). Figure 2 condenses all the above information on sustainability science in the form of characteristics of problems and solutions.

Figure 2: Characteristics of problems and solutions in sustainability science



#### **1.1.4 System Thinking, Approach & Dynamics**

Senge (1990) states that systems approach is at the heart of sustainability. Systems thinking, which Senge (1990) refers to as the fifth discipline, is a conceptual framework for visualizing the invisible interrelationships and patterns of transition and transformation of systems. Examples of systems include businesses, humans, nitrogen cycle, transportation, plants, animals, information, cities, states, et cetera. He opines that nature is not a sum of parts (within a whole) but a sum of wholes, resulting in something larger than a whole. Boardman and Sauser (2008) note that people from different fields such as physics (Albert Einstein) and biology (Ludwig von Bertalanffy) used systems as an approach to simulate thinking, even before the emergence of systems as an academic discipline or field.

In 1961, the seminal publication titled "Industrial Dynamics" by Jay Forrester initiated the development of the field of System Dynamics. The field seeks to understand better and manage complex non-linear systems that exhibit dynamic behavior (e.g.: economic systems, ecological systems, social systems, managerial systems, et cetera). The System Dynamics Society defines system dynamics as "a computer-aided approach to policy analysis and design", and notes that it applies to "any dynamic systems characterized by interdependence, mutual interaction, information feedback, and circular causality" (System Dynamics Society, 2016). Concepts such as feedback thinking, feedback loop dominance, stocks and flows, and endogenous point-of-view are integral to the systems dynamics approach (System Dynamics Society, 2016). Forrester (2007) notes that system dynamic models can retain the richness of process information collected, including dynamic behaviors based on different policies, unlike case-studies (pioneered by Harvard) that are unable to capture the dynamic complexity involved. The primary form of analysis for system dynamics is dynamic simulation analysis.



Systems thinking, which is an increasingly popular term in industrial engineering and sustainability, has come to mean more than just thinking, talking, and acknowledging systems. Forrester (1994) notes that in the U.S., systems thinking “implies a rather general and superficial awareness of systems.” Forrester (2007) observes that systems thinking is not quantitative, and does not provide an understanding of why dynamic behavior occurs, but it demonstrates the existence of complexity. Forrester (2007) refers to systems thinking as a gateway to system dynamics and estimates potential knowledge gain from the two areas through a ratio of 5:95. Forrester (1994) states that systems thinking and soft operations research help organize and guide processes when system dynamics interfaces with society in the system under consideration. At the same time, Forrester (1994) warns that superficial enthusiasm of systems thinking may misguide users to think that systems thinking is sufficient to solve complex problems. Boardman and Sauser (2008) distinguish two types of systems thinking: (1) thinking about systems and (2) thinking from systems. Thinking about systems refers to focusing thinking on the systems, which guides our otherwise chaotic thinking. Thinking from systems refers to focusing our thinking on the systemic descriptions of the problem and its treatments, along with stakeholders of the problem.

The book ‘Limits to Growth’ by Donella Meadows, published in 1972, is considered one of the seminal books on sustainability and systems, and a driver for action on sustainable development. This book, funded by the Club of Rome, demonstrates the impacts of the exponential growth of five variables (world population, industrialization, pollution, food production and resource depletion) using system dynamics based computer simulation – World3 model developed by Jay Forrester. The book is a successor to Forrester’s World Dynamics, which was

published nine months earlier, improved on the assumptions used and was written appropriately for public consumption (Forrester, 2007).

Meadows (1997) highlights the importance of leverage points in systems analysis, by stating that it is what practitioners are looking for in complex systems. She also highlights Jay Forrester's favorite quote that "People know intuitively where leverage points are..." but they are pushing in the wrong directions. She also cites Forrester's word to describe complex systems as 'counterintuitive'. In other words, finding leverage points are difficult, and when one finds it, no one will believe that it is the leverage point. Meadows (1997) identifies the following ten places to intervene in a system, as a means to think more broadly about system change: (1) power to transcend paradigms, (2) mindset or paradigm out of which the goals, rules, feedback structure arises, (3) goals of the system, (4) power of self-organization, (5) rules of the system, (6) information flows, (7) driving positive feedback loops, (8) regulating negative feedback loops, (9) material stocks and flows, and (10) numbers. Meadows' modeling work "Groping in the Dark – The First Decade of Global Modelling" (D. H. Meadows, Richardson, & Bruckmann, 1982) has served an integral part in the Brundtland Commission's report "Our Common Future" (WCED, 1987) towards igniting the SD movement.

United Kingdom's Department for Environment, Food and Rural Affairs (DEFRA) notes that in the 1990s and 2000s, several pervasive environmental problems emerged on top of existing problems, such as resource depletion, climate change, and biodiversity reduction. These newer problems were identified to be widely different from the older problems and called for shifts in systems in order to obtain the desired improvements in environmental efficiency (Geels, Monaghan, Eames, & Steward, 2008). It has been recognized that in order to understand the environmental impact of a single product or process, the environmental impacts of

the larger system must be first understood. Further to this recognition is that the reduction of environmental impacts of one product may be accompanied by an increase in systemic environmental impact associated with increased consumption. They note that 'system change' is a newer approach to environmental policy, when compared to (1) end-of-pipe – reactive solutions, (2) process efficiency measures and industrial ecology – process solutions, and (3) product life cycle – product solutions. The Systems approach targets society as a whole towards a certain vision as a driving philosophy, with attributes such as (1) co-evolutionary and multi-dimensional, (2) multi-actor, (3) multi-level, (4) radical, (5) long-term and (6) non-linear. Sustainable Consumption and Production (SCP) incorporates the many of the attributes of the systems approach, especially the concept that sustainable solutions necessitate social and technological change (Geels et al., 2008).

### **1.1.5 Production and Consumption Systems**

Production and consumption systems are integral to sustain human society. Production is often associated with supply chains, and consumption is often associated with the purchase, use, and end-of-life. Production and consumption have the potential to affect all facets of society (e.g.: income inequality, power, politics) and nature (e.g.: ecosystem services, biodiversity, resource depletion). European Commission (2010) states that, currently, we do not produce and consume products in a sustainable manner. In other words, we utilize production practices and technologies that are detrimental to the environment to produce products that affect human and environmental health during their use and end-of-life. Kates (2000) notes that both over-consumption and under-consumption exists side-by-side in the real world.

There are several approaches to sustainability in production and consumption: (1) sectoral approaches such as improvement of productivity in

transportation and agriculture by reducing the pollutants into the air, soil and water, (2) place-based approaches that focus on local environmental challenges by addressing the drivers in an optimal manner, (3) product-oriented approaches that focus on minimizing use of resources and minimizing emissions in the supply chain that are hazardous to nature, and (4) consumer-oriented approaches that focus on behavioral change related to purchase or use of products that lead to reduced impacts on the environment (Lebel, Lorek, & Daniel, 2010).

The Oslo symposium, in 1994, first defined sustainable consumption and production (SCP) as "the use of services and related products, which respond to basic needs and bring a better quality of life while minimizing the use of natural resources and toxic materials as well as the emissions of waste and pollutants over the life cycle of the service or product so as not to jeopardize the needs of further generations" (UN-DESA, 2016). SCP has gained further momentum by being recognized at the Johannesburg World Summit (2002), by being central to the 10-year framework for SCP that was adopted at the Rio+20 conference on sustainable development. Most recently, the achievement of SCP has been made an integral part of the SDGs in the post-2015 development agenda (United Nations Environmental Programme, 2015).

The following are the four fundamental principles of sustainable consumption and production (European Environment Agency, 2013):

- advance quality of life into the future, whilst preventing the increase in environmental degradation and conserving resource use
- remove the inversely linear relationship between economic growth and environmental degradation by:

- improving efficiency in the use of energy and resources and decreasing emissions to soil, water, and air
- advocating a shift in consumption patterns towards resource-efficient products and processes without affecting the quality of life
- exercise life cycle thinking approaches in production and consumption
- prevent the occurrence of rebound effects, when increased consumption negates the gains from increased efficiency

Traditionally, the tools used to mitigate the environmental impacts were focused on production, but SCP takes it a step further and includes consumption. SCP utilizes LCT approaches and industrial ecology (IE) instruments to achieve its principles.

### **1.1.6 Industrial Ecology**

Industrial Ecology seeks to transform industrial systems by so that they mimic ecological systems – all waste is reused – this is currently being referred to as ‘circular economy’. The term ‘Industrial Ecology’ was first used by Frosch and Gallopoulos (1989), in the form of ‘industrial ecosystem’, at a time when the anthropogenic impacts on ecology were barely understood. The driver for the emergence of Industrial Ecology was the need to understand the complicated interlinkages between industrial systems, ecological systems and human systems (Gradel and Allenby, 1995; Clift and Druckman, 2016). The International Society for Industrial Ecology has adopted a definition from White (1994), which states “the study of flows of materials and energy in industrial and consumer activities, of the effects of these flows on the environment, and of the influences of economic, political, regulatory and social factors on the flow, use and transformation of

resources". Allenby (2006) defines industrial ecology as "a systems-based, multidisciplinary discourse that seeks to understand emergent behavior of complex integrated human/natural systems". Clift and Druckman (2016) note that this definition utilizes a systems approach and multi-disciplinary approach. Given that industrial ecology is concerned with ecological limits, impacts associated with the related industrial system, it is concerned with sustainability. Graedel and Allenby (1995) state that industrial ecology seeks to guide our future trajectory to sustainable development. They also bring to focus the IPAT equation, which was established by Ehrlich and Holdren (1971), as a suggested avenue for sustainable living.

$$\text{Impact} = \text{Population} \times \text{Affluence} \times \text{Technology}$$

This equation was deployed to understand the environmental impacts caused by the combination of technological progress, income inequality, and population growth. For example, the actionable parameter in this equation for industry is technology, especially cleaner technology for the purposes of energy generation, waste production and such.

Life Cycle Assessment (LCA) has been one of the essential tools for industrial ecology, as it delves with identifying and quantifying the potential environmental impacts across the product supply chain, while ensuring that burden shifting does not occur. Other industrial ecology tools include Design for Environment, Industrial Symbiosis, eco-industrial parks, Urban Metabolism, Input-Output Analysis, Socio-Economic Metabolism, and Material Flow Analysis.

### **1.1.7 Life Cycle Thinking**

Life Cycle Thinking has been suggested as a critical approach to identify improvements in products in the form of reduced health and environmental impacts across all life cycle stages of a product (European Commission, 2010). The principal aim of life cycle thinking is to avoid shifting of environmental impacts from (1) one life cycle stage to another, (2) one geographic region to another, and (3) one impact category to another. The several tools that utilize the life cycle approach include: LCA, carbon footprinting, ecological footprinting, environmental input-output analysis, material flows, and life cycle costing (European Commission, 2010).

The emergence of life cycle thinking (LCT) can be traced back to the 1960s, with the increased concerns of limited natural resources. The earliest studies using this approach were referred to as "Resource and Environmental Profile Analysis" (European Commission, 2010). The need for LCT is attributed to the need for accurate information to make informed decisions.

The benefits of life cycle approach include market-oriented policies, innovation in design, identifying hot spots in the supply chain, developing resource management strategies, informing consumer through labels and declarations, closer interactions with suppliers and customers, better relations with environmental groups and governmental entities, et cetera (European Commission, 2010).

### **1.1.8 Life Cycle Assessment**

The Johannesburg Summit report called out, specifically, for the use of life cycle analysis/assessment (LCA) and national indicators for measuring progress towards sustainable consumption and production (Hertwich, 2005; United Nations, 2002). The Natural Step framework, developed in 1989, is a highly regarded framework for strategizing institutional sustainability through back-casting. It

highlights the need for LCA as one of the tools to transition to sustainability (Holmberg, 1998). LCA offers the best framework for estimating the potential environmental impacts of goods and services, throughout its life cycle. This information can then be driven throughout the supply chain and the value chain to drive innovation and behavioral change towards reducing our pressure on the earth resources and ecosystem services. The use of LCA as a means to SCP, advances the idea of reducing the negative environmental and health impacts that are related to the consumption of materials and resources (European Commission, 2010). A study by the Grocery Manufacturer's Association (GMA) indicated that sustainability factors drive or influence the purchasing decisions of more than 50% of the surveyed shoppers, but that it is only secondary to other dominant purchasing drivers (GMA & Deloitte, 2009).

ISO 14040 (International Standards Organization, 2006a) and 14044 (International Standards Organization, 2006b) are international standards that provides the principles and framework for life cycle assessment, and requirements for practitioners to perform life cycle assessment, respectively. They enable the identification of environmental aspects and quantification of potential environmental impacts (relative to the functional unit considered) of a product or process over one or more life cycle stages (raw material extraction, production, transportation and distribution, use, and end-of-life). There are four phases to the framework of life cycle assessment (Figure 1): (1) goal and scope definition, (2) inventory analysis, (3) impact assessment, and (4) interpretation. The goal and scope definition phase determines the objective, breadth, and depth of the study. In the life cycle inventory analysis phase (LCI phase), all the inputs and outputs to/from the defined system boundary are aggregated and analyzed. The life cycle impact assessment phase (LCIA phase) provides additional information on the inventory analysis results so as



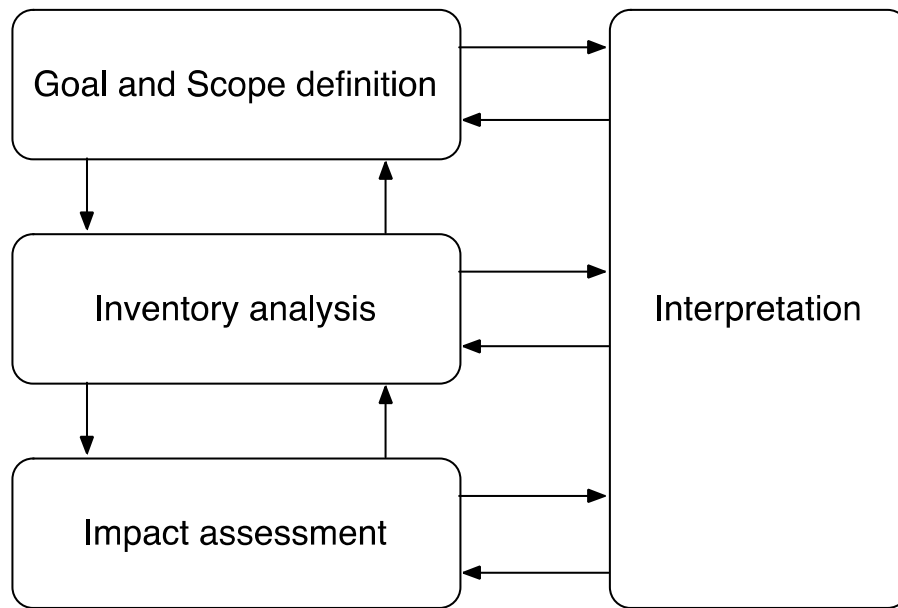
to better comprehend the environmental implications. In the interpretation phase, the results from the inventory analysis phase and the impact assessment phase are understood with respect to the goal and scope phase to arrive at the conclusions and recommendations. The recommendations are then utilized for decision-making applications such as product improvement, public policy, product comparison, marketing, et cetera. It must be noted that not all LCA's require the LCIA phase and those studies are referred to as LCI studies, as opposed to LCA studies when LCIA phase is included.

ISO 14040 (International Standards Organization, 2006a) identifies seven fundamental principles for life cycle assessment to guide decision-making when planning and executing an LCA. These principles include: (1) life cycle perspective, (2) environmental focus, (3) relative approach and functional unit, (4) iterative approach, (5) transparency, (6) comprehensiveness, and (7) priority of scientific approach.

LCA requires life cycle inventory (LCI) data for various product systems that includes several unit processes interlinked together using intermediate flows. These unit processes are linked to other product systems using product flows and to the environment using elementary flows (input and output flows). LCI datasets are highly complex and may have as many as 10,000 data points or more. The specific data relating to the products and process that is the focus of the LCA is referred to as the foreground data or primary data. Usually, a practitioner is able to collect data the primary data, directly, for the analysis. Other data that is not specific to the specific product or process that is the focus of the analysis is called background data or secondary data. The secondary data is often generic in nature and obtained from LCA databases. In the process of inventory analysis, various inputs such as resources used and outputs such as emissions to soil, water, and air are aggregated across

various environmental aspects. Using various types of analyses such as contributory analysis, dominance analysis, influence analysis and anomaly assessment, the LCA practitioner can identify and prioritize significant environmental issues for improvement, concerning the goal and scope definition.

Figure 3: Framework for life cycle assessment



The LCIA phase involves the conversion of LCI results into impact assessment results through the use of characterization factors (CF). This requires the classification of LCI results to one or more impact categories (also referred to as mid-point categories). The LCI results are then multiplied with the characterization factors for each impact category to obtain impact indicator results that have unique units. These characterization factors are produced using complex fate, exposure, and effects models, as part of an impact assessment characterization methodology. Of the many published characterization methodologies, some also have endpoint

categories and the associated endpoint indicators, which are the result of classification one of more impact categories to endpoint categories. Normalization is an optional step which calculates the magnitude of the results with respect to some reference information. Weighting is another optional step whereby the priorities of the stakeholders with respect to the environmental impacts can be embedded into the indicator results. Additionally, after the performance of normalization, all impact categories or endpoint categories will have the single unit of measure; thereby making it convenient to convert the indicator results from several impact or endpoint categories into a single score by use of weighting.

There are many LCA tools that make the process of performing an LCA easier by combining several inventory databases and several characterization methodologies into a convenient software platform. The LCA software tool eliminates several laborious tasks for the LCA practitioner, which eliminates certain sources of uncertainty and introduces new sources of uncertainty.

#### **1.1.8.1 Area of Focus: Attributional LCA**

There are two forms of process-LCA (1) attributional LCA (retrospective or accounting perspective), and (2) consequential LCA (prospective perspective) (Ekvall, Tillman, & Molander, 2005; Finnveden et al., 2009; Tillman, 2000). Attributional LCA includes environmentally relevant flows that are part of the product system to determine the potential environmental impact of the product, using normative allocation and cut-off rules. On the other hand, consequential LCA includes environmentally relevant flows to the extent that they are expected to change based on the change in demand for the product. In other words, attributional LCA describes the product system as-is, whereas consequential LCA describes the consequences of the product system. Further, consequential LCA models the consequences of making one choice over another. Clearly, the two types of process-

LCA have different purposes. Ekvall et al. (2016) note that it is important to choose the right type of LCA for the specific purpose, as it has a definite influence on the LCA results.

De Camillis et al. (2013) states that attributional approach is the most widely applied LCA modeling approach. Williams, Weber, & Hawkins (2009) stated that attributional LCA is the more standardized approach to LCA, based on the amount of critical review that the method has undergone through numerous research articles and case studies. European Commission (2010b) refers that attributional LCA as ISO LCA, based on information provided in the ILCD Handbook (European Commission Joint Research Centre, Institute for Environment and Sustainability, 2010a).

According to Weidema (2014), ISO 14049 clause 6.4 (International Standards Organization, 2012) provides the basis for consequential LCA. Finnveden et al. (2009) highlights that there is still no consensus or guidance on when performing a consequential LCA is more appropriate than performing an attributional LCA. Ekvall et al. (2016) have found in their analysis that The International Reference Life Cycle Data System (ILCD) handbook (European Commission Joint Research Centre, Institute for Environment and Sustainability, 2010) is inconsistent with their recommendations on how to choose between attributional and consequential LCA (Zamagni, Buttol, Porta, Buonamici, Masoni, Guinée, & Ekvall, 2008a).

The author has developed two methodologies for this thesis. Both methodologies are applicable to attributional LCA, and one of the two methodologies – to assess the sensitivity of product-evolution – is applicable to consequential LCA. This limitation is the primary reason for constraining the scope of this thesis to attributional LCA. Additionally, since attributional LCA is more popular and standardized, these methodologies will serve a larger population and advance the standardized methodology.

### **1.1.8.2 Area of Focus: Cradle-to-Manufacturing Gate**

There are roughly six stages in the life of a product: (1) resource extraction, (2) processing, (3) manufacturing, (4) distribution, (5) use, and (6) end-of-life. LCAs that include all life cycle stages are called 'cradle-to-grave,' those that include from resource extraction to any intermediate stage are called 'cradle-to-gate', and those that include any one or two consecutive stages are called 'gate-to-gate,' provided they do not include any end stages such as resource extraction and end-of-life. Predominantly, LCA's are performed by product manufacturers so that they can either innovate new products or improve upon existing products. Accordingly, they utilize a 'cradle-to-manufacturing gate' approach beginning with resource extraction and ending with manufacturing. Manufacturers tend to select this scope because they realize that they have the ability to influence change within their facility and potentially within their supply chain, towards eliminating the environmental hotspots. Manufacturers are in a position to influence their supply chain based on their ability to stipulate conditions when purchasing raw materials from their suppliers. Manufacturers often do not have the sufficient control over how products are shipped to the retailers or how consumers wish to use and determine the end-of-life of their products.

There are cases when manufacturers include the entire supply chain, so as to understand the environmental impacts of their product cycle. One major hurdle to including the entire supply chain within an LCA, is the general lack of information on how products are used (consumer behavior) and how products meet their end-of-life. Obtaining information on the final two stages of LCA, is often expensive and requires a separate survey-based study.

## 1.2 Uncertainty

Uncertainty is not just pervasive in the scientific process (Costanza & Cornwell, 1992; Fowle & Dearfield, 2000), but everywhere (D. V. Lindley, 2014). On the contrary, people like to be sure and confident about the information and knowledge that they possess (D. V. Lindley, 2014). Uncertainty disappears when certainty takes its place (Bedford & Cooke, 2001). True knowledge and good information is almost always treated as desirable (Smithson, 1989). Bedford (2001) states that one becomes certain of a declarative sentence when (1) the condition of truth exists, and (2) the value conditions for "true" are valid. Lindley (2008) notes that in the interrelationship between theory and experiment, it is uncertainty that guides scientists on future steps.

The standard JGCM 100 (Joint Committee for Guides in Metrology, 2008) states that the terms "measurand", "error" and "uncertainty" are the most commonly misunderstood. Smithson (1989) provides guidance into the understanding of uncertainty through the following definition: "Ignorance is usually treated as either the absence or the distortion of true knowledge, and uncertainty as some form of incompleteness in information or knowledge". He refers to uncertainty as a manageable type of ignorance, that which can be subdivided into ambiguity, probability, vagueness, fuzziness, and non-specificity, based on wide-spread usage in philosophical and scientific literature. Bedford (2001) argues that ambiguity is not a type of uncertainty, but associated with linguistic conventions and truth conditions. As such, there are many taxonomies for uncertainty, such as those based on probabilistic concepts, psychological and phenomenological arguments, and such (Smithson, 1989; Bedford, 2001). Smithson (1989) also noted that ignorance is referred to uncertainty in some academic disciplines. According to Bedford (2001), ambiguity must be removed in order to discuss uncertainty meaningfully.

Uncertainty occurs in qualitative and quantitative form (Curry, Nembhard, & Bradley, 2009). There are certain complex issues (e.g.: organizational change, perceptions of quality, et cetera) that cannot be measured by quantitative values. The following are the core differences between quantitative and qualitative research. Qualitative approaches focus on complexity and range of occurrences, whereas quantitative approaches focus on the count of occurrences (Curry et al., 2009). Qualitative approaches to uncertainty generate the hypothesis using observations – inductive, whereas quantitative approaches create the hypothesis and then tests it using the observations (Curry et al., 2009). Qualitative approaches occur in natural settings and generates text-based data through discussions and observations, whereas quantitative approaches occur in natural and experimental settings and generates numeric data through standardized processes and tools (Curry et al., 2009).

The Joint Committee for Guides in Metrology comprehends 'uncertainty' to be doubt and 'uncertainty of a measured value' to be doubt in the validity of the measured value, which is expressed as standard deviation. This standard defines 'uncertainty in measurement' as "parameter, associated with the result of a measurement, that characterizes the dispersion of the values that could reasonably be attributed to the measurand" (Joint Committee for Guides in Metrology, 2008).

The term 'Uncertainty' has multitudes of definitions, as it is embedded in different academic disciplines and studied by varied scientific researchers. With reference to the term 'sustainability', scientists such as Kidd (1992) suggest that there should not be a single definition, but that it is important that stated definitions precisely communicate what the term means. Accordingly, it is important that researchers don't get embroiled in the diversity of definitions, but seek to understand the definitions provided under the relevant context. In this thesis, the definition of

uncertainty established by the Joint Committee for Guides in Metrology is used as a basis for comprehension and expression.

Suppression of uncertainty is evident in everyday life examples – hearing the newscaster say that it will rain as opposed to it may rain – false confidence. Lindley (2014) recommends that it important not to neglect or suppress uncertainty due to discomfort but to openly discuss it. Given that uncertainty is disliked by us, the only way address this problem is to either remove or reduce uncertainty. In order to do so, one is expected to collect and process facts through analytical experiments. Lindley (2014) notes that while we do dislike uncertainty, there are instances (e.g.: gambling) where we do like uncertainty – “without it life would be duller”. When analyzing our dislike of uncertainty, Lindley (2014) points out people are more concerned about the negative outcome due to the uncertainty. Despite the negative connotations associated with uncertainty, it has found many uses: to create an advantage in sports and war, to promote curiosity amongst scientists, to question the veracity of witness statements by jurors, et cetera. In order to create an overall solution, the uncertainties need to be combined – which is where the quantification of uncertainty comes to play. The arithmetic combination of uncertainty provides limited challenges to measuring the overall uncertainty (D. V. Lindley, 2014). It is evident that uncertainty concerns a statement whose validity or truth is weighed by a person. Evidence also demonstrates that uncertainty is personal – the uncertainty for one person can be different from uncertainty for another person (D. V. Lindley, 2014). The term usually used to describe the uncertainty event is “degree of belief”. If one believes the truth of the event, then one has high degree of belief. Belief communicates the relationship between the person and the event that takes place in the world. The strength of the belief or relationship is referred to as “probability”. Thus, one’s belief in the uncertainty of an event is described as ‘your probability for



the event' (D. V. Lindley, 2014). Using beliefs one can guide one's actions, such as taking an umbrella if one believes that it is going to rain. Decision Analysis is the study of analyzing beliefs to decide from the various courses of action (D. V. Lindley, 2014).

The National Institute of Standards and Technology, an organization under the United States Department of Commerce, presents the international view of how to express measured uncertainty based on the CIPM (International Committee for Weights and Measures) approach (Bureau International des Poids et Mesures, 1994) through the NIST Technical Note 1297. According to CIPM, the uncertainty of a measured result can have many components, and these components can either arise from random or systemic effects. When the uncertainty is expressed as a standard deviation of the measured value, then it is termed 'standard uncertainty. Evaluation of uncertainty by statistical means is termed 'Type A evaluation of standard uncertainty' and assessment of uncertainty in other ways is termed 'Type B evaluation of standard uncertainty' (Taylor & Kuyatt, 1994).

### **1.2.1 Origins and Evolution of Uncertainty**

The origins of uncertainty can be traced back the development of critical judgment amongst Greek philosophers and the resulting realization that infallible knowledge is very limited in scope (Tarnas, 1991). Philosophical publications by Heraclitus (~500 BCE) on the constantly changing nature of the world (Graham, 2015), and Zeno of Elea (490 - 430 BCE) on the irresolvable paradoxes (Huggett, 2010) further expanded the exposure to uncertainties. Tarnas (1991) notes that the advent of reason opened everything to doubt, with every generation of philosophers offering different solutions. The resulting ethical ambiguity forced stoic philosophers to rationally deal with the situation, but they could not provide certainty in philosophy for people to live by. During this time of moral and ethical instability, the

religion of Christianity provided an ideal certainty for the human dilemma. The intellectual ascension of a philosopher was replaced by the emotional and communal relationship with God (Tarnas, 1991). "But again, with the truth so firmly established, the philosophical inquiry was seen by the early Church as less vital to spiritual development, and intellectual freedom, basically irrelevant, was carefully circumscribed" (Tarnas, 1991) – this was a transition from uncertainty to certainty.

The time between 14th and 17th century was an immensely transformative period with the intermingling of cultural epochs such as renaissance, reformation, scientific revolution, and the scientific revolution. Humans were able to explore the planet, discovering new land, cultures, and species. They explored space and reflected nature with mathematical sophistication (Tarnas, 1991). Smithson (1989) notes that modern probability theory emerged in 1660. Stigler (2015) brings up the work of Jerome Cardan (a.k.a. Cardano) who wrote an article on the game of chance, which was published much later in 1663. He notes that because it was released more than 100 years later, it had no impact on the development of probability but provides insight into the level of understanding of uncertainty at that time. During this period, there was a resurgence of uncertainty in the fields of science, philosophy, humanities, epistemology and such. With the decline of religion and metaphysics/philosophy in the eighteenth century, science seemed to be the only avenue to address uncertainty for the modern mind. Tarnas (1991) conveys the transitive implications through the following words. "In the face of science's supreme cognitive effectiveness and the rigorously impersonal precision of its explanatory structures, religion and philosophy were compelled to define their positions in relation to science, just as, in the medieval era, science and philosophy were compelled to do so in relation to the culturally more powerful conceptions of religion."

In the nineteenth century, scientists predominantly believed that uncertainty could be eradicated by facts, laws and ultimate predictability without exceptions. They also believed that nature was ultimately knowable, even if it is not known by this generation of scientists, then it would be by future generations. They perceived their limitations to be the lack of computational power (human, in this case) and the complexity of the problem (D. Lindley, 2008). In 1927, Werner Heisenberg proposed an uncertainty principle, based on a thought experiment, in the field of physical sciences, also referred to as Heisenberg's Uncertainty Principle or Indeterminacy Principle. The principle states that the position and momentum of a particle cannot be measured with complete precision at the same time – derived from the wave and particle nature of quantum objects. It is more commonly stated as 'the act of observing changes the observed.' This principle upended the scientific assumption that everything in nature cannot be defined with immeasurable precision, and their interconnections understood to the fullest extent (Lindley, 2008). He also states that 'Uncertainty' represents the apex of quantum mechanics, which arose because the physics of the nineteenth century could not address many problems that were posed (Lindley, 2008).

### **1.2.2 Dealing with Uncertainty**

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### **1.2.3 Uncertainty in Life Cycle Assessment**

The topic of uncertainty was first approached by Reinout Heijungs in a seminal article titled “Identification of key issues for further investigation in improving the reliability of life-cycle assessments” in 1996 (Heijungs, 1996). Cirolto et al. (2004) describe uncertainty as the quantitative difference between measured value and true value, due to probabilities. It must be noted that the term ‘uncertainty’ has not been clearly defined in any LCA literature – peer-reviewed

journal articles, reports, books, or standards. Despite the lack of a precise definition, the number of publications on uncertainty has been progressively increasing.

Ciroth (2004), when announcing the new section on 'Uncertainties' in the International Journal of Life Cycle Assessment, stated that the stability of a result is equally as important as the factors that change the ranking of the alternatives. Uncertainty is not just important because some academics think it is important, but more so, because divergence in LCA results (including interpretation) can provide misleading outcomes; which when used to make decisions, can have adverse impacts on the environment and society.

At the same time, there are several different taxonomies for uncertainty in life cycle assessment, which leaves many LCA practitioners confused. To provide clarification to the inconsistencies in LCA methodologies and uncertainty in life cycle assessment, several journal articles, and reports have been published on the consolidated understandings of uncertainty in LCA. Yet, there are inconsistencies and lack of clarity amongst these consolidated publications due to the broadening nature of the scope of LCA, and diversified opinions. The UNEP/SETAC Life Cycle Initiative led a single, major, multi-stakeholder initiative to resolve the issue of inconsistency in uncertainty assessment in LCA, but the project failed due to reasons unknown.

Hellweg and Canals (2014), in their overarching review of LCA, note that despite the growing number of publications on uncertainty in life cycle assessment, uncertainty analysis is rarely performed in LCA's.

How does uncertainty analysis differ between attributional LCA and consequential LCA? To answer this question, one must understand the differences and identity between the two types of process-LCA. Some of these differences are found in section 1.1.5.1. Firstly, it is important to recognize that the life cycle stages and phases in attributional and consequential are the same. Secondly, the major

differences between the two types are (1) inventory included, and (2) cut-off and allocation rules, Thirdly, both types are static, linear and homogenous models (Consequential-LCA, 2015). It must be noted that inventory analysis in attributional LCA and consequential LCA is identical, except that the scope of the included inventory is different. Thus, the sources of uncertainty are not expected to vary much between the two types, with regards to inventory. With respect to the cut-off and allocation rules, the sources of uncertainty are expected to vary.

### **1.2.3.1 Uncertainty in Life Cycle Phases**

The four phases of life cycle assessment are (1) goal and scope definition, (2) life cycle inventory analysis, (3) impact assessment, and (4) interpretation. Sources of uncertainty exist in all phases of life cycle assessment, as demonstrated by Reap et al. (2008a; 2008b). More importantly, despite LCA being an iterative process, it is still sequential in nature, and therefore uncertainty from the earlier phase is propagated into the subsequent phases.

In the goal and scope definition phase, uncertainty can occur in the product system definition, functional unit definition, reference flow estimation, system boundaries definition, scenarios created, assumptions used, choices made, allocation procedures, and cut-off criteria. They may be more sources of uncertainty in this phase, that which has not yet been identified.

In the life cycle inventory analysis phase, uncertainty can occur in form of poor data quality, data collection errors, existence of data gaps, used of proxy data to fill data gaps, use of unrepresentative data, insufficient understanding of underlying physical processes, inaccurate data, inaccurate emission factors, inaccurate emission measurements, apparent mistakes, variability around the mean, temporal variability in emission inventories, spatial variability in emission inventories, technological variability, difference in performance between equivalent

processes, life cycle inventory modelling technique, model used to describe unit processes, improper or broken linkages between unit processes, non-linearity in calculations, appropriateness of input or output flows, internally recurring unit processes in life cycle inventories, and static as opposed to dynamic modelling. They may be more sources of uncertainty in this phase, that which has not yet been identified.

In the life cycle impact assessment phase, uncertainty can occur in the form of choice of impact assessment methodology, selection of impact categories, use of more than one characterization methodology for one or more impact categories, choice of characterization model for an impact category, improper linkages between the mid-point indicators and the end-point indicators, lack of standardization of impact categories, omission of known impact categories, omission of known end-point categories, inconsistent impact category indicators, inaccurate characterization factors, spatial variability of fate factors, temporal change in the environmental systems, spatial variability in the environmental sensitivity, variation in susceptibility of humans, with and without respect to spatial factors, inadequate characterization models, absence of characterization factors, insufficient knowledge on the lifetime of substances, value choices in time horizon of the characterization methodology, use of static model as opposed to dynamic modeling, use of linear instead of non-linear modeling, inaccurate normalization data, variation in normalization data, limitations of normalization methodology, bias in normalization, data gaps in reference emissions, choice in weighting methodology, inoperative weighting criteria, unrepresentative weighting criteria, variability of in environmental preferences, variability in weighting factors, omission of unknown impact categories, contribution to impact category is unknown, and incorrect choice of probability distribution. They



may be more sources of uncertainty in this phase, that which has not yet been identified.

In the interpretation phase, uncertainty can occur in the form of improper use of interpretation methods, inability to easily and effectively track all steps, processes, assumptions of an LCA, inconsistency in names of elementary flows in the LCI datasets and the LCIA methods, insufficient visualization of data, linguistic impression, use of deterministic mean to communicate results, and difficulty in comparing products based on relative trade-offs between alternatives. They may be more sources of uncertainty in this phase, that which has not yet been identified.

### **1.2.3.2 Uncertainty in Life Cycle Stages**

As mentioned in section 1.1.8.2, there are roughly six stages in the life of a product. The relevant life cycle stages of the study are established in the Goal & Scope definition phase of the LCA. Sources of uncertainty exist in all life cycle stages. Uncertainty from each life cycle stage is propagated to the next stage in the supply chain. Uncertainty exists in the stages primarily in the form of data, modeling, choices, variability, mistakes, et cetera. All the sources of uncertainty from the included life cycle stages is captured in all the four life cycle phases, as modeled by the LCA practitioner. Table 1 correlates the broad sources of uncertainty between life cycle stages and life cycle phases. These sources of uncertainty are based on existing typology as established by Huijbregts et al. (1998) and reinforced in a general forum by Rosenbaum et al. (2009). It must be noted that all the sources of uncertainty are applicable to all life cycle stages and may occur repeatedly based on the life cycle phase. In other words, the sources of uncertainty are irrespective to the life cycle stages and are respective to the life cycle phases.

Table 1: Sources of uncertainty in LCA with respect to life cycle stages and phases

Life Cycle Stages \ Life Cycle Phases	Goal & Scope definition	Inventory analysis	Impact Assessment	Interpretation
Raw material extraction	Choice uncertainty	Model uncertainty	Model uncertainty	Inconsistency
Processing	Inaccurate system boundaries	Data uncertainty	Data uncertainty	Incomplete
Manufacturing	Mistakes	Temporal variability	Temporal variability	Anomalies
Distribution		Spatial variability	Spatial variability	Discrepancies
Use		Source-object variability	Source-object variability	
End-of-life		Mistakes	Mistakes	

### 1.3 Research Focus

Given the growing demand for environmentally responsible products from consumers and commercial buyers (Waste Management, 2016), product manufacturers have increasingly adopted the use of LCA to assess the “environmental score” of products for purposes of responsible innovation and improvement. At the same time, the complexity associated with decreased supply chain visibility, data inaccuracy and imprecision, model inaccuracy and imprecision, et cetera, has increased doubt in the reliability of LCA to serve as a reliable decision-support tool. To address this issue, researchers, have in the past, and presently, continue to identify sources of uncertainty in LCA, propose taxonomies for uncertainty in LCA, propose methods to address the uncertainty and variability, and so on. The focus of this thesis is to contribute to this effort of advancement in identification and addressment of uncertainty and variability in ‘attributional’ LCA, which is a more widely used form of LCA, and which conforms to ISO 14040 and 14044 standards.

The question that this thesis seeks to answer is, **“What is the present state of knowledge on uncertainty and variability in ‘attributional’ LCA, and how can the author contribute to the quantitative assessment of uncertainty and variability?”**

First, a thorough literature review was performed to consolidate the progress made on uncertainty in LCA. The literature review includes not only peer-reviewed publications, books, and reports but also activities undertaken by public service organizations (e.g.: United Nations, European Commission – Joint Research Center – Institute for Environment and Sustainability, et cetera). Based on the literature review and the author’s in-depth understanding of the laundry detergent supply chain, this thesis delves into two LCA-uncertainty issues that are demonstrated using the laundry detergent supply chain, that which are also evident in many different product supply chains.

### **1.3.1 Gaps in Literature**

The process of research dictates that before deciding to work on a problem, a literature review be performed to build a foundation of prior works and to identify gaps in literature that need to be filled. Accordingly, with regards to this thesis, a literature review on uncertainty in LCA is to be performed. This review, which can be seen in Chapter 3, will build on other literature reviews, scientific reports, and books on uncertainty and variability in LCA, that are not limited to: Reap et al. (2008a; 2008b), Heijungs and Huijbregts (2004), Llyod and Ries (2007), Björklund (2002), Zamagni et al. (2008b), Ross et al. (2002), Heijungs (1996), Heijungs and Lenzen (2014), Finnveden et al. (2009), Hauschild and Huijbregts (2015), Klöpffer (2014), Schaltegger et al. (1996), and Klöpffer and Grahl (2014).

Based on the identified gaps in the literature review of uncertainty and variability in ‘attributional’ LCA, and hurdles faced when performing LCA’s on laundry

detergents, two critical issues of concern that required addressing were identified and selected. These two gaps are:

- Lack of formal methodology to determine surrogate LCI data for missing LCI data
- Lack of consideration of product-evolution in LCA

CHAPTER 2  
RESEARCH METHODOLOGIES

### 2.1 Introduction

In this chapter, the various research methodologies that have been utilized in this thesis research are discussed, their novel contribution to science, along with how other researchers have used them.

The question that this thesis attempts to answer is, ***"What is the present state of knowledge on uncertainty and variability in 'attributional' LCA, and how can the author contribute to the quantitative assessment of uncertainty and variability?"***

This question can be split into two halves: (1) What is the present state of knowledge on uncertainty (theory and practice) in addressing uncertainty and variability in 'attributional' LCA, and (2) What can the author do to contribute to the quantitative assessment of uncertainty and variability in 'attributional' LCA? The second question can be further divided into (2a) what can the author do to contribute to the quantitative assessment of uncertainty, and (2b) what can the author do to contribute to the quantitative assessment of variability? In summary, the thesis seeks to answer three questions, within one.

As a result, the methodologies involved to answer these questions will also be unique to each of the questions. Each of these three questions are addressed using various methodologies separately in chapters 3, 4 and 5, respectively. One research methodology that is common across the three questions is literature review. Even while this is the case, literature review is performed in various scales and various related fields of science and brought together towards their applicability to 'attributional' LCA, and to the problem under consideration. In all cases, established research methods have been applied to known and unknown problems in a unique

manner, without over stepping the bounds of necessity, to address the problem of concern in a sufficient manner. The sufficiency of addressment or of the methodologies used can be argued differentially by many researchers, but is limited by the author in order ensure practicality in replication, that which many novel methodologies fail at. For example, there is no known application of the “new approach for modular valuation of LCA’s” proposed by Ciroth et al. (2003) or the “combined model of simulation and approximation” to quantify uncertainty in life cycle assessment that was proposed by Ciroth et al. (2004). Both methodologies proposed by Andreas Ciroth are scientifically commendable but have not found use by other researchers or LCA practitioners. In light of such situations that are commonly present in the field of LCA and potentially other academic fields, the author has sought out methodologies that are easy to replicate and at the same time sufficient to address the problem of concern, by general LCA practitioners. Additionally, many researchers propose novel methodologies that go beyond the scope of the international standards that govern LCA (ISO 14040 and ISO 14044). For example, Zhai and Williams (2010) attempt to capture the dynamics of the supply chain using hybrid LCA (a combination of process-sum LCA and input-output LCA), which does not conform to the ISO standards for LCA. The author has thus ensured that the methodologies used in this thesis do not extend beyond the methodological bounds of ISO 14040 and ISO 14044.

### **2.1.1 Sustainability Assessment Methodologies**

Sustainability can be assessed at different scales, application targets, and so on. The Organization for Economic Co-operation and Development (OECD) states that the main steps to sustainability assessment are relevance analysis, scoping analysis, impact analysis, comparative analysis, associative analysis, and political analysis. Sustainability assessment tools focusing on economic aspects include cost-

benefit analysis, regression, scenarios, et cetera. Sustainability assessment tools focusing on environmental aspects include life cycle analysis, material flow analysis, resource accounting, and ecological footprinting. Sustainability assessment tools focusing on social aspects include sustainable livelihoods, human and social capital measurement, and multi-stakeholder engagement (Stevens, 2016).

### **2.1.2 Uncertainty Quantification Methodologies**

The methodologies used to quantify uncertainty most often depends on the typologies and/or sources of uncertainty. Uncertainty quantification, generally, includes a sequence of steps such as problem definition, model verification, identification of uncertain inputs, identify and integrate observational/experimental data, identify uncertain parameters, perform response surface analysis, perform sensitivity analysis and risk analysis, and documentation and review (Lin, Engel, & Eslinger, 2012). Probability and statistics are two leading academic areas, related mathematics, using which uncertainty is quantified. Probability takes into consideration the likelihood of events in the future whereas statistics takes into consideration the frequency of past events. In other words, both fields have different purposes and are applied based on the problem definition. It must be noted that the use of probability distributions in statistics is quite common. Given that LCA focuses on environmental impacts that occurred in the past, statistics is used to quantify the uncertainty. Lloyd and Ries (2007) have surveyed the statistical methodologies utilized for the quantification of uncertainty in life cycle assessment, with the following observations:

- Sources of information used to characterize uncertainty, include: life cycle inventory (LCI) data, data quality indicators (DQI) – directly and indirectly, expert judgement, and other supporting information.

- Methods to quantify uncertainty propagation include: fuzzy data sets, probabilistic simulation, Bayesian statistics, scenario analysis, stochastic sampling – Monte Carlo simulation – Latin hypercube sampling – parametric bootstrapping, analytical uncertainty propagation, interval calculation, et cetera.
- Sampling iterations ranged from 100 to 30,000.
- Probability distribution functions used to quantify uncertainty include almost every distribution form (normal, triangle, uniform, log normal, beta, defined parameter, intervals, trapezoidal, bootstrapping, t-distribution, pert, gamma)
- Various forms of graphs used to communicate uncertainty include: box-and whisker plot, histogram, error bars, et cetera.

## **2.2 Consolidating Addressment of Uncertainty and Variability in Attributional Life Cycle Assessment Modeling**

In order to consolidate how uncertainty and variability have been addressed in 'attributional' LCA modeling, the primary research methodology utilized was literature review. According to Rapple (2011) and Pautasso (2013), the ever growing number of scientific publications have resulted in the demand for literature reviews since readers cannot be expected to read all publications in order to keep themselves up to date on scientific advances. Hampton and Parker (2011) highlight that scientific synthesis offers numerous other advantages such as (1) offering counter-weight to hyper specialization, (2) coping with too many discoveries in short periods of time, (3) enables to conceptualization of complex problems beyond the scope of current endeavors, (4) the inherent diversity in the synthesis offers opportunities for



transformative research and spontaneous discoveries, and lastly, (5) it is a significant social investment. Timely synthesis provides new insights, as comparable to primary research, and are widely read due to the convenience factor (Hampton and Parker, 2011). In order to facilitate the professional complication of a literature review, Pautasso (2013) has shared the following ten rules: (1) Define a topic and an audience, (2) search and re-search literature, (3) take notes while reading, (4) choose the type of review you wish to write, (5) keep the review focused, but make it of broad interest, (6) be critical and consistent, (7) find a logical structure, (8) make use of feedback, (9) include your own relevant research, but be objective, and (10) be up-to-date, but do not forget older studies.

Literature review on the topic of uncertainty and variability in LCA has been performed by several researchers that include Heijungs (1998a), Björklund (2002), Ross et al. (2002), Heijungs and Huijbregts (2004), Llyod and Ries (2007), Reap et al. (2008a, 2008b), and Williams et al. (2009). These articles focused on (1) identifying sources of uncertainty and organizing them within a proposed typology of uncertainty and variability with respect to life cycle phases (Heijungs, 1998a), (2) expansion of typologies and classifying sources of uncertainty and variability accordingly with respect to life cycle phases; and identification of tools for sensitivity analysis, and uncertainty analysis (Björklund, 2002), (3) survey of how LCA and LCI studies deal with uncertainty (Ross et al., 2002), (4) summary of tools and techniques used to address uncertainty, without justification of appropriateness (Heijungs and Huijbregts, 2004), (5) newly proposed typology of uncertainty and variability; and in-depth quantitative analysis of how uncertainty is dealt with from 24 studies – summary without guidance (Llyod and Ries, 2007), (6) in-depth overview of unresolved problems that are not sources of uncertainty, and sources of uncertainty in each of the four phases of life cycle assessment – without lack of

clarity in systematically addressing uncertainty issues (Reap et al., 2008a, 2008b), (7) focus on uncertainty theory and uncertainty typology in the LCI analysis phase with the proposed use of hybrid methods to address it (Williams et al., 2009), and (8) review various sources of uncertainty with respect to the typology: parameter, scenario and model; other limitations and research needs with respect to ISO-LCA that questionably includes consequential LCA, EIO LCA and hybrid LCA (Zamagni et al., 2008a).

When these literature reviews were analyzed, it was evident that the following was lacking: (1) definitions of uncertainty and other uncertainty related terms, (2) consistency in typology of uncertainty and variability, (3) consistency in the sources of uncertainty and variability, (4) organized list of methods and guidance to address various identified sources of uncertainty, (5) specific and/or consistent focus on issues relating to 'attributional' LCA, that which conforms to ISO 14040 and ISO 14044, (6) reasons why uncertainty assessment was not being performed, (7) previously unidentified and/or recently identified sources of uncertainty, (8) previously unidentified and/or recently identified methods and guidance documents to address uncertainty using primary research (9) recent multi-stakeholder activities towards addressing uncertainty in specific areas of LCA, (10) updated sources of uncertainty that require primary research, (11) focus on communication of uncertainty information, and ultimately, (12) a defined set of critical questions to accelerate primary and collective action towards improving reliability and credibility of LCA.

In order to address these issues in a comprehensive manner, a literature review was performed using roughly 347 references (includes old publications and the most recent publications). The review refrained from making definitive suggestions for terminologies, typologies, and methodologies as it was the author's

view point that such decisions should be the outcome of a multi-stakeholder engagement process. In order to set the basis for a multi-stakeholder discussion, the review consolidated (1) various definitions of uncertainty from different disciplines and implied definitions from within the field of life cycle assessment, (2) roughly thirty typologies of uncertainty from various disciplines, and eight typologies of uncertainty that have been proposed for use in LCA. The authors attempted to define commonly used uncertainty-related terms in LCA, that were not previously defined anywhere or within LCA (for e.g.: uncertainty characterization). Unresolved issues in LCA that are not sources of uncertainty and variability have been excluded from the study, to ensure on practical issues of reliability and credibility, and not on developmental issues of reliability and credibility.

The authors aggregated the various sources of uncertainty and variability, along with the published methods and guidance to address those issues, with respect to each of the four phases of life cycle assessment, and another category for overall applicability.

The authors tie all the research together by putting forth several logical questions to set the basis for future multi-stakeholder and primary research activities to improve the reliability and credibility of LCA.

The use of literature review, in this case, does not just provide an overview of the state of knowledge of uncertainty and variability in 'attributional' LCA, but provides the state of the related situation. It does so by pulling together all the available information into logical situational statements and questions that sets the basis for multi-stakeholder groups to sit together and decide how they want to move forward. Given the success of multi-stakeholder groups in the LCA community coming together to create guidance documents (e.g.: Product Category Rule Guidance, Global Guidance for LCA databases, Global Guidance on LCIA Indicators),

this document is designed to be a precursor for such a guidance document on uncertainty and variability.

### **2.3 Patching LCI Data Gaps of Consumer Goods Through Expert Elicitation**

In this study, the authors have proposed a formal method to determine proxy (or surrogate) LCI data for missing LCI data, through the use of expert elicitation. In this method, experts were asked to suggest the best proxy with respect to Cumulative Energy Demand (CED) for target chemical products that already have LCI data but which was not disclosed to the experts. In the process of selecting proxies, the experts were asked to provide scientific criteria based on which they select proxies, which practitioners can later use as the basis of selection of the best proxy. The difference in CED impacts between the best proxy and the target proxy was then calculated to be the uncertainty associated with the use of the proxy.

Expert elicitation is a method that is traditionally used when confronted with the lack of data. It is a systematic approach that synthesizes the subjective judgments of experts (Slottje et al., 2008). The use of expert knowledge and choices is not uncommon in life cycle assessment. Coulon et al. (1997) and Heijungs (2010) identify expert elicitation as one of schools of processing uncertainty in LCA. Kennedy et al. (1996) and Weidema and Wesnaes (1996) use expert judgment to quantify inherent uncertainties using pedigree-based approaches (Coulon et al. 1997). The use of social panels in the weighting stage of LCA is a means of eliciting “value-based” choices that are supported by a list of criteria, from experts. De Haes (2000) states that social panels are considered to be more robust than the other methods of weighting. Koffler et al. (2008) developed a methodology for group decision making in panel based LCA studies, which is based on the elicitation of the perspectives from each panelist. Given that any and all LCA practitioners perform proxy selections, the authors decided to crowd source the proxy selections from

experts based on the hypothesis that some experts make better choices and that the criteria that they use could guide proxy selections by novices. Expert elicitation was performed through Institutional Review Board (IRB) approved (See Appendix B) web surveys, with participants located around the world, over a period of two months.

While expert elicitation has been used in other areas of life cycle assessment, it has not been used in fill data gaps. This is the first instance wherein the expertise of people is used in a consistent and process-oriented manner to determine surrogate data, and the uncertainty associated with its use is quantified.

#### **2.4 Sensitivity of Product-evolution in Life Cycle Assessment**

In this study, the author has identified a unique problem of product-evolution, wherein the bill of materials of a product changes in a non-uniform manner. Thus so, an LCA performed on a product might be out-of-data before the LCA is published. In order to demonstrate this issue of variability, within the scope of ISO 14044, the authors use sensitivity analysis to quantify it in the form of a range. Using a case of laundry detergents, the sources of variability were identified, generalized and quantified. Using three tiers of laundry detergents, and consequently base-case formulations, these variabilities are analyzed using sensitivity analysis. The implications of individual variabilities and coupled variabilities are obtained from calculated LCIA results for each of the three base-case formulation (also referred to base-impacts).

Sensitivity analysis is a systematic process of determining the model output based on the sensitivity to the model input (International Standards Organization, 2006b; Groen et al., 2014). ISO 14044 (International Standards Organization, 2006b) recommends the use of sensitivity analysis when (1) defining and refining the system boundaries – including allocation and cut-off criteria, (2) analyzing the implications of different reference systems, (3) LCIA data quality analysis, (4)

selection of impact categories, (5) classification of inventory results, (6) assessing the implications of value-choices and weighting methods, (7) determining limitations of the LCA for use in the interpretation phase, et cetera. As recommended by ISO 14044, sensitivity analysis is commonly used to assess the implications of methodological choices, assumptions and such (Huang et al., 2012, Cellura et al., 2011). Markwardt and Wellenreuther (2016) have used sensitivity analysis to quantify the end-of-life management as applicable to different country-specific situations, thereby extending the applicability of the LCA findings.

In this case, sensitivity analysis is used to quantify product-evolution, which when interpreted appropriately with the results of a static LCA, will not be considered out-of-date. The approach of using sensitivity analysis for this particular problem is novel, and therefore contributes to science. Additionally, the easily replicable nature of this methodology for this commonly occurring problem will find use amongst LCA practitioners in the industry.

CHAPTER 3  
CONSOLIDATING PROGRESS ON UNCERTAINTY AND VARIABILITY IN  
'ATTRIBUTIONAL' LCA

### **3.1 Introduction and Motivation**

Models are simplifications of a reality that is highly complex and immensely vast, and therefore they are subject to imprecision and inaccuracy. Since the usefulness of models depends on the reliability of results, the identification, prioritization, quantification, and communication of uncertainty is crucial (Loucks, van Beek, Stedinger, Dijkman, & Villars, 2005).

Uncertainty is pervasive in the scientific process (Costanza & Cornwell, 1992; Fowle & Dearfield, 2000). Uncertainty, a synonym for doubt, can be very confusing to many life cycle assessment (LCA) practitioners. According to Walker et al. (2003), one cannot simplify uncertainty to the absence of knowledge for in fact more information may lead to more uncertainty.

Life Cycle Assessment (LCA) quantitatively tracks the potential environmental impacts of international value chains, while ensuring that burden shifting is avoided (Finnveden et al., 2009; Hellweg & Milà i Canals, 2014a). ISO 14040 (International Standards Organization, 2006c) and ISO 14044 (International Standards Organization, 2006d) are the international standards that defines the rules for performing an LCA.

As a decision tool, LCA has found uses in business decision-making (design, supply chain optimization, marketing, et cetera), public policy (European Commission's Energy-using-Products Directive, European Waste Framework Directive, et cetera), purchasing policy by retailers, assessing alternatives (technologies, consumer products, fuels, transportation modes), and identification of areas that require further research (Hellweg & Milà i Canals, 2014b). Given that LCA

has also been reported to contain many unresolved issues (Reap, Roman, Duncan, & Bras, 2008b; 2008a) and sources of uncertainty (Björklund, 2002; Heijungs & Huijbregts, 2004; Huijbregts, 1998a; Lloyd & Ries, 2007) that affects the reliability of its results, it is only logical to question, how can one depend on LCA results for critical decisions when the results are not certain?

Firstly, one must come to terms with the fact that practitioners are attempting to quantify the impacts on the environment due to complex international supply chains using cause-effect models that may or may-not sufficiently reflect the actual environment. For example, the sources of uncertainty in climate science range from the planet's axis of rotation to change in atmospheric composition (Shome & Marx, 2009).

Ciroth (2004), when announcing the new section on 'Uncertainties' in the International Journal of Life Cycle assessment, stated that the stability of a result is equally as important as the factors that change the ranking of the alternatives. Uncertainty is not just important because some academics think it is important, but more so, because divergence in LCA results (including interpretation) can provide misleading outcomes; which when used to make decisions, can have adverse impacts on the environment and society. Thissen (2008) states that the knowledge of the existence of uncertainty and its quantification, can guide decision makers to make deliberate informed choices amongst alternatives or creating new alternatives based on the uncertainties.

Many statisticians often repeat a quote by Johnson (1787) to establish that uncertainty in numbers was long important: "Round numbers, said he, are always false". Björklund (2002) stated that reliability of LCA results is affected by use of point estimates (without standard deviations or as ranges). Twenty years since, it is still common to find LCA's published in leading journals to just consider whole



numbers or averages as results. According to Thissen (2008), it is ethically undesirable to put forth impact assessment results without uncertainty considerations or with minimal attention to uncertainty considerations.

Thissen (2008) states that, most commonly, scientific motives push for reducing uncertainties by investing in more detailed research but some of such uncertainties may not be reducible, referred to as irreducible uncertainties. In such cases, it may be appropriate to quantify them and develop actionable approaches based on the quantified uncertainty. If any LCA practitioner were seriously considering performing uncertainty analysis as part of their LCA, they would have read several or all of the articles mentioned in Table 2. These articles clarify and/or consolidate uncertainty issues in life cycle assessment, with a general perspective, and therefore, it can easily apply to LCA studies that a practitioner is performing. The UNEP/SETAC's 'LCA Training Kit, Module K: Uncertainty in LCA' (Heijungs, Udo de Haes, White, & Golden, 2008) is of little help on its own, to an LCA practitioner interested in performing uncertainty analysis. None of these articles are detailed methodology articles, which there are many of, but these articles provide some clarity into the uncertainty-related issues, sources of uncertainty, typologies of uncertainty, technicalities, and possible methods to address uncertainty issues. In other words, a novice practitioner might be able to get a rough idea on what uncertainties and variabilities affect the practitioners LCA study, the next steps to take, and so on. In addition to these articles, CALCAS's 'Critical Review of the Current Research Needs and Limitations of ISO-LCA Practice' (Zamagni, Buttol, Porta, Buonamici, Masoni, Guinée, Heijungs, et al., 2008b) provides an in-depth overview of parameter uncertainty, model uncertainty, and scenario uncertainty, along with a literature review of these three uncertainties in Annex II (Zamagni, Buttol, Porta, Buonamici, Masoni, Guinée, & Ekvall, 2008a).

Despite the availability of such information, Hellweg and Canals (2014a) state that methods to address uncertainty in LCA are rarely used. The authors believe that these are some of the reasons why:

- Confusion about uncertainty terminologies and typologies
- Lack of detailed guidance on how to perform uncertainty analysis – step by step process
- One of the major flaws in the LCA studies that perform uncertainty analysis is the lack of justification as to why the particular methodology, a particular choice, a particular assumption was part of the study.
- Resources (economic and human) required to perform uncertainty analysis
- Absence of recommended practices for addressing uncertainty
- Limited knowledge on the strategies to reduce uncertainty
- Inadequate guidance on how to communicate uncertainty

In order to address the reasons provided, in 2008, the UNEP/SETAC Life Cycle Initiative (UNEP/SETAC Life Cycle Initiative (LCI), 2016) commenced a four-year project titled “Towards Uncertainty Management in LCA – Consensus Building and Practical Advice for Handling Uncertainty in LCA” under Phase II (2007-2012) of its activities (UNEP/SETAC Life Cycle Initiative (LCI), 2010). The core goal of this project was to provide consistent & compatible guidance to reduce, quantify (input, propagation & output), and interpret uncertainty across all life cycle stages, to practitioners and method developers. Other goals included creating a wiki of existing methods and case-studies, training courses, recommendations of methods/practice, identification of dominant sources of uncertainty, guidance on unquantifiable uncertainty, et cetera. In other words, the project aimed to nurture and guide the growth and use of uncertainty analysis in LCA. The first workshop on Uncertainty Management in LCA took place in November 2008 in Tampa, Florida, USA, and

followed by a second consensus building workshop at the LCA IX conference in September 2009 in Boston, Massachusetts, USA to discuss the first draft of the uncertainty management framework and guidance document (Rosenbaum, Ciroth, Mckone, Heijungs, Jolliet, & Freire, 2009b) (Rosenbaum, Ciroth, Mckone, Heijungs, Jolliet, & Freire, 2009a). Unfortunately, this project did not reach its completion for reasons unknown. The project page does not appear in the revamped UNEP/SETAC LCI website, nor does the existence of the project acknowledged under Phase II (2007-2012) activities (UNEP/SETAC Life Cycle Initiative, 2016).

In 2011, Reinout Heijungs and Manfred Lenzen, as part of the 'Uncertainty Group' of The Sustainability Consortium (TSC) proposed a task titled "Uncertainty propagation" wherein they would summarize and fill gaps in the behavior of uncertainty as it propagates through LCA calculations. They proposed to provide an overview and characterizations of various means to propagate qualitative and quantitative uncertainty, within the context of life cycle assessment. The outcomes of the project were to be published in a peer-reviewed journal but unfortunately, this did not happen, implying that the project may not have reached its planned completion.

Table 2: Core articles focused on general uncertainty issues in LCA.

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Heijungs, R. 1996. Identification of key issues for further investigation in improving the reliability of life-cycle assessments. *Journal of Cleaner Production* 4(3-4): 159-166.

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Huijbregts, M. A. 1998. Application of uncertainty and variability in LCA. Part I: A General Framework for the Analysis of Uncertainty and Variability in life cycle assessment. *International Journal of Life Cycle Assessment* 3(5): 273-280.

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Ross, S., Evans, D., Webber, ME. 2002. How LCA studies deal with uncertainty. *International Journal of Life Cycle Assessment* 7(1):47-52.

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Björklund, A. E. 2002. Survey of approaches to improve reliability in LCA. *International Journal of Life Cycle Assessment* 7(2): 64-72.

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Heijungs, R. and M. A. J. Huijbregts. 2004. A review of approaches to treat uncertainty in LCA. In *Complexity and integrated resources management. Proceedings of the 2nd biennial meeting of the International Environmental Modelling and Software Society (iEMSs)*, edited by C. Pahl-Wostl et al. Manno, Switzerland: International Environmental Modelling and Software Society.

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Llyod, S.M. and Ries, R. 2007. Characterizing, Propagating, and Analyzing Uncertainty in Life-Cycle Assessment. A Survey of Quantitative Approaches. *Journal of Industrial Ecology* 11(1): 161-179.

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Reap, J., Roman, F., Duncan, S., Bras, B. 2008. A survey of unresolved problems in life cycle assessment. Part 1: goal, scope, and inventory analysis. *International Journal of Life Cycle Assessment* 13: 290-300.

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Reap, J., Roman, F., Duncan, S., Bras, B. 2008. A survey of unresolved problems in life cycle assessment. Part 2: goal, scope, and inventory analysis. *International Journal of Life Cycle Assessment* 13: 290-300.

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Williams, E.D., Weber, C.L., Hawkins, T.R. (2009) Hybrid Framework for Managing Uncertainty in Life Cycle Inventories. *Journal of Industrial Ecology* 13:928-944.

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### **3.1.1 Scope of this Article**

The focus of this article is to provide an overview of the current science regarding uncertainty and variability within attributional Environmental Life Cycle Assessment modeling including the methods that are used to quantify and address uncertainty and variability. Additionally, the authors consolidate and provide LCA practitioners with (1) an operational list of uncertainties and variabilities to consider when performing an LCA, (2) document published methods to quantify and address considered uncertainties and, (3) review the methods to communicate quantified LCA results under uncertainty.

It must be noted that one or more sources of uncertainty and variability listed in following tables, in each section, maybe connected to either due to similarity, causality, general applicability, and so on. Therefore, some might argue that some sources that are too close to each other should be bundled together and others that are not sufficiently close to each other should be kept separated. The authors have made their best effort to bundle or separate various sources of uncertainty and variability based on their differences and similarities. Additionally, methods to addresses uncertainty and variability issues are not necessarily focused on one issue at a time. Since uncertainties propagate through the LCA model (inventory, impact assessment), new or proposed methods often seek to address more than one source of uncertainty and variability.

De Camillis et al. (2013) states that attributional approach is the most widely applied LCA modeling approach. Furthermore, based on an informal survey, the authors found that a large majority of LCA studies that are published are attributional in nature – the more standardized approach to LCA (Williams, Weber, & Hawkins, 2009). In a hypothetical example to express the relevance of the attributional approach, the sum of attributional LCA of all products and services in

the world will be equivalent to the observed environmental impacts worldwide (Sonnemann & Vigon, 2011). To that end, the authors limit the scope of this study to attributional LCA (also referred to as retrospective LCA), to ensure focus and facilitate a large number of attributional LCA practitioners to take advantage of the information presented here.

This article does not assess the accuracies, duplicity, overlap of typologies or terminologies of uncertainties in LCA. It does not assess the advantages and drawbacks of the methods to address uncertainty and variability (identify, characterize, quantify, communicate) that have been proposed by researchers in the peer-reviewed journal articles, books, or reports. This article does not include unresolved issues in LCA that do not cause uncertainty and variability (e.g.: inconsistent database format).

## **3.2 Uncertainty and Variability Definition, Terminology and Typology**

### **3.2.1 Uncertainty and Variability Definitions**

The term 'uncertainty', even though used in every day conversation, does not have a clear and consistent definition. The U.S. Environmental Protection Agency (2011) defines uncertainty "as the lack of precise knowledge, either quantitative or qualitative". While there are numerous definitions of uncertainty based on their field of origin (see Appendix), Downey et al. (1975) argue that the frequent use of the term uncertainty makes it easy to assume that everyone knows what uncertainty means. Milliken (1987) argues that scientists who assume that there is agreement on the definition of environmental uncertainty, tend to interpret scientific literature as though there was agreement, when in fact, there is confusion and inconsistency. This results in difference in interpretation of scientific literatures, which is uncertainty in itself.

Heijungs (1996) implies that uncertainty refers to unintentional deviations. Björklund (2002) states that the source of uncertainty is the "lack of knowledge about the true value of a quantity". First, it is clear that both authors clearly refrain from defining uncertainty. Next, it can be observed that the explanation provided by Heijungs (1996) is vague, and the one provided by (Björklund, 2002) is focused solely on the quantitative aspect. Unfortunately, while the term 'uncertainty' is used widely, there lacks a unifying definition and approach to uncertainty in attributional environmental life cycle assessment modeling.

Similarly, there are several uncertainty-related terms used frequently in LCA, often without a clear and consistent definition, and with the implicit assumption that the meaning is understood. Examples of such terms include level of uncertainty, degree of imprecision, degree of precision, degree of doubt, degree of confidence, degree of unpredictability, level of agreement or consensus, ignorance, indeterminacy, and so on. Heijungs (2013) points out that the use of technical terms incorrectly in life cycle assessment (LCA), when compared to the same terms in other disciplines and daily language, is causing confusion.

Various documents (reports, books, peer-reviewed journal articles, et cetera) on uncertainty highlight different typologies of uncertainty – some overlap in terminology but not always in definition. Roughly thirty typologies of uncertainty have been published since the year 1984 (see Appendix). Researchers continue to identify and increasing number of sources of uncertainties, when exploring various case studies (Heinemeyer et al., 2008).

It is evident that there is confusion as to whether 'uncertainty' and 'variability' should be discussed together as a single issue or as two separate issues. Uncertainty and variability have often been bundled together, on the basis that (1) variability is a type/component of uncertainty (Deser, Knutti, Solomon, & Phillips, 2012; Sabrekov,

Runkle, Glagolev, Kleptsova, & Maksyutov, 2014) – ISO 14044 (International Standards Organization, 2006d) states that data variability, along with input uncertainty and model imprecision cause uncertainty (Lloyd & Ries, 2007), (2) convenience – simply stating that the term ‘uncertainty’ includes both uncertainty and variability (Björklund, 2002; Krupnick et al., 2006), (3) stating that despite the different definitions and sources, the approaches to address them overlap (Heijungs & Huijbregts, 2004).

According to the U.S. Environmental Protection Agency (2011), ‘Variability’ is defined as “a quantitative description of the range or spread of a set of values”, whose measures include mean, standard deviation, variance, and interquartile range, and is caused due to inherent heterogeneity/diversity across various factors such as person, place and time (Food and Agriculture Organization of the United Nations, 2016). As with the term ‘uncertainty’, ‘variability’ too has many variations of definitions (Begg, Welsh, & Bratvold, 2014; Huijbregts, 1998a; National Research Council (NRC), Committee on Models in the Regulatory Decision Process, 2015), but they all roughly mean the same. Variability is also referred to as aleatory uncertainty, stochastic uncertainty, irreducible uncertainty (Uncertainty Quantification Laboratory, Stanford University, 2016), and Type A uncertainty (Food and Agriculture Organization of the United Nations, 2016).

Many articles (Begg et al., 2014; Lehmann & Rillig, 2014; U.S. Environmental Protection Agency, 2011) have been published over time distinguishing the difference between uncertainty and variability, and why shouldn’t be bundled together. Lehman (2014) distinguishes ‘uncertainty’ to be unexplained variation and ‘variability’ to be explained variation (e.g. spatial and temporal variability), though an example of soil carbon content. Similarly, the Food and Agriculture Organization of the United Nations (2016) identifies variability as heterogeneity and uncertainty as



lack of precise knowledge. Lehman (2014) calls the misinterpretation of known variability as uncertainty, as “a flaw in scientific communication that blurs the lines of scientific knowledge”. Uncertainty and variability are quantified using probability distributions and frequency distributions, respectively (Begg et al., 2014; Frey, 1992). The fact that both uncertainty and variability use distributions is a major source of confusion for many and that can lead to some researchers using frequency distributions to quantify uncertainty, resulting in erroneous assessments (Begg et al., 2014).

Frey (1992) argues that in certain cases when (1) there is uncertainty about the variability, and (2) there exists a possibility to interpret variability as uncertainty, the distinction between uncertainty and variability is unclear. In other words, frequency distributions assist in determining population subsets that merits further research, whereas probability distributions measure the uncertainty characteristics of the population that can aid in better understanding the issue of concern and determining strategies to reduce the uncertainty (Frey, 1992). The National Research Council’s Committee on Models in the Regulatory Decision Process (2015) deviates by stating that quantitative uncertainty doesn’t always use probability distribution.

Heinmeyer et al. (2008) highlights that it is not always possibility to quantify all sources of uncertainty and variability and therefore the expression of them may be qualitative or quantitative (to the extent scientifically possible). It is generally agreed upon that some uncertainties can be reduced by further research and more/better data (National Research Council, Committee on Models in the Regulatory Decision Process, 2015) but ultimately cannot be eliminated. Uncertainty that can be reduced are also referred to as epistemic uncertainty. At the same time, there are uncertainties cannot be reduced, that which are not variabilities. These uncertainties, that are specifically focused on distant futures, are referred to as “Knightian

uncertainty”, based on work by economist Frank Knight (Dizikes, 2010; Knight, 1964).

On the other hand, there is inconsistency in what researchers say about variability: (1) cannot be reduced (Björklund, 2002; National Research Council (NRC), Committee on Models in the Regulatory Decision Process, 2015; Webster & Mackay, 2003), (2) unlikely to be reduced (Deser et al., 2012), (3) hard to reduce, and (4) usually not reducible (Loucks et al., 2005; National Research Council (NRC).Committee on Models in the Regulatory Decision Process, 2007). The authors interpret the four aforementioned phrases to be (1) impossible to be reduced, (2) probability of reduction is low, (3) it can be reduced, but it is resource intensive, and (4) the frequency of reduction is low. Ultimately, all researchers agree that variability can be better characterized through further research (Björklund, 2002; National Research Council (NRC).Committee on Models in the Regulatory Decision Process, 2007).

### **3.2.2 Relevant Uncertainty Terminologies**

When reviewing uncertainty in the literature, or when discussing about uncertainty in forums, we frequently hear the following terms “characterizing uncertainty”, “uncertainty propagation”, “uncertainty analysis”, “uncertainty quantification”, which can be confusing to many. Definitions of uncertainty-related terms that may seem confusing or are not commonly found are explored here briefly.

As with the term ‘uncertainty’, ‘uncertainty analysis’ or ‘uncertainty assessment’ has many definitions (see Appendix). Heinemeyer et al. (2008) state that “the objective of an uncertainty analysis is to determine differences in the output of the assessment due to the combined uncertainties in the inputs and to identify and characterize key sources of uncertainty”. They also recommend that

sensitivity analysis be part of uncertainty analysis in order to prioritize key uncertainties and variabilities.

*Characterizing uncertainty* refers to the qualitative and/or quantitative description of the inherent properties of the uncertainties. O'Reilly et al. (2011) states that characterizing uncertainty serves the following purposes: "(1) articulate what you know, (2) indicate the precision of what you believe you do know, and/or, (3) quantify how much not knowing something (or only knowing it within a certain range of precision) matters to a given audience." The authors found very few articles defining what uncertainty characterization was, even though many use the term frequently.

Propagation refers to spreading or transferring. In the context of, *Uncertainty propagation*, the input uncertainty follows the numbers through the model, and is consolidated as output uncertainty in the final results. It is also referred to as Error propagation. Definitions for this term were not very easily found.

*Degree of uncertainty* was found to be a colloquial term used to express the deviation from the numerical value.

According to Heinemeyer et al. (2008), *Levels of uncertainty* is an expression of degree of severity of uncertainty, from an assessor's perspective. Riesch (2012) states that their terming of the typology of uncertainty as 'levels of uncertainty' in Spiegelhalter and Riesch (2011), as unwise given that other researchers have used 'levels of uncertainty' for other dimensions of uncertainty.

The authors have not found any difference between the terms 'uncertainty' and 'true uncertainty'.

*Errors* are the recognizable deficiencies in the models or algorithms that are not because of the lack of knowledge (Oberkampf & Trucano, 2002). The Uncertainty Quantification Laboratory, Stanford University (2016) states that errors are generally

associated with the translations of the mathematical formulas into computational code or numerical algorithm, and also referred to as computational error (Oberkampff & Trucano, 2002). This is very close in meaning to computational uncertainty proposed by Renouit Heijungs for the Co-ordination Action for innovation in Life-Cycle Analysis for Sustainability (CALCAS) study (Zamagni, Buttol, Porta, Buonamici, Masoni, Guinée, & Ekvall, 2008a). Oberkampff and Trucano (2002) indicates that there are two types of errors: (1) unacknowledged error (programming error, compiling error, et cetera), and (2) acknowledged error (known approximations to simplify modeling of processes).

In order to prevent confusion in terminology, the Intergovernmental Panel for Climate Change (IPCC) has mapped linguistic terminology translating degree of confidence into likelihood scale (e.g.: 'virtually certain' equivalent to '>99% probability of occurrence', 'exceptionally unlikely' equivalent to '<1% probability') and quantitatively calibrated levels of confidence (e.g.: 'very high confidence' equivalent to 'at least 9 out of 10 chance of being correct', 'very low confidence' equivalent to 'less than 1 out of 10 chance' (Spiegelhalter & Riesch, 2011). Similarly,ecoinvent 3.0 LCI Database (Weidema et al., 2013) uses statistical terms as defined in ISO 3534 (International Standards Organization, 2006a; 2006b), whenever applicable.

### **3.2.3 Uncertainty Typologies**

Sometimes, simple phrases are made confusing by researchers. For example, the phrase 'typologies of uncertainty' has been expressed in the following different ways: classes of sources of uncertainty (Heinemeyer et al., 2008), classifying uncertainty (Loucks et al., 2005), characterization of uncertainties (Kiureghian & Ditlevsen, 2009), levels for objects of uncertainty (Spiegelhalter & Riesch, 2011), kinds of uncertainty (Wynne, 1992), dimensions of uncertainty and so on. It is

important to know that proposals for new typologies of uncertainty have not reduced in the last thirty years. As with the definition of uncertainty, so far, researchers have come up with roughly thirty typologies (see Appendix) based on disagreements with pre-existing typologies.

Walker et al. (2003) state that uncertainty is a three dimensional concept: (1) *location of uncertainty* is where the uncertainty occurs, (2) *level of uncertainty* is the spectrum between deterministic knowledge and ignorance, and (3) *nature of uncertainty* is with respect to inherent variability or imperfection in human knowledge. The typology of *location of uncertainty* includes: context uncertainty, model uncertainty, input uncertainty, parameter uncertainty, and model-outcome uncertainty. The typology of the *level of uncertainty* includes: statistical uncertainty, scenario uncertainty, recognized ignorance, and total ignorance. The typology of *nature of uncertainty* includes: epistemic uncertainty, and variability uncertainty.

Typologies of uncertainty as proposed in field of life cycle assessment are shown in Table 3.

The earliest classification of uncertainty in LCA goes back to 1994, when van Hess (1994) listed five classifications of sources of uncertainties in LCA in the Fourth SETAC-Europe Congress (Lindfors, Christiansen, Hoffmann, Virtanen, Juntilla, Hanssen, Rønning, Ekvall, & Finnveden, 1995b). Later in 1995, Lindfors et al. (1995b) stated that the three types of uncertainty established by Funtowicz and Ravetz (1990) is visible in the various LCA steps. According to Lindfors et al. (1995b), *technical uncertainty* corresponds to inexactness or measurements and is often normally or log-normally distributed. It sub-divided into (1) measurement errors, (2) variation between measurements, and (3) variations of measurements in time. Measurements errors are further sub-divided into calculation errors, measuring errors, and function errors. *Methodological uncertainty* corresponds to unreliability or

bias is experimental design and is often exhibits non-continuous distributions. Lastly, *epistemological uncertainty* corresponds to ignorance or lack of knowledge.

Table 3: Suggested typologies of uncertainty and variability in LCA.

<p><b>Uncertainty in LCA (van Hess, 1994)</b></p> <ul style="list-style-type: none"> <li>• Missing data</li> <li>• Measurement accuracy</li> <li>• Differences between processes</li> <li>• Old data</li> <li>• System boundaries</li> </ul>	<p><b>Uncertainty in LCA (Lindfors, Christiansen, Hoffmann, Virtanen, Juntilla, Hanssen, Rønning, Ekvall, &amp; Finnveden, 1995b)</b></p> <ul style="list-style-type: none"> <li>• Technical uncertainty</li> <li>• Methodological uncertainty</li> <li>• Epistemological uncertainty</li> </ul>
<p><b>Uncertainty and variability in LCA (Huijbregts, 1998a)</b></p> <ul style="list-style-type: none"> <li>• Parameter uncertainty</li> <li>• Model uncertainty</li> <li>• Uncertainty due to choices</li> <li>• Spatial variability</li> <li>• Temporal variability</li> <li>• Variability between sources and objects</li> </ul>	<p><b>Uncertainty in LCA (Hertwich, Mckone, &amp; Pease, 2000), adopted from Uncertainty in risk management (Finkel, 1990)</b></p> <ul style="list-style-type: none"> <li>• Decision rule uncertainty</li> <li>• Model uncertainty</li> <li>• Parameter uncertainty and variability</li> </ul>
<p><b>Uncertainty in LCA (Zamagni, Buttol, Porta, Buonamici, Masoni, Guinée, Heijungs, et al., 2008b)</b></p> <ul style="list-style-type: none"> <li>• Parameter uncertainty</li> <li>• Model uncertainty</li> <li>• Scenario uncertainty</li> <li>• Suggestion to include 'Computation uncertainty', as proposed by Renuit Heijungs</li> </ul>	<p><b>Uncertainty in life cycle inventory (Williams et al., 2009)</b></p> <ul style="list-style-type: none"> <li>• Data</li> <li>• Cut-off</li> <li>• Aggregation</li> <li>• Geographical</li> <li>• Temporal</li> </ul>
<p><b>Uncertainty in LCA (Nicholson, 2014), seemingly adopted from Uncertainty in sustainability assessment (Huijbregts, 2011)</b></p> <ul style="list-style-type: none"> <li>• Statistical uncertainty</li> <li>• Decision rule uncertainty</li> <li>• Model uncertainty</li> </ul>	<p><b>Uncertainty in LCA (O. Jolliet, Saadé-Sbeih, Shaked, Jolliet, &amp; Crettaz, 2016)</b></p> <ul style="list-style-type: none"> <li>• Parameter and input data</li> <li>• Model uncertainty</li> <li>• Uncertainty due to choices and assumptions</li> <li>• Spatial variability</li> <li>• Temporal variability</li> <li>• Technological/population variability</li> </ul>

According to Lindfors et al. (1995b), systematic presence of uncertainty in LCA can be determined from three aspects: (1) types of uncertainty (stated above), (2) point of introduction (process, system, comparison, characterization, and valuation), (3) sources of uncertainty. The five points of introduction of uncertainty are hereby expanded briefly. Process uncertainty point refers to the uncertainty in the specification of input/output data for a process, and the uncertainty in the normalization of the input/output data to the component that it belongs to. System uncertainty point refers to the uncertainty in the normalization of input/output data for the component to the product, and the uncertainty in the summation of input/output data for all components of the product. Comparison uncertainty point refers to the normalization of the input/output to the functional unit of the product, in order to compare two products. Characterization uncertainty point refer to uncertainty due to (1) difference in spatial scales, (2) choice of models, and (3) time scales covered by the models. The valuation uncertainty point refers to the uncertainty in the weighting of the LCIA results that can carried out using various methods (Lindfors, Christiansen, Hoffmann, Virtanen, Juntilla, Hanssen, Rønning, Ekvall, & Finnveden, 1995b)

In 1998, Huijbregts (1998a), built on the work by Morgan & Henrion (1990), Funtowitz & Ravetz (1990), and US EPA (1997) to establish a typology that is shown in Table 3. According to Huijbregts (1998a), parameter uncertainty occurs due to data-related issues (inaccurate data, unrepresentative data, lack of data, et cetera). Imperfections in the LCA model, including that of the characterization model, due to simplifications of reality causes model uncertainty. Differing choices result in varying LCA results, and the uncertainty associated with this issue is called uncertainty due to choices. Spatial variability occurs due to the lack of geographic specificity in the inventory datasets, characterization models, et cetera. Temporal variability occurs

due to changes in inventory datasets and characterization factors, et cetera, over a given time period. Variability between sources and objects refers to the changes in interaction between the source of emissions and receiver of emissions due to the characteristics of the source and/or the receiver. In 2000, Hertwich et al. (2000), acknowledged the existence of the various frameworks for the analysis and typology of uncertainty, and chose to adopt an already existing uncertainty typology that was proposed by Finkel (1990).

In proposing another typology of uncertainty for LCA, Nicholson (2014) seems to have adopted the typology of uncertainty in sustainability assessment (not including variability) from Huijbregts (2011), who pieced it together the three types of uncertainty from three different sources, one being himself. This uncertainty typology includes: (1) statistical uncertainty (Walker et al., 2003; Warmink, Janssen, Booij, & Krol, 2010), (2) decision rule uncertainty (Hertwich et al., 2000) and (3) model uncertainty (Huijbregts, 1998a). Statistical uncertainty is applicable to any numerical value, and that which can be characterized in probabilities. Decision rule uncertainty occurs when there is difference in opinion about how to quantify or compare social objectives. Model uncertainty is as explained previously. Lastly, Jolliet et al. (2016) appear to have adopted the typology proposed by Huijbregts (1998a), but with few modifications to the terms.

There does not exist a consensus or even a generally agreed upon typology for uncertainty, but more recently, some researchers in LCA (Gregory, Montalbo, & Kirchain, 2013; Lloyd & Ries, 2007; Zamagni, Buttol, Porta, Buonamici, Masoni, Guinée, Heijungs, et al., 2008b) and tending to coalesce around one typology: (1) parameter uncertainty, (2) model uncertainty, and (3) scenario uncertainty - which could either be because they agree, or out of convenience, or because they assume others agree. This classification is sourced (Lloyd & Ries, 2007) from U.S.-



Environmental Protection Agency (1989) but it limited to just uncertainty and does not include variability.

The typologies of variability provided by U.S. Environmental Protection Agency (1989) include: (1) spatial variability, (2) temporal variability, and (3) inter-individual variability. Heinemeyer et al. (2008) states that their classification of uncertainties (parameter, model, scenario) is not strict and that any uncertainty that arises can overlap (e.g. model and parameter uncertainty can overlap and cannot be clearly distinguished). The only difference U.S. Environmental Protection Agency (1989) and Huijbregts (1998a) is the lack of equivalence between 'inter-individual variability' in the former and the 'variability between sources and objects' in the latter. 'Inter-individual variability' is focused on individuals, which can applicability in attributional life cycle assessment in weighting and may be even other value choices. In comparison, 'variability between sources and objects' is stated to be influential in the inventory and impact assessment phases of LCA (Huijbregts, 1998a). At the same time, when reviewing each of the roughly thirty uncertainty typologies in the Appendix, it is evident that each of them can be adapted for the field of Life Cycle Assessment.

Krupnick et al. (2006) states that the classification of uncertainties provides theoretical dividing lines and that users need not be overly concerned about classification and need to focus more on identification and treatment of uncertainties. Many have attempted to backtrack the evolution of the various typologies of uncertainty (Riesch, 2012), and discuss the benefits, detriments and thought process behind of each approach (Krupnick et al., 2006). But, in the end, it comes down to the question: Why is uncertainty typology important? How is it advantageous to the practitioner to classify uncertainty into categories?

Typologies provide a systemic platform using which the sources of uncertainty for the problem under consideration can be identified (Krupnick et al., 2006). In other words, it might eliminate the possibility for one to not consider a particular source of uncertainty. Only after identification of the uncertainties, can the actor characterize the uncertainty, prioritize it, and then seek ways to address it. It can also be argued that typology is the first step in the characterization of an uncertainty.

### **3.3 Uncertainty in Standards and Guides for LCA**

According to Finkbeiner (2013), the ISO standards serve as the constitution of LCA by representing consensus on best practice and state of art. As evidenced from the uncertainty-related statements in ISO 14044 (see Appendix), the requirements to perform uncertainty analysis attempt to be stringent with the use of several 'shall' statements. At the same time, the lack of detail in the statements can allow for varied interpretations that which can be argued against conformance to the standard. For example, ISO 14044 does not distinguish between a robust method of uncertainty analysis and a lazier method. In reality, there is huge difference in the rigor between a lazier method (using ranges to express uncertainty, while using secondary data for foreground and background systems) and a comparatively more robust method like the one proposed by Gregory et al. (2013) or Heijungs and Tan (2010), in the case of parameter uncertainty.

It is continually evident that ISO 14044 does not fulfill its core purpose of reducing or eliminating variation in its use, due to (1) vagueness of the text, (2) lack of guidelines on specific topics (Weidema, 2014b), and (3) limitations for analyzing highly complex and broad systems with interrelations and dynamics (Zamagni, Buttol, Porta, Buonamici, Masoni, Guinée, Heijungs, et al., 2008b). These reasons have resulted in many forms of LCA. Firstly, there are two forms of process-LCA (1)

attributional LCA (retrospective or accounting perspective), and (2) consequential LCA (prospective perspective) (Ekvall, Tillman, & Molander, 2005; Finnveden et al., 2009; Tillman, 2000). Secondly, Other forms of LCA that have cropped up over time, which include (1) Economic Input-Output LCA (EIO) or Environmentally extended Input Output Analysis (Hendrickson et al., 1997), (2) Hybrid Input-Output LCA (Lenzen, 2002; Peters & Hertwich, 2006; Suh, 2004), (3) Integrated Hybrid Analysis (Suh & Huppes, 2004), (4) Dynamic LCA (Pehnt, 2006), (5) Fire LCA (Andersson, Simonson, & Stripple, 2007), (6) Meso-scale LCA (Sarigiannis & Triacchini, 2000), (7) Risk-based LCA (Khan, Sadiq, & Husain, 2002), et cetera. The other forms of LCA exist to address the inability of the traditional process-LCA to comprehensively address one or more problems on a case-by-case basis. Clearly, ISO 14040 and ISO 14044 standards refer to the process to perform attributional LCA. EIO LCA (Hendrickson, Lave, & Matthews, 2006).

Hybrid Input-Output LCA and Integrated Hybrid Analysis (Suh et al., 2004) are the only other methods that claim compliance with ISO 14040/44. According to Weidema (2014b), ISO 14049 clause 6.4 (International Standards Organization, 2012) provides the basis for consequential LCA. Finnveden et al. (2009) highlights that there is still no consensus or guidance on when performing a consequential LCA is more appropriate than performing an attributional LCA. Ekvall et al. (2016) have found in their analysis that The International Reference Life Cycle Data System (ILCD) handbook (European Commission Joint Research Centre, Institute for Environment and Sustainability, 2010c) is inconsistent in their recommendations on how to choose between attributional and consequential LCA (Zamagni, Buttol, Porta, Buonamici, Masoni, Guinée, & Ekvall, 2008a).

One reason that can be attributed to lack of detail in ISO 14040 and 14044 standards is the geo-politics involved when sub-committees from 119 member

countries (full members that participate in ISO technical committees or subcommittees) come together to create and edit standards (International Standards Organization, 2015) – roughly four years process.

Noting the insufficiency in detail of the ISO standards such as ISO 14040, ISO 14041 (replaced by ISO 14044 in 2006), ISO 14042 (replaced by ISO 14044 in 2006), and ISO 14043 (replaced by ISO 14044 in 2006), several supplementary guides have been published – here are some notable publications. In 1995, the Nordic Council of Ministers published ten technical reports and two special reports (Lindfors, Christiansen, Hoffmann, Virtanen, Juntilla, Hanssen, Rønning, Ekvall, & Finnveden, 1995c; 1995b) which provided detailed information on each aspect of LCA, including uncertainty (special report 1). In the same year, the “Nordic Guidelines on Life Cycle Assessment” was published (Finnveden & Lindfors, 1996; Lindfors, Christiansen, Hoffman, et al., 1995a).

In 1997, the European Environmental Agency put forth a guidance document titled “Life Cycle Assessment (LCA). A guide to approaches, experiences and information sources” (Jensen et al., 1997). Following this, in 2001, the Center of Environmental Science - University of Leiden and the Ministry of Housing, Spatial Planning and the Environment published a supplemental guide titled “Handbook on life cycle assessment. Operational guide to the ISO standards” (Guinée et al., 2002). Further, U.S. EPA also published a guidance document titled “Life Cycle Assessment: Principles and Practice” (Scientific Applications International Corporation (SAIC), 2006), to support LCA practitioners. In 2004, Henrikke Baumann and Anne-Marie Tillman put forth the very popular “Hitch Hiker’s Guide to LCA. A orientation in life cycle assessment methodology and application” (Tillman & Baumann, 2004).

In 2008, the European Commission’s Co-ordination Action for Innovation in Life-Cycle Analysis for Sustainability (CALCAS) initiative found the simplifications in

the ISO 14040 series standards to be too restrictive and therefore has published a report titled, "Critical Review of the Current Research Needs and Limitations related to ISO-LCA Practice", as part of Deliverable 7 of Work package 5 (Co-ordination Action for innovation in Life-Cycle Analysis for Sustainability) *Critical review of the current research needs and limitations related to ISO- LCA practice*, 2008; European Commission Joint Research Centre, Institute for Environment and Sustainability, 2008; Zamagni, Buttol, Porta, Buonamici, Masoni, Guinée, & Ekvall, 2008a), where the intrinsic limits of ISO based LCA was identified (assumptions and simplifications, elements not aligned with new scientific developments or best practices, and missing or insufficient guidance). The report was also to serve as a basis to guide future directions of research in order to improve the reliability, usability and significance of LCA applications.

In order to address the shortfall of the ISO 14040/44 standards, the European Commission published the International Reference Life Cycle Data System (ILCD) Handbook – General Guide for Life Cycle Assessment – Detailed Guidance (European Commission Joint Research Centre, Institute for Environment and Sustainability, 2010c) to serve as the basis for its efforts towards product footprinting via the Product Environmental Footprint (PEF) Guide (Manfredi, Allacker, Chomkham Sri, Pelletier, & Tendall, 2012). But not everyone agrees with the additional details, requirements, and interpretations provided in the ILCD handbook (Lindfors, Ekvall, Eriksson, Jelse, & Rydberg, 2012).

There is currently an effort to create an encyclopedia of Life Cycle Assessment with additional sub-volumes on related topics such as other forms of LCA, applications of LCA, Life Cycle Management (LCM), Life Cycle Sustainability Assessment (LCSA), et cetera (Klöpffer, 2012). This encyclopedia titled "LCA Compendium – The Complete World of Life Cycle Assessment", edited by Walter

Klöpffer and Mary Ann Curran, is estimated to be roughly ten volumes, of which three (Background and Future prospects of Life Cycle Assessment (Klöpffer, 2014), Life Cycle Impact Assessment (Hauschild & Huijbregts, 2015), Life Cycle Management (Margni, 2015)) have been already published (Masoni, 2016). The more recently published guides include "Life Cycle Assessment (LCA): A Guide to Best Practice" (2014), "Environmental Life Cycle Assessment: Measuring the Environmental Performance" (Schenck & White, 2014), and Environmental Life Cycle Assessment (O. Jolliet et al., 2016).

Heijungs (2013) cites two example 'shall' statements from standards that are difficult to perform with a limited time, limited budget and limited word-limit, and therefore LCA studies not performing them should not claim 100% conformance with ISO 14044 or ILCD Handbook.

Based on discussions within the ISO community, there is a broad consensus not to revise the ISO 14040 and ISO 14044 standards in short term, based on the evaluation of proposals with respect to "criteria risk vs. opportunity, priority level, added value, and level of consensus", but that there was an indication that a modest revision in the medium term maybe on the horizon (2013). Given the vagueness in the text of the ISO standards, varied interpretations of the ISO standards, and the unclear guidance (Weidema, 2014b), it is clearly evident that the first source of uncertainty in LCA are the standards themselves, based on which LCA is performed. Finkbeiner (2013) states that while it is fair to ask for more detail, it can happen only if global consensus on those issues evolve. Alternately, if we seek to push for more standardization when global consensus has not evolved, it may backfire with the dilution of existing standards.

Despite the fact that certain first generation standards such as ISO 14040 (1997), ISO 14041 (1998), ISO 14042 (2000a), ISO 14043 (2000b), ISO 14047

(2003), and ISO 14049 (2000c) have been “technically revised, cancelled and replaced”, and revised standards have been released (Finkbeiner, Inaba, Tan, Christiansen, & Klüppel, 2006; Klöpffer, 2014), authors continue to quote and cite the first generation standards. For example, Seto et al. (2016) quote from ISO 14040:1997, Reap et al. (2008a) discuss problems in system boundaries in ISO 14041:1998, and so on. Does it matter that authors continue to cite and quote contents of standards that have been withdrawn? Maybe in some instances it may not matter and other instances it does, but do we clearly know which are those instances and which are not? According to Finkbeiner (Klöpffer, 2014, p. 88), the parallel development of the first generation of standards led to some inconsistencies between the standards. In the revision of ISO 14040:1997, ISO 14041:1998, ISO 14042:2000, and ISO 14043: 2000, the focus clearly remained on improving readability, the removal of inconsistencies and errors, and some formal (for example, reduced number of annexes, and alignment of definitions) and technical changes (for example, addition of principles of LCA, and addition of several definitions), while the main technical content remained unaffected (Finkbeiner et al., 2006). It is doubtful that authors who quote or cite the first generation of standards, check for the inconsistencies and errors and then use them.

### **3.4 Sources of Uncertainty and Variability: LCA Software Tool**

The widespread performance of LCA’s can be attributed in large part to the convenience of LCI data-containing LCA software (Klöpffer & Curran, 2013), also known as LCA software package or LCA software tool. Oftentimes, one might choose an LCA tool right after deciding to perform an LCA – mostly because one or more LCI databases are conveniently bundled with the software. Additionally, LCI data-containing LCA software’s are often expensive and may require resources (funding) in some form or the other to be obtained at the time of or in advance. As of 2007,

there were 42 LCA software tools and 26 LCI databases available amongst the worldwide LCA community (European Commission Joint Research Centre, Institute for Environment and Sustainability, 2008). Citroth (2012) identifies four characteristics to an LCA software without data: (1) platform (web-based or desktop-based), (2) pricing model (commercial or free), (3) development model (open-source or closed-source), and (4) purpose (general LCA or specialized tools or add-on's)

Few software tools such as Open LCA (OpenLCA.org, 2014), and Brightway 2 (Mutel, 2016) are available for free, where users will have to purchase the LCI database(s) independently. Commonly used commercially-sold LCI data-containing LCA software's include SimaPro (PRé Sustainability, 2013), GaBi (Speck, Selke, Auras, & Fitzsimmons, 2016; Thinkstep, 2016), Umberto (ifu Hamburg GmbH, 2016), Aveny LCA 2 (Aveny GmbH, 2016), and eBalance (IKE Environmental Technology Co., 2016). The choice of the LCA software package is influenced by factors such as financial resources available, goal of the current project and future projects, the know-how of the user, user-experience, mentor influence, convenience of access, internet-availability, reliability, ability to import/export different data formats, service-support, access to source-code, et cetera (Seto et al., 2016).

Herrmann and Moltesen (2015) compared two of the most commonly used LCI data-containing LCA software's, SimaPro 7.3.3 and GaBi 4.4.139.1 which used the same Ecoinvent database and the same version of the LCIA methods, using 100 randomly selected aggregated unit process, from a perspective of an ordinary or skilled LCA user. The LCIA methods used for comparison were EDIP 2003 (Hauschild & Potting, 2005), CML 2001 (Guinée et al., 2002), and Eco-indicator 99(H) (Goedkoop, Effting, & Collignon, 2000), which included all impact categories available in the two software's. It was found that the two software's introduce different types of errors in different stages of the calculation in their databases



(inventory and impact assessment), resulting in differences in the inventory level and the impact assessment level. When comparing the effects of the software's on already published studies such as Herrmann and Moltesen (2012) and Yusoff and Hansen (2007), it was found that the differences in impacts were so large that it could change the conclusions of the study.

Herrmann and Moltesen (2015) highlight concerns of the influence of economic factors when the absolute differences are found using the two software's for comparing alternatives. Similarly, Speck et al. (2016) performed a study comparing GaBi and SimaPro, using the creation and disposal of 1kg of aluminum, corrugated board, glass, and polyethylene terephthalate. The LCIA methods utilized in the study were Impact 2002+ (O. Jolliet et al., 2003), ReCiPe (Goedkoop et al., 2009), and TRACI 2 (Bare, 2012).

The differences in impacts in some impact categories were traced back to the difference in characterization factors used, which was also one of the outcomes of Herrmann and Moltesen (2015). Seto et al. (2016) states that it is important to select the right LCA tool for the particular project through evaluation, before performing the LCA. In order to evaluate LCA software tools, Seto et al. (2016) developed a questionnaire to assess the quality of analysis (adequate flexibility, sophistication, and complexity of analysis) for all life cycle stages, along with quantitative ratings. The questionnaire was then used to evaluate five LCA software tools for the purpose of performing comparative LCA for seven concrete mix designs.

### **3.5 Sources of Uncertainty and Variability: Goal and Scope Definition**

The 'goal and scope definition' phase is the most critical step of a life cycle assessment, where the practitioner establishes the direction, boundaries and methods used in the study. This phase requires that the following be clearly stated: (1) product system under consideration, (2) functions that are and are not

considered, (3) functional unit, (4) system boundary, (5) allocation procedures, (6) LCIA methodology and impact categories, (7) data requirements and data quality requirements, (8) assumptions, (9) value choices, (10) limitations, (11) interpretation methods, (12) critical review, et cetera (International Standards Organization, 2006d). In this section, the authors consolidate all sources of uncertainty relevant to the Goal and Scope phase of a life cycle assessment (Table 4).

Table 4: Sources of uncertainty and variability in Goal & Scope phase and methods to address them.

<b>Sources of uncertainty and variability, as provided by various scientific articles, reports, and books</b>	<b>Methods and guidance to address uncertainty and variability, as provided by various scientific articles, reports, and books</b>
Temporal change in product due to product evolution (Subramanian, Golden, & Meier, 2016)	(Subramanian et al., 2016)
Inaccurate functional unit and reference flow (Reap, Roman, Duncan, & Bras, 2008a; Rosenbaum, Citroth, Mckone, Heijungs, Jolliet, & Freire, 2009a)	(Cooper, 2003), (Weidema, Wenzel, Petersen, & Hansen, 2004), (Ciroth & Srocka, 2008), (Deng & Williams, 2011), (International Standards Organization, 2012)
Inaccurate selection of system boundaries & cut-off criteria (Reap, Roman, Duncan, & Bras, 2008a; Rosenbaum, Citroth, Mckone, Heijungs, Jolliet, & Freire, 2009a; Williams et al., 2009)	(Tillman, Ekvall, Baumann, & Rydberg, 1994), (Raynolds, Fraser, & Checkel, 2000), (J. H. Schmidt, 2008), (International Standards Organization, 2012),
Scenarios and Assumptions (Tillman et al., 1994)	(Pesonen, Ekvall, & Fleischer, 2000), (Heijungs & Guinée, 2007)
Choices (Finkbeiner, 2009; Huijbregts, 1998a)	(Huijbregts, 1998a), (Benetto, Dujet, & Rousseaux, 2006), (Steubing, Mutel, Suter, & Hellweg, 2016)
Allocation procedures (Luo, Voet, Huppel, & Udo de Haes, 2009; Reap, Roman, Duncan, & Bras, 2008a)	(Weidema, 1999) ,(Weidema, 2000), (Weidema & Norris, 2002), (Guinée, Heijungs, & Huppel, 2004), (International Standards Organization, 2006d), (International Standards Organization, 2012), (Heijungs & Guinée, 2007), (Reap, Roman, Duncan, & Bras, 2008a), (Luo et al., 2009), (Pelletier, Ardente, Brandão, De Camillis, & Pennington, 2015), (Cruze, Goel, & Bakshi, 2014), (Hanes, Cruze, Goel, & Bakshi, 2015), (Andrianandraina et al., 2015), (Schrijvers, Loubet, & Sonnemann, 2016a), (Schrijvers, Loubet, & Sonnemann, 2016b), (Beltran, Heijungs, Guinée, & Tukker, 2016)

### **3.5.1 Specification of Functional Unit and Reference Flow**

After stating the goal of the LCA study, the first steps involved is to (1) identify and prioritize product functions and product alternatives, (2) define the function unit and (3) determine the reference flows (International Standards Organization, 2012; Reap, Roman, Duncan, & Bras, 2008a; Weidema et al., 2004). ISO 14044 (International Standards Organization, 2006d) defines the functional unit as “quantified performance of a product system for use as a reference unit”, and the reference flow as “measure of the outputs from processes in a given product system required to fulfill the function expresses by the functional unit.

Subramanian et al. (2016) have highlighted that the product system under consideration may evolve over time in a non-uniform manner. Therefore, the LCA of a product may not accurately represent the product, sometimes even within the span of performing the LCA. Product evolution may or may not affect the functionality of the product. They recommend quantifying the inventory variability and interpreting the results accordingly, apart from a host of other solutions.

The interpretation of the definitions of functional unit and reference flows vary amongst different guides, but consistently provides additional detail to the ISO definitions. For example, Cooper (2003) states that the functional unit includes the magnitude and duration of service, and the product life span. Günther and Langowski (1997) interprets the quantified performance in a functional unit as technical function, whereas Weidema (2004) refers the quantified performance in the functional unit as properties that include functionality, stability, durability, appearance, ease of maintenance, et cetera – all properties that are necessary to study the alternatives, which are determined by the market requirements where the products are sold. Lindfors et al. (1995a) states that three aspects (efficiency,

durability, and performance quality standard) must be considered when specifying a functional unit.

According to Weidema (2004), reference flow refers to the product flows (product and product parts) necessary to deliver the product performance described in the functional unit, so that there is equivalence in the comparison of product alternatives. On the other hand, Cooper (2003), states that the reference includes the quantity and type of the energy and materials with respect to the functional unit, and the number of times the material is replenished over the analysis lifetime. While these and other definitions of functional unit and reference flow seem right, they are inconsistent, and its efficacy can be proved only when it is tested under a wide range of scenarios.

The functional unit is the first quantitative datum of an LCA (Ciroth & Srocka, 2008), and therefore the foundation of an LCA - and any mistakes in it would propagate through the study, leading to inaccurate results. Uncertainty in the functional unit can occur through potential error from (1) missing functions, (2) misspecified functions, (3) missprioritized functions, (4) insufficient functional unit for multiple functions (Reap, Roman, Duncan, & Bras, 2008a), (5) insufficient functional unit for difficult-to-quantify or non-quantifiable functions (Cooper, 2003; Günther & Langowski, 1997), (6) inadequacy of functional unit to handle strict functionally-equivalent comparisons, (7) irrelevant market segment (geographically, temporally, and customer), and (8) disregard for relevant alternatives or inclusion of irrelevant alternatives (Weidema et al., 2004), (9) product lifetime subject to non-systematic variations, (10) influence of consumer habits on product performance and product lifetime (Günther & Langowski, 1997).

Uncertainty in reference flows can occur through the following (1) insufficiency of the reference flow in handling multiple functions, (2) inaccuracy in

quantifying the reference flow due to use-scenarios, and system dependencies (Reap, Roman, Duncan, & Bras, 2008a), (3) disregard for relevant properties or inclusion of irrelevant properties, (4) bias in test conditions, and (5) uncertainty in measurement methods (Weidema et al., 2004).

ISO 14049 (2012) provides additional detail, supporting ISO 14044 (2006d), on how to define a functional unit and determine the reference flow. On a side note, ISO 14049 (2000c) was editorially updated in 2012 to reference to ISO 14044 instead of ISO 14041 (International Standards Organization, 1998) – no technical changes were performed (Finkbeiner, 2013). Noting the insufficiency in detail provided by the ISO standards, the Danish LCA-Methodology and Consensus Project published one among many reports titled “The Product, Functional Unit, and Reference Flows in LCA” (Weidema et al., 2004) that provides a detailed iterative step-by-step procedure to establish the goal of the study, define the functional unit, and determine the reference flows.

Similarly, Cooper (2003) has suggested requirements for specifying functional units and reference flows. Ciroth and Srocka (2008) established a method using statistical sampling to quantify precise and representative estimates (including uncertainty information) for a functional unit. ISO 14049 (2012) states that the functional unit maybe expressed as quantified product flows, in which case, it will be identical to the reference flow. Deng and Williams (2011) explore the use of an alternate measure “typical product” instead of functionality, thereby allowing the functional unit to be dynamic and in sync with the evolution of the product.

### **3.5.2 Specification of System Boundaries and Cut-off Criteria**

The selection of system boundaries determines the processes (foreground and background) and their level of detail that are included in the study, that which is closely associated with the goal of the study (Tillman et al., 1994). The specification

of system boundaries are also referred to as delimitation of system boundaries or system delimitation (J. Schmidt, 2004). Reap et al. (2008a) states that the boundaries must reflect the right breadth and depth in order for the study to reflect reality sufficiently and thereby ensure that the decision maker is confident with making decisions based on the LCA results.

According to Tillman et al. (1994) there are five dimensions that are part of system boundaries: (1) temporal boundaries, (2) spatial boundaries, (3) production of capital goods, (4) boundaries between technological system and nature, and (5) system boundaries between the product under consideration and other connected products. On the other hand, Lindfors et al. (1995a) states that there are three boundaries: (1) geographical boundaries, (2) life cycle boundaries, and (3) boundaries between Technosphere and biosphere (Jensen et al., 1997).

Ideally, the inputs to the system boundaries and the outputs from the system boundary should be elementary flows (nature to technological system, and technological system to nature) (Tillman et al., 1994).

Given that the reduction of all flows to elementary flows would be resource intensive, Tillman et al. (1994) suggests that processes that have negligible influence on the results and those identical processes between comparative systems can be omitted. Per ISO 14044, omissions of processes are acceptable provided they don't significantly change the overall conclusions of the study – such omissions shall be clearly stated, and justification and implications shall be provided. Jensen et al. (1997) states the defining a system boundary is subjective in nature, and therefore transparency in the process and in the assumptions is critical. Ignorance about pertinent aspects of the product systems under consideration can lead to subjectivity in the specification of system boundaries (Björklund, 2002).

The main issue of contention in specifying system boundaries is “cut-off criteria”, which is defined by ISO 14044 (2006d) as “specification of the amount of material or energy flow or the level of environmental significance associated with unit processes or product system to be executed from a study”. ISO 14044 highlights three types of cut-off criteria (mass, energy, and environmental significance) which should be used at the same time, to ensure that important results are not omitted from the study. The cut-off criteria are a cumulative limit based on which certain processes can be excluded from the study. Sensitive analysis is used to assess significance of important processes and is iteratively included within the system boundary. While this sounds straight forward, Reap et al. (2008a) cites the reasons provided by several researchers (Raynolds et al., 2000; Suh, 2004), who state that using cut-off criteria is very challenging in practice due to the difficulty in presenting justifications.

Reap et al. (2008a) states that using cut-off requires the LCA practitioner to have a holistic knowledge about all possible consequences of each decision on a product system, including that of the category impacts – which would result in intense consumption of resources and man-hours – maybe not very realistic. Truncation error is a result of not including pertinent processes within the system boundary due to the use of cut-off criteria.

According to Reap et al. (2008a), there are four categories of approaches to addressing boundary selection: (1) qualitative or semi-quantitative, (2) quantitative approach guided by data availability, (3) quantitative process based approach, and (4) input-output based approach. The authors summarize from Raynolds et al. (2000) that the first two approaches are unreliable, and that the process-based approach, despite being rigorous and repeatable, yields high truncation errors, increases data needs, and usually cuts off capital goods. The input-output approach



suffers from a unique set of problems but is excluded from this review as it would go beyond the attributional-LCA scope of this study (it constitutes Hybrid-LCA).

Tillman et al. (1994) propose three methods (process tree, technological whole system, socio-economic whole system) of specifying system boundaries along with multiple examples. Schmidt (2008) analyzes the differences between system delimitation in attributional and consequential approaches, and highlights that the use of attributional approach is more precise but has blind spots in the processes to be included, whereas consequential approach is more accurate and complete, but less precise. Schmidt (2008) has proposed a decision tree methodology for consequential LCA that identifies the blind-spotted processes of attributional LCA.

### **3.5.3 Assumptions**

AN LCA study usually contains several assumptions, that which increases depending on the size of the study. ISO 14044 states the following with respect to assumptions: (1) must be consistent with the goal & scope, (2) shall be clearly stated and explained, (3) use of assumptions in LCIA should be minimized, (4) uncertainty in assumptions is to be quantified as part of uncertainty analysis, and (5) variation in assumptions are to be analyzed using sensitivity analysis. Several assumptions about particular situation, which could be about the future or alternate reality and so on, leads to the formation of several different scenarios, which can be analyzed using scenario analysis (1994). Reap et al. (2008a) highlights some practical problems with scenario analysis such as (1) difficulty in predicting the future through assumptions (Pesonen et al., 2000), (2) not including the 'zero' alternative for establishing the baseline (Hauschild & Wensel, 1999), and (3) lack of transparency in the scenario elemental to the LCA study (Pesonen et al., 2000).

Scenarios are established in the 'goal and scope' phase of an LCA and its influences are visible in other phases as well. Therefore, when making comparisons

of scenarios, it is pertinent that the decision-maker is aware of the uncertainty underlying each scenario. The Working Group 'Scenario Development' in LCA of SETAC-Europe (2000) has proposed the classification of scenarios into the following: (1) what-if scenarios (compare two or more alternatives to obtain operational information; short term) and (2) cornerstone scenarios (new way of seeing the world for strategic information; long term). Pesonen et al. (2000) offer guidance to LCA practitioners on how to apply scenario analysis with respect to life cycle assessment. When assumptions are not clearly stated, explained, and analyzed using sensitivity analysis or scenario analysis, then it becomes a source of uncertainty.

#### **3.5.4 Choices**

In ISO 14044 (International Standards Organization, 2006d), one can find different types of choices: value-choices, methodological choices, data-set choices, and cut-off choices. When there are multiple choices for a particular selection, then it can lead to multiple results, and thereby uncertainty due to choices. Huijbregts (1998a) states that choices are unavoidable in LCA and provides multiple examples of uncertainty due to choices such as functional unit, allocation procedure for multiple output processes, differing weighting methods, differing characterization methodology for same impact points, and so on. Similarly, in the earlier sections, we discussed uncertainty due to choices in LCA software tool (SimaPro vs GaBi). Huijbregts (1998a) identifies several approaches to reducing uncertainty due to choices: (1) use of standardization procedures such as guidance documents which mimics unity in LCA, (2) use of peer-review to judge choices based on merit, and (3) scenario analysis, when use of standardization procedures is not possible.

Benetto et al. (2006) proposes the use of possibility theory to model the uncertainty due to methodological choices. ISO 14044 (2006d) proposes the use of sensitivity analysis to assess the outcome of methodological choices and data-set

choices. It also implies the use of scenario analysis to assess the implications of allocation rules and cut-off choices. When there are multiple choices in several value chains, the number of alternative value chains can quickly increase – the modeling becomes resource intensive and cumbersome using standard LCA software. Steubing et al. (2016) reason that the mathematical structure for the value chains in the traditional LCI databases are not appropriately designed for extensive scenario analysis. Therefore, in order to improve the efficiency in performing scenario analysis and necessary optimizations as it relates to key choices in LCA, they have introduced a modular approach to LCA. A simpler approach to decrease the number of choices was proposed by Huijbregts (1998b), which involves the formulation of several options for each choices, followed by the selection of two extreme options for each choice, and then construct two scenarios that contains the all of the selected two extreme options, and lastly, assess the effect of the two scenarios on the LCA results.

### **3.5.5 Allocation**

ISO 14044 (2006d) defines allocation as the "partitioning of input or output flows of a process or a product system under study and one or more other product systems". In other words, allocation or partitioning approach determines the environmental burden attributable to the products or functions of a multi-functional process in an accurate manner (Reap, Roman, Duncan, & Bras, 2008a; Schrijvers, Loubet, & Sonnemann, 2016b). Allocation procedures do not just apply to the LCA model that the practitioner is creating but also to the creation of new data sets and aggregated data sets. Specific attention has been paid to allocation procedures for closed loop recycling, open loop recycling, and energy recovery because the environmental burdens are shared by more than one product system (International Standards Organization, 2006d). Procedures for allocation for life cycle inventory

have been debated heavily, even as early as the year 2000 in articles such as Weidema (2000), Weidema et al. (2002). Inaccurate allocation of environmental burdens to products or functions will lead to uncertainty in the LCA results. Allocation procedures are also referred to as allocation schemes, allocation approaches, allocation methods, methods to handle multi-functional products, and so on, by various authors.

ISO 14044 (2006d) provides a three-step hierarchical process that to deal with allocation: (1) avoid allocation by utilizing either sub-division or system expansion approach (Heijungs & Guinée, 2007), (2) partitioning based on physical causality (e.g.: mass, energy), and (3) partitioning based on non-causal relationships (e.g.: cost) (Schrijvers, Loubet, & Sonnemann, 2016b). An equivalent approach to system expansion approach is the avoided burdens approach, also referred to as substitution approach or subtraction approach (Azapagica & Clift, 1999). Heijungs and Guinée (2007) states that 'what-if' assumptions in the system expansion approach is so large that it lead to divergent LCA results. At the same time, they also state that the partitioning approach cannot avoid the use of arbitrary assumptions, especially in the case of allocation factors. Another approach to partitioning is the cut-off approach, whereby the impacts are completely attributed to the functional unit, and no impacts are attributed to the co-products (Schrijvers, Loubet, & Sonnemann, 2016b).

Reap at al (2008a) has detailed the problems associated with this step-wise process. Other allocation schemes include: weight, volume, market-value, energy and demand (Curran, 2007). When comparing several approaches to allocation using a case study of comparing environmental impacts of fuels, Curran (2007) found that the choice of allocation procedures didn't have any impact on the results, using a case of three hypothetical fuel systems. On the contrary, Luo et al. (2009) have

found that choice of allocation procedures impact the outcomes of the LCA, especially for global warming potential (GWP). In order to establish consistency in how to deal with multi-functional products, Pelletier et al. (2015) recommend additional clarity and guidance in ISO 14044. They question the feasibility of the privileged recommendation of system expansion in ISO 14044, and suggest ISO to provide clear rationale for privileging natural science-based approach (e.g.: physical allocation) over socio-economic approach (e.g.: economic allocation). They state that the choice of allocation procedure should not be arbitrary but based on clear rationale with respect to the goal and scope of the LCA.

Methods of handling co-products in LCA are continually being explored via different cases such as Ayer et al. (2007), Luo et al. (2009), Wiedemann et al. (2015), who explore the co-production of wool and meat from sheep. Schrijvers et al. (2016b) acknowledges the current state of affairs, as it relates to allocation procedures, with the following points: (1) presence of various guidelines providing divergent recommendations on selection of allocation procedures, (2) lack of sufficient guidance, and (3) difficulty in selecting the best procedure for allocation from a mix of methods available from scientific literature. Consequently, they developed a systematic framework for consistent allocation procedures in attributional and consequential LCA, using recycling as a case-study. They conclude by stating that, for attributional LCA, system expansion and partitioning (including cut-off approach) can solve the issue of multi-functionality (Schrijvers, Loubet, & Sonnemann, 2016a; 2016b).

### **3.6. Sources of Uncertainty and Variability: Inventory Analysis**

The inventory analysis creates a compilation of inputs (raw materials, energy, et cetera) and emissions (to air, water, and soil) with respect to the system boundary of the study (International Standards Organization, 2006d). Life Cycle

Inventory is very data intensive using data from a wide range of sources and differing accuracy (De Smet & Stalmans, 1996). Consequently, the sources of uncertainty and variability with respect to life cycle inventory can be many, as seen in Table 4. Weidema and Wesnaes (1996) state that there are two types of uncertainty in LCI: (1) basic and (2) additional. Basic uncertainty refers to typical measurement errors and normal fluctuations in measurements, and additional uncertainty refers to lack of optimal quality of data with respect to reliability, completeness, temporal correlation, geographical correlation, and technological correlation. Williams et al. (2009) state that there are five types of uncertainty in LCI: (1) data collection errors, (2) cut-off errors, (3) aggregation errors, (4) spatial variation, and (5) temporal variation. Uncertainty in the life cycle inventory (measured or simulated) is also referred to as parameter uncertainty (Gregory et al., 2013; Lloyd & Ries, 2007). According to Lloyd and Ries (2007), parameter uncertainty is the most commonly addressed typology of uncertainty.

### **3.6.1 LCI Data Quality**

Given that a LCI contains thousands of data points, the quality of each of the data points influences the overall data quality of the LCI. Weidema and Wesnaes (1996) identify three types of data that are part of a LCI: (1) environmental data related to the investigated processes, (2) system data related to the flow of materials, energy, et cetera, through the investigated processes, and (3) performance data related to the functional unit.

Table 5: Sources of uncertainty and variability in Life Cycle Inventory Analysis Phase and Methods to Address them. n/a indicates that no guidance is available and that more research is needed.

<b>Sources of uncertainty and variability, as provided by various scientific articles, reports, and books</b>	<b>Methods and guidance to address uncertainty and variability, as provided by various scientific articles, reports, and books</b>
<ul style="list-style-type: none"> <li>Data quality (Finnveden &amp; Lindfors, 1998)</li> </ul>	(Kennedy, Montgomery, & Quay, 1996), (Weidema & Wesnaes, 1996), (Chevalier & Le Téo, 1996), (Coulon, Camobreco, Teulon, & Besnainou, 1997), (Finnveden & Lindfors, 1998), (Huijbregts, Norris, Bretz, Ciroth, et al., 2001a), (Lewandowska, Foltynowicz, & Podlesny, 2004), (Weidema et al., 2013), (Sekar, Sreenivasan, Sivakumar, Vakil, & Gondkar, 2013), (Ciroth, Muller, Weidema, & Lesage, 2013), (C. L. Weber, 2012)
<ul style="list-style-type: none"> <li>Data collection errors (Williams et al., 2009)</li> </ul>	(Weidema, Frees, Petersen, & Ølgaard, 2003), (Sonnemann & Vigon, 2011)
<ul style="list-style-type: none"> <li>Different types of data gaps (Finnveden &amp; Lindfors, 1998)</li> <li>Use of proxy data (Milà i Canals et al., 2011)</li> </ul>	(Chevalier & Le Téo, 1996), (Huijbregts, Norris, Bretz, Ciroth, et al., 2001a), (Hischier, Hellweg, Capello, & Primas, 2004), (Geisler, Hofstetter, & Hungerbühler, 2004), (Curran & Notten, 2006), (Steen & Dahllof, 2007), (Wernet, Hellweg, Fischer, Papadokonstantakis, & Hungerbühler, 2008; Wernet, Papadokonstantakis, Hellweg, & Hungerbühler, 2009), (Milà i Canals et al., 2011), (Sonnemann & Vigon, 2011), (Wernet, Hellweg, & Hungerbühler, 2012), (Henriksson, Guinée, Heijungs, de Koning, & Green, 2014), (Subramanian & Golden, 2015)
<ul style="list-style-type: none"> <li>Unrepresentative data (Henriksson et al., 2014)</li> </ul>	(Weidema & Wesnaes, 1996), (Huijbregts, Norris, Bretz, Ciroth, et al., 2001a), (Milà i Canals et al., 2011), (Weidema et al., 2013), (Subramanian & Golden, 2015)

<ul style="list-style-type: none"> <li>• Lack of understanding of underlying physical processes (R. R. Tan, 2008)</li> </ul>	n/a
<ul style="list-style-type: none"> <li>• Incorrect choice of probability distribution</li> </ul>	(Huijbregts, 1998a), (Benetto et al., 2006), (Zhang et al., 2016)
<ul style="list-style-type: none"> <li>• Inaccurate data, also referred to as inherent uncertainty (Henriksson et al., 2014)</li> <li>• Inaccurate emission factors (Rosenbaum, Ciroth, Mckone, Heijungs, Jolliet, &amp; Freire, 2009a)</li> <li>• Inaccurate emission measurements (Björklund, 2002)</li> <li>• Apparent mistakes (Finnveden &amp; Lindfors, 1998)</li> <li>• Variability around the mean, also known as spread (Henriksson et al., 2014)</li> </ul>	(Chevalier & Le Téo, 1996), (Coulon et al., 1997), (Huijbregts, Norris, Bretz, Ciroth, et al., 2001a), (Ciroth, 2004), (Koffler, Baitz, & Koehler, 2012), (Henriksson et al., 2014), (Sekar et al., 2013), (Sonnemann & Vigon, 2011), (Zhang, Wu, & Wang, 2016), (C. L. Weber, 2012)
<ul style="list-style-type: none"> <li>• Temporal variability in emission inventories (Björklund, 2002; Rosenbaum, Ciroth, Mckone, Heijungs, Jolliet, &amp; Freire, 2009a)</li> <li>• Spatial variability in emission inventories (Björklund, 2002; Rosenbaum, Ciroth, Mckone, Heijungs, Jolliet, &amp; Freire, 2009a)</li> <li>• Technological variability (Björklund, 2002; Rosenbaum, Ciroth, Mckone, Heijungs, Jolliet, &amp; Freire, 2009a)</li> <li>• Difference in performance between equivalent processes (Björklund, 2002)</li> </ul>	(Hellweg, Hofstetter, & Hungerbühler, 2003), (Udo de Haes, Heijungs, Suh, & Huppes, 2004), (Pehnt, 2006), (Levasseur, Lesage, Margni, Deschênes, & Samson, 2010), (P. Zhai & Williams, 2010), (Sonnemann & Vigon, 2011), (Collinge, Landis, Jones, Schaefer, & Bilec, 2012), (Pinsonnault, Lesage, Levasseur, & Samson, 2014), (Yuan, Wang, Zhai, & Yang, 2015),
<ul style="list-style-type: none"> <li>• Life cycle inventory modelling technique (Björklund, 2002; Koffler et al., 2012)</li> <li>• Model used to describe the unit process (Weidema et al., 2013)</li> <li>• Improper or broken linkages between unit processes</li> <li>• Non-linearity in calculations (Björklund, 2002; Ciroth, 2004)</li> <li>• Appropriateness of input or output flows (Frischknecht et al., 2007)</li> <li>• Internally recurring unit processes in life cycle inventories (Heijungs &amp; Suh, 2006)</li> </ul>	(Heijungs & Suh, 2006), (Sonnemann & Vigon, 2011), (O. Jolliet et al., 2016),



<ul style="list-style-type: none"> <li>• Static as opposed to dynamic modeling (Björklund, 2002)</li> </ul>	
<ul style="list-style-type: none"> <li>• Consolidation of some sources of uncertainty and variability listed above</li> </ul>	(Huijbregts, Norris, Bretz, Citroth, et al., 2001a), (International Standards Organization, 2006d), (Koffler et al., 2012), (Heijungs, Suh, & Kleijn, 2005), (R. R. Tan, 2008), (Heijungs & Tan, 2010), (Hong, Shaked, & Rosenbaum, 2010), (Gregory et al., 2013)

Weidema and Wesnaes (1996) state that data quality refers to data characteristics such as (1) meta-data, (2) spread and distribution pattern of the data, (3) reliability with respect to the methods used for measurement, calculation, et cetera, (4) completeness with respect to data collection points, representativeness of the population, et cetera, (5) age of the data, (6) geographical compatibility, and (7) technological compatibility. According to De Smet and Stalmans (1996), factors that affect the data quality of the each of data points include: (1) data sourced from different geographical locations around the world, (2) data sourced from national statistics literature, industry reports, manufacturers, peer-reviewed literature, books, et cetera, (3) analyst’s knowledge of the product or process under consideration, (4) assumptions used, (5) calculations performed, and (6) validation procedures (De Smet & Stalmans, 1996).

Data quality of the LCI is dependent on the goal and scope of the study in which it is to be used. The various data points obtained from numerous sources of varying accuracy are compiled together to form a LCI, and therefore a systematic data quality analysis and documentation is critical for the interpretation phase of the LCA.

Formal activities on data quality management include establishing (1) goals for data quality, and (2) data collection strategy (Weidema & Wesnaes, 1996). De Smet and Stalmans (1996) state that LCI data of good quality must be (1) relevant

to the study in terms of age, technological scope, spatial scope, et cetera, and (2) compatible with other LCI data with respect to system boundaries, level of detail, assumptions, cut-off rules, allocation rules, recycling rules, availability of data quality documentation, et cetera. In 2003, the Danish Environmental Protection Agency published a report (based on a 1998 - 1999 study) on data collection strategy which provides guidance on collecting data with adequate quality such that the overall uncertainty is reduced to an acceptable level.

This involves the following (1) identification and estimation of the largest uncertainties that dominate the overall uncertainty, (2) ascertaining reducible uncertainty from irreducible uncertainty, and (3) reduction of uncertainty that results in an overall uncertainty-based data collection strategy. In 2011, the UNEP/SETAC Life Cycle Initiative published a guidance document titled "Global Guidance Principles for Life Cycle Assessment Databases. A Basis for Greener Processes and Products" (Sonnemann & Vigon, 2011), that was created using a multi-stakeholder process. This guidance, also referred to as 'Shonan Guidance Principles', provides specific guidance on development of new data sets through data collection, developing datasets from multiple sources of existing data, and for data quality management (Sonnemann, Vigon, Rack, & Valdivia, 2013).

In order to address the need to quantify uncertainty due to data quality, Weidema and Wesnaes (1996) propose the use of pedigree matrix (PM), which originated from Post-normal science as part of the Numerical Unit Spread Assessment Pedigree (NUSAP) (Ravetz & Funtowicz, 1990). The second version of PM takes into consideration basic uncertainty (epistemic error) and additional uncertainty (imperfect data: reliability, completeness, temporal correlation, geographical correlation, and technological correlations) to convert uncertainty factors (estimated using empirical data (Ciroth et al., 2013)) to numerical values and

their deviations, based on Monte Carlo simulation with a defined probability distribution and defined number of trials. One of the limitations of the first version of PM was that it was designed for use only with lognormal distributions. Muller et al. (2014) demonstrate a new methodology which shows that PM also works with other distributions such as beta, gamma, and binomial distributions in Ecoinvent 3 (Moreno Ruiz et al., 2013).

In 2015, Muller et al. (2015) presented additional work on improving PM by deriving uncertainty factors for basic uncertainty and additional uncertainty based on type of flow or industrial sector. They state that currently used uncertainty factors in the second version of the PM, tend to underestimate uncertainty.

Kennedy et al. (1996) have proposed the use of stochastic LCA model instead of a traditional deterministic LCA model to address variable input data quality using expert judgement.

### **3.6.2 Data Gaps**

Data gaps can either be lack of data for a product or process, that can either be gate-to-gate or cradle-to-gate. Data gaps can occur due to confidential nature of industry data, technologically new product or process, data has not been collection due to lack of resources and interest, difficulty in collecting data, lack of knowledge on product or process, et cetera (Nicholson, 2014). De Eicker (2010) assessed the applicability of non-local LCI by comparing Brazilian LCI with European LCI for Triple Superphosphate, and found that the European LCI considered a broader spectrum of background processes and environmental processes – another source of data gap.

Most often, when an LCA practitioner ventures to perform an LCA, it is associated with certain resource constraints. As a result of which, foreground data is collected but background data almost always not collected (Koffler et al., 2012). LCA practitioners tend to use background data (data from commercial LCI databases, also

referred to as secondary data) in conjunction with the collected foreground data (also referred to as primary data).

Several methods that have been proposed to address data gaps include: (1) new data collection (Sonnemann & Vigon, 2011), (2) creation of aggregated data sets (Sonnemann & Vigon, 2011), (3) extrapolated data (Milà i Canals et al., 2011), (4) proxy or surrogate data (Milà i Canals et al., 2011; Subramanian & Golden, 2015), (5) molecular structure based neural network model that estimates selected inventory and impact assessment results (Wernet et al., 2008; 2009), (6) estimating gate-to-gate life cycle information using engineering process design techniques (Jiménez-González, Kim, & Overcash, 2000), (7) estimating inventory through the use of stoichiometric equations (Hischier et al., 2004), (8) buy from commercial LCA databases (Bretz & Frankhauser, 1996), (9) estimating of LCI using a generic input-output scheme for product production, with parameter values derived from on-site data and heuristics (Geisler et al., 2004), (10) use of intervals defined by experts (Chevalier & Le Téno, 1996), et cetera. Wernet et al. (2012) have proposed a tiered approach to estimate LCI and impacts using four different methods (all mentioned above), for relative quick and simple estimations of LCA results. Given that estimation of process flows are resource intensive, Steen and Dahllof (2007) propose a method for estimating process flows of chemical substances using available data for process flows, chemical properties, chemical reactions and production procedures, but concluded that there was no significant improvement in estimation when compared to the method of grouping (by chemical properties and physical properties and collect process flow data to estimate environmental impact of production based on rule of thumb) proposed by Sun et al. (2003).

Milà i Canals et al. (2011) state that the use of proxy data is the easiest and quickest way to fill LCI data gaps but they are associated high uncertainty. They

identify four types of surrogate data: (1) scaled proxies exist when known LCI's of the product, under consideration, are linearly scaled to fill data gaps created by unknown LCI's – functional equivalence is not considered, (2) direct proxies exist when a known LCI provides one-on-one replacement for an unknown but functionally similar LCI, (3) averaged proxies (or generic proxies) exist when the average (weighted or un-weighted) or median of a group of functionally similar LCI's are used as a replacement, and (4) extrapolated proxies exist when one or more LCI's are modified to create an unknown LCI (Milà i Canals et al., 2011).

Extrapolated proxies are also referred to as aggregated data in the Shonan Principles (Sonnemann & Vigon, 2011), where horizontal averaging (combining several unit processes that supply a common reference flow) (Henriksson et al., 2014) and vertical averaging (combining multiple unit processes that follow each other in the product life cycle, and are connected by intermediary flows) are utilized. Subramanian and Golden (2015) propose a method that uses expert elicitation to establish guidance on selecting the best direct proxy and also quantify the uncertainty associated with the use of the proxy. The use of data extrapolation to fill data gaps were found to require extensive expert knowledge, and therefore more robust (Milà i Canals et al., 2011). Curran and Notten (2006) have provided a summary of life cycle inventory databases, available worldwide, updated to the year 2006, that LCA practitioners can use to guide their search for spatially sensitive LCI data.

### **3.6.3 Unrepresentative Data**

Unrepresentative data can either be proxy LCI data or data whose quality (with respect to the goal and scope) has been affected by temporal difference, technological difference, and spatial difference. These issues have been sufficiently covered in the previous two sections.

### **3.6.4 Inaccurate Data**

Inaccuracy refers to errors in LCI data that be attributed to measurement error (systematic error, random error), data entry mistakes, deliberate errors, inherent randomness, and so on (Björklund, 2002). While these sources of inaccuracy may be independent of one another, they may occur at the same time. Therefore, it is incumbent on the data collector or LCA practitioner to assess these sources of data accuracy and address them appropriately.

Random errors or statistical variation are random fluctuations in the data due to improper measuring technique, equipment limitations, et cetera (Morgan et al., 1990). They can be reduced through repeated measurements and quantified as standard deviation, confidence intervals, et cetera (Morgan et al., 1990). Systematic error refers to the systemic shift in data due to consistent bias in the measuring equipment, empirical procedure.

Inherent randomness is a result of indeterminacy based on available knowledge. Morgan and Henrion (1990) state that there may be hidden variables and logical mechanisms but we don't know of their existence or understand them, and therefore we are unable to solve the indeterminacy.

Apparent mistakes (also referred to as deliberate errors) are those that are easily noticeable, that which mostly occur due to errors in estimation and data entry. Finnveden and Lindfors (1998) highlights that one of the reasons for large variations in data can be apparent mistakes. For example, a process output maybe larger than the sum-total.

According to Chevalier and Téno (1996), the use of point values in LCA data, especially that of industrial proprietary data, results in the loss of realism. The data that represents realism is called as 'fuzzy data'. Henriksson (2014) refers to this as variability around the means or spread. An example of fuzzy data is the quantity

greenhouse gas (GHG) emissions from a home's heating, ventilation and Air-conditioning (HVAC) systems, which varies based on the HVAC settings and the reaction of the inhabitants on the local climate. The following methods can be used to restore realism to average data: computation of error bounds, modeling of data fuzziness, intervals, fuzzy sets, and probability distributions (Chevalier & Le Téo, 1996). Henriksson et al. (2014) have proposed a protocol for horizontal averaging of data, while taking into consideration, the inherent uncertainty, variability around means, NUSAP pedigree, and user influence on results, thereby reducing quantitative uncertainty.

Significant figures, often confused with number of decimals, is the number of digits that provide certainty to the numerical value. Significant figures are regularly used to report on the certainty of the repeatability of the numerical values.

### **3.6.5 Variability (Spatial, Technological, Temporal, and Others)**

McKone et al. (2011) indicates that the biggest challenge to addressing uncertainty in LCA is the provision and tracking of data quality metrics, data validation and ability of data to capture the evasive trio (technological, temporal and spatial variations). Peereboom et al. (1999) identifies geographical, temporal and technological representativeness as few of the many differences in LCI data (from different databases) that caused different LCA results. Wiedemann and McGahan (2011) highlights that the natural variability in the system will subject the results of the LCA to certain degree of uncertainty.

Lack of temporal variation, also referred to as temporal homogeneity, in LCI data is referred to as one of major problems in LCA (Hellweg et al., 2003). The natural environment changes over time, and therefore the data collected (elementary flows) may not be representative of the current changes. Similarly, product supply chains are frequently changing wherein the nature of the market

demands that suppliers and buyers constantly change relationships in the supply chain (K. C. Tan, 2001) in order to remain financially viable. In other words, the properties of the intermediary flows change with respect to the changes in the supply chain. This results in temporal variability of the LCI data. Reap et al. (2008a) highlight that the temporal factors include timing and rate of emissions, time-dependent environmental processes, and temporal patterns in cradle-to-grave phases of a product, have the potential to influence the accuracy of the LCA.

Huijbregts (1998a) states that short term variations (e.g.: weekdays vs weekends) in emissions are often not considered within LCA because of how data is obtained: the averaging of yearly emissions with yearly production. At the same time, he also says that yearly variations (e.g.: over several years) may not necessarily be captured due to resource constraints. If temporal resolution does not exist in the LCI data, then the associated uncertainty is propagated to the LCIA phase (Huijbregts, 1998a). In pursuance of considering time in life cycle assessment, Levasseur et al. (2010) considers the temporal profile of emissions to compute the dynamic life cycle inventory. Pinsonnault et al. (2014) assesses the relevance of including temporal resolution in the background LCI data and notes that the inclusion is resource intensive and may not be advantageous to every study.

Spatial variation of processes has implications on elementary flows and intermediary flows. For example, the fifty miles of flat plains and fifty miles of rocky plains has implications on the amount of fuel consumed by a truck and the resulting emissions. Emissions can take place in various spatial settings such as indoors, outdoors, urban areas, rural areas, land, sea, air, fresh water lakes, and so on. Additionally, there are implications of wind characteristics, water current characteristics, et cetera on spatial variation. Difference in technology for the same



process can lead to differing elementary flows and intermediary flows, and therefore differing LCI data.

Several methods to address aggregate variability in LCI have also been proposed. Finnveden and Lindfors (1998) provide rules of thumb for variation in results for various inventory parameters (e.g. total amount of solid waste, other energy related air emissions) when no other information is available. In order to compute parametric data variability represented by fuzzy numbers, Tan (2008) has integrated fuzzy numbers with matrix-based LCI computation. He identifies this approach to be an alternative or complementary to interval analysis and probabilistic techniques for parametric uncertainty assessment. Researchers such as Pehnt (2006) and Zhai and Williams (2010) have used dynamic LCI to assess technological variation of renewable energy technologies over time (past and future). Collinge et al. (2012) utilize dynamic process modeling to incorporate temporal and spatial variations in the industrial and environmental systems that fall within the scope of the LCA. But their major contribution comes in the form of proposing a framework for dynamic life cycle assessment. Other examples of incorporating dynamic LCA includes Garcia et al. (2015) who emphasizes the dynamic behavior of a fleet of vehicles, technological improvements, operational changes of the vehicles, and background processes.

### **3.6.6 Life Cycle Inventory Modeling Imprecision**

A model is a simplification of reality and therefore, it is bound to have uncertainty associated with it. It has been noted that several LCA models provide a linear response to a non-linear phenomenon. While the use of a non-linear model can reduce the uncertainty due to this issue, Olivier et al. (2016) note that the presence of asymptotes in a non-linear model can skew the results to the higher end. In such a case, they suggest that a simple linear model may lead to more realistic results.

Improper or broken linkages between unit processes is a source of uncertainty, which can be eliminated if proper data validation is carried out. For industrial systems that deal with feedback and recirculation, internally recurring processes would be present. Matrix-based LCI's can adequately address this issue, which has been extensively reviewed by Heijungs and Suh (2006) and operationalized in ecoinvent, GaBi, and other commercial LCA databases. The latest version of ecoinvent (version 3.0) is able to explicitly account for temporal and spatial variability (O. Jolliet et al., 2016).

### **3.6.7 Methods to Address Uncertainty and Variability in Life Cycle Inventory**

Several methods have been proposed that seek to address uncertainty and variability relating to life cycle inventory results in an aggregate manner, which is often referred to as parametric uncertainty. Some methods also quantify uncertainty propagation and therefore can be used either for LCI or LCI and LCIA, in which case, they are discussed here and the citation is present both in Table 5 and Table 6.

Koffler et al. (2012) state that the uncertainty associated with the primary data can be quantified using a mean and standard deviation (best measure of spread, apart from variance, quartile, range, et cetera) over a definite number of data points. On the other hand, they say that quantifying the uncertainty in background processes, which contains hundreds of processes, is impractical and infeasible given the resource (cost, time, human) constraints. They reference Thilo Kupfer's PhD work to state that the "best achievable uncertainty in LCA is 10%", as exemplified in the case of forecast of environmental impacts in the design of chemical equipment. In other words, the minimum uncertainty for a model containing high quality data and low errors is +/- 10%.

Ciroth et al. (2004) introduce a method that combines approximation formulas and Monte Carlo simulation to calculate uncertainty in LCA (input

uncertainty, uncertainty propagation and output uncertainty). Sekar et al. (2013) propose three methods to address uncertainty due to statistical variations in LCI data and statistical variations of impacts due to differing assumptions. The first method is 'Monte Carlo based paired sampling', which works only when comparing products with similar value chains (same population). For example, two different types of steel can be compared, but steel cannot be compared with plastic. In order to address the limitation of this method, they propose the use of 'Monte Carlo based confidence interval' method. The confidence interval (CI) method linearly decreases the CI width from 95% to determine the statistical difference between comparable alternatives if the CI's do not overlap. The last method is 'parametric bootstrapping', which quantifies the variability around the mean by creating a distribution of means through resampling.

Huibregts et al. (Huijbregts, Norris, Bretz, Citroth, et al., 2001a) presents a framework for modeling data uncertainty in LCI that was put forth by the SETAC working group 'Data Availability and Quality'. In here, the working group provides suggestions to address lack of data, unrepresentative data, and data inaccuracy. Several techniques to calculate intervals have been discussed by Chevalier and T eno (1996) to quantify the true nature of data. Koffler et al. (2012), recommend a two-step approach their clients (users of GaBi LCA software) to address uncertainty in LCI data. The first step involves the performance of hot-spot analysis to identify the largest contributors of impacts and sensitivity analysis to identify the parameters that influence the largest contributors.

The second step involves the quantification of the identified parameters. In order to do that, the practitioner is expected to establish the upper and lower bounds through additional research, which are then used with Monte Carlo analysis to produce a mean and standard deviation, over 10,000 simulation runs. ISO 14044

(2006d) recommends that uncertainty analysis be performed in order to characterize the uncertainty introduced by data uncertainty and data variability into the LCI results. They also suggest that the results be expressed in the form of ranges or probability distributions. Heijungs et al. (2005) recommends the use of random sampling methods such as Monte Carlo analysis and Latin hypercube modeling or analytical formulas for error propagation, to quantify the propagation of input uncertainties.

In order to address the drawbacks of the use of Monte Carlo analysis to quantify uncertainty propagation (computationally intense, does not automatically assess sensitivity and individual parameter attribution to overall uncertainty), Hong et al. (2010) propose the use of Taylor series expansion to lognormally distributed parameters. They found that the analytical Taylor series expansion produces simpler results compared to Monte Carlo analysis, and provides individual parameter contributions to overall uncertainty.

When multiple datasets are available for a single product/process, then Weber (2012) proposes a simple process to quantify the underlying uncertainty: (1) PM approach for one dataset, (2) uniform distribution for two datasets, and (3) normal distribution (data relatively unskewed) or triangular distribution (data is relatively skewed). He uses this approach by treating temporal variability, spatial variability, lack of technological specificity, and other types of uncertainty similar to parameter uncertainty.

The use of fuzzy arithmetic integrated with matrix-based LCI has been proposed by Tan (2008) to quantify data variability in LCI, as an alternative to interval analysis, Monte Carlo analysis (probabilistic) and Taylor series (analytical). Heijungs and Tan (2010) provide rigorous proof that the assumptions used by Tan (2008) for the propagation of parametric uncertainties is valid under specific

conditions. In order to effectively compare alternative drying systems, Gregory et al. (2013) performed (1) stochastic parametric uncertainty analysis using the PM method to assess data uncertainty, and (2) probabilistic scenario analysis which targeted value choices and a selected set of parameters, to quantify their influence on the results.

Huijbregts (1998b) illustrates the influence of parametric uncertainty (in inventory and characterization factors of GWP) and uncertainty due to choices (different allocation choices) through the use of Latin Hypercube sampling in the matrix inventory method. He also uses uncertainty importance analysis to distinguish which verifies the parameter that puts forth the largest uncertainty.

### **3.7 Sources of Uncertainty and Variability: Impact Assessment**

LCIA is the most complex phase of life cycle assessment as it includes several different characterization models for various midpoint and endpoint categories, which are created based on the simplifications of the natural environment and also our limited knowledge of the natural environment. There are four or five steps in life cycle impact assessment (LCIA), depending on the source. The number of steps don't necessarily matter because it either involves consolidation of steps (e.g.: selection and classification) or exclusion of optional steps (e.g. grouping). When consolidation of steps and exclusions do not occur, these are the seven steps in LCIA: (1) selection of impact categories, category indicators and characterization models, (2) classification of LCI results to one or more impact categories, (3) calculation of impact category indicators, which is also referred to as characterization, (4) optional calculation of damage category indicators, also referred to as characterization, (5) optional use of normalization, (6) optional use of grouping, and (7) optional use of weighting (European Commission Joint Research

Centre, Institute for Environment and Sustainability, 2010b; Hauschild & Huijbregts, 2015; International Standards Organization, 2006d; O. Jolliet et al., 2016).

In the impact assessment phase, the LCI results are assigned to impact categories at an intermediary level, which are also referred to as midpoint categories. Examples of midpoint indicators include climate change, stratospheric ozone depletion, human toxicity, particulate matter formation, photochemical ozone formation, ecotoxicity, acidification, eutrophication, land use, water use, abiotic resource use, et cetera (Hauschild & Huijbregts, 2015). Then, the impact category indicators are calculated by means of multiplying the characterization factors generated by the characterization models with the inventory flows (International Standards Organization, 2006d; O. Jolliet et al., 2016).

While each impact category gives us information on targeted impacts on the environment, there can be many such impact categories, which tends to make it difficult to comprehend, absorb and communicate. Endpoint categories or damage categories represent the damage to different areas of protection such as human health, natural environment, and natural resources (Hauschild & Huijbregts, 2015). These endpoint categories are formed by allocating impact categories to one or more endpoint categories on the basis of stressors present in the inventory that have already been established to adversely impact the endpoint categories and some assumptions (O. Jolliet et al., 2016). The quantitative indicators associated with the endpoint categories are referred to as endpoint indicators. Some impact assessment methods consolidate all endpoint indicators into a single value using the process of weighting, which is commonly referred to as 'single overall score'.

Jolliet et al. (2016) argue that the importance of life cycle impact assessment comes to light when practitioners are not unable to determine the better of two emission scenarios using life cycle inventory analysis. Therefore, the magnitude or

severity of impacts from each substance is evaluated using the emissions that are aggregated based on their potential to cause environmental impacts. Life cycle impact assessment utilizes several complex models to accurately link the impact pathways of each substance in the inventory to all the associated potential environmental, thereby resulting in the midpoint indicator results for each of the considered impact categories in the impact assessment method. Jolliet et al. (2016) argue that inventory analysis utilizes implicit equivalent weighting in most cases and assigns importance to some flows in an arbitrary manner. They observe that a life cycle impact assessment that is grounded on “consistent and explicit” criteria is more appropriate than the use of implicit evaluation in inventory analysis.

Given the complexity of the characterization models, there are many sources of uncertainty in this phase, as shown in table 6. Llyod and Ries (2007) have evidenced that uncertainty is generally reported for impact assessments, always report on mid-point indicators, end-point indicators and overall scores. It is also clear that any advancement in life cycle impact assessment methods seeks to effectively (1) reduce uncertainty and/or (2) quantifying uncertainty, in the results.

Table 6: Sources of uncertainty and variability in Life Cycle Impact Assessment phase and methods to address them. n/a indicates that no guidance is available and that more research is needed.

<b>Sources of uncertainty and variability, as provided by various scientific articles, reports, and books</b>	<b>Methods and guidance to address uncertainty and variability, as provided by various scientific articles, reports, and books</b>
<ul style="list-style-type: none"> <li>• Choice of impact assessment methodology</li> <li>• Selection of impact categories (Laurin et al., 2016; Reap, Roman, Duncan, &amp; Bras, 2008b)</li> <li>• Use of more than one characterization methodology for</li> </ul>	(Halleux, Lassaux, & Germain, 2006), (Landis & Theis, 2008), (Weidema, 2014a), (Dreyer, Niemann, & Hauschild, 2003), (European Commission Joint Research Centre, Institute for Environment and Sustainability, 2010a), (Benetto et al., 2006), (Huijbregts,

<p>one or more impact categories (Huijbregts, 1998a)</p> <ul style="list-style-type: none"> <li>• Choice of characterization model for an impact category (Björklund, 2002; Rosenbaum, Ciroth, Mckone, Heijungs, Jolliet, &amp; Freire, 2009a)</li> <li>• Improper linkages between the mid-point indicators and the end-point indicators; endpoint characterization factors (International Standards Organization, 2006d)</li> <li>• Lack of standardization of impact categories</li> <li>• Omission of known impact categories Goedkoop:srcXL11j</li> <li>• Omission of known endpoint categories (Goedkoop et al., 2009)</li> <li>• Inconsistent impact category indicators (O. Jolliet, Frischknecht, Bare, &amp; Boulay, 2014)</li> </ul>	<p>1998a), (Reap, Roman, Duncan, &amp; Bras, 2008b),</p>
<ul style="list-style-type: none"> <li>• Inaccurate characterization factors (Herrmann &amp; Moltesen, 2015)</li> <li>• Spatial variability of fate factors (Rosenbaum, Ciroth, Mckone, Heijungs, Jolliet, &amp; Freire, 2009a)</li> <li>• Temporal change in the environmental systems (Huijbregts, 1998a; Rosenbaum, Ciroth, Mckone, Heijungs, Jolliet, &amp; Freire, 2009a)</li> <li>• Spatial variability in the environmental sensitivity (Huijbregts, 1998a; Rosenbaum, Ciroth, Mckone, Heijungs, Jolliet, &amp; Freire, 2009a)</li> <li>• Variation in susceptibility of humans, with and without respect to spatial factors (Huijbregts, 1998a; Rosenbaum, Ciroth, Mckone, Heijungs, Jolliet, &amp; Freire, 2009a)</li> <li>• Inadequate characterization models (Hauschild et al., 2012)</li> </ul>	<p>(Hauschild &amp; Potting, 2005), (Potting &amp; Hauschild, 2005), (Pinsonnault et al., 2014), (Rosenbaum &amp; Jolliet, 2013), (Manneh, Margni, &amp; Deschênes, 2010), (Rosenbaum et al., 2008), (Hauschild et al., 2008), (Brent &amp; Hietkamp, 2003), (Heijungs, de Koning, Ligthart, &amp; Korenromp, 2004), (Heijungs et al., 2004)</p>
<ul style="list-style-type: none"> <li>• Absence of characterization factors (Huijbregts, 1998a; Rosenbaum, Ciroth, Mckone, Heijungs, Jolliet, &amp; Freire, 2009a)</li> </ul>	<p>(Rosenbaum et al., 2008), (Hauschild et al., 2008)</p>
<ul style="list-style-type: none"> <li>• Insufficient knowledge on the lifetime of substances (Huijbregts, 1998a)</li> </ul>	<p>(Huijbregts, Guinée, &amp; Reijnders, 2001b)</p>



<ul style="list-style-type: none"> <li>Value choices in time horizon of the characterization methodology or impact assessment model (De Schryver, Humbert, &amp; Huijbregts, 2012)</li> </ul>	(De Schryver et al., 2012)
<ul style="list-style-type: none"> <li>Use of static modeling as opposed to dynamic modeling (Björklund, 2002)</li> <li></li> </ul>	(Collinge et al., 2012), (Pehnt, 2006)
<ul style="list-style-type: none"> <li>Use of linear instead of non-linear modeling (Björklund, 2002)</li> <li></li> </ul>	(van Zelm et al., 2012)
<ul style="list-style-type: none"> <li>Inaccurate normalization data (Huijbregts, 1998b; Rosenbaum, Ciroth, Mckone, Heijungs, Jolliet, &amp; Freire, 2009a; Wegener Sleeswijk, van Oers, Guinée, Struijs, &amp; Huijbregts, 2008)</li> <li>Variation in normalization data (Laurent, Lautier, Rosenbaum, Olsen, &amp; Hauschild, 2011a)</li> <li></li> </ul>	(Laurent, Lautier, Rosenbaum, Olsen, & Hauschild, 2011a), (Laurent, Olsen, & Hauschild, 2011b), (Lautier et al., 2010), (Bare, Gloria, & Norris, 2006),
<ul style="list-style-type: none"> <li>Limitations in normalization methodology</li> </ul>	(Norris, 2001), (Stranddorf & Hoffmann, 2005), (Stranddorf, Hoffmann, & Schmidt, 2005), (Curran, 2012), (Prado-López, 2015), (SETAC North American LCA Advisory Group, 2015), (Laurin et al., 2016), (Prado-López et al., 2013), (Prado-López et al., 2015), (Prado-López, 2015)
<ul style="list-style-type: none"> <li>Bias in Normalization (Heijungs, Guinée, Kleijn, &amp; Rovers, 2007)</li> <li>Data gaps in reference emissions</li> </ul>	(Heijungs et al., 2007), (Wegener Sleeswijk et al., 2008), (Laurent, Olsen, & Hauschild, 2011b), (Lautier et al., 2010)
<ul style="list-style-type: none"> <li>Choice of weighting methodology (Huijbregts, 1998a)</li> </ul>	(Udo de Haes, 2000), (Stranddorf & Hoffmann, 2005), (Stranddorf et al., 2005), (Prado-López et al., 2013), (Prado-López et al., 2015), (Prado-López, 2015), (Koffler, Schebek, & Krinke, 2008), (W.-P. Schmidt & Sullivan, 2002), (Huppel, van Oers, Pretato, & Pennington, 2012)
<ul style="list-style-type: none"> <li>Inoperative weighting criteria (Huijbregts, 1998a; Rosenbaum, Ciroth, Mckone, Heijungs, Jolliet, &amp; Freire, 2009a)</li> <li>Unrepresentative weighting criteria (Hauschild &amp; Huijbregts, 2015)</li> </ul>	(Hauschild & Huijbregts, 2015), (Itsubo et al., 2015), (Johnsen & Løkke, 2012)
<ul style="list-style-type: none"> <li>Variability of environmental preferences (Huijbregts, 1998a)</li> </ul>	(Itsubo, Sakagami, Kuriyama, & Inaba, 2012), (Hauschild & Huijbregts, 2015)

<ul style="list-style-type: none"> <li>• Variation in weighting factors (Hauschild &amp; Huijbregts, 2015)</li> </ul>	(Itsubo et al., 2012)
<ul style="list-style-type: none"> <li>• Omission of unknown impact categories (Rosenbaum, Ciroth, Mckone, Heijungs, Jolliet, &amp; Freire, 2009a)</li> </ul>	n/a
<ul style="list-style-type: none"> <li>• Contribution to impact category is unknown (Huijbregts, 1998a)</li> </ul>	n/a
<ul style="list-style-type: none"> <li>• Incorrect choice of probability distribution</li> </ul>	(Huijbregts, 1998a), (Benetto et al., 2006), (Zhang et al., 2016),
<ul style="list-style-type: none"> <li>• Consolidation of two or more uncertainties and variabilities listed above</li> </ul>	(Huijbregts, 1998b), (Hong et al., 2010)

### **3.7.1 Impact Assessment Methods, Selection of Impact Categories and Characterization Models**

ISO 14044 states that selecting impact categories, category indicators and characterization models must be clearly justified and described, including the appropriateness of the characterization model used to determine the indicators.

In reality, practitioners don't often choose impact categories, choose impact indicators, perform classifications of LCI results, and choose characterization models, rather they choose an impact assessment methodology that contains a characterization model for each selected impact category. There are roughly twelve impact assessment methods, for life cycle assessment, publicly available to be used by LCA practitioners (European Commission Joint Research Centre, Institute for Environment and Sustainability, 2010a).

These methods are often bundled in LCI data-containing LCA software packages. Some of these methods are limited to midpoint categories, whereas others extend to endpoint categories. These methods have varying number of midpoint

(impact) categories and endpoint categories, some of which overlap across methods. For example, 'ReCiPe' LCIA methodology (Goedkoop et al., 2009) has eighteen midpoint categories and three endpoint categories, whereas 'IMPACT World+' LCIA methodology (IMPACT World+, 2013) has ten midpoint categories and three endpoint categories. Global warming, ozone depletion, human toxicity are some examples of midpoint categories that are common between the two methodologies. IMPACT World+ (2013) has one midpoint category called 'ecotoxicity', while in ReCiPe, it appears as terrestrial ecotoxicity, freshwater ecotoxicity, and marine ecotoxicity. The endpoint categories vary slightly from each other: (human health = human health), (ecosystem diversity ≠ ecosystem quality), and (resource availability ≠ resource and ecosystem services).

Over the last 20 years, LCIA methodologies have been evolving and improving by building on top of each other. IMPACT World+ is an update to IMPACT 2002+ (O. Jolliet et al., 2003), EDIP, and LUCAS. It incorporates information necessary to quantify spatial variability and model uncertainty (IMPACT World+, 2013). Impact 2002+ was an update to Eco-indicator 99, with the exception for toxicity impact categories. Stepwise 2006 (Weidema, 2009; Weidema, Wesnaes, Hermansen, Kristensen, & Halberg, 2008) was modeled based on IMPACT 2002+ (O. Jolliet et al., 2003) and EDIP2003. ReCiPe 2008 was modeled on endpoint-oriented Eco-indicator 99 and the midpoint-oriented CML 2002 method (Goedkoop et al., 2009). Given the choices associated with the selection of impact assessment methodologies, several researchers have compared them to figure out the difference between them.

Reap et al. (2008b) highlights the lack of standardization in the impact categories that have lead to slightly different impact categories and different characterization models. Dreyer et al. (2003) concludes, from their comparative

analysis of EDIP97, CML2001, and Eco-indicator 99, that choice of impact assessment methodology matters in some cases, with respect to diverging impact category indicators. Bulle et al. (2014) compared four LCIA methodologies which included IMPACT World+ (IMPACT World+, 2013), Eco-indicator99 (H) (Goedkoop et al., 2000), Stepwise2006 ("Impact assessment with option of full monetarisation - 2.-0 LCA consultants," 2006; Weidema et al., 2008), and ReCiPe (H)(Goedkoop et al., 2009), and noted that the overall tendency of the methodologies with respect to high importance and low importance of impact categories are respected. At the same time, they noted some differing behaviors between methodologies that required additional research. Weidema (Weidema, 2014a) compared three LCIA methods which included Eco-indicator99 (H) (Goedkoop et al., 2000), Stepwise2006 (Weidema, 2009; Weidema et al., 2008), and ReCiPe (H) (Goedkoop et al., 2009) using the monetary evaluation of the commonly shared endpoints of the three methods, which was 30%, 28% and 165% of the gross domestic product. He observed that the main differences between the methods were due to assumptions used and the data used in the models, especially as it relates to human health, technology shifts, land-related issues and so on. Landis et al. (Landis & Theis, 2008) compared LCIA methodologies that included IMPACT 2002+, TRACI, and CML and observed that the difference in results were due to the following (1) inconsistent characterization factors for substances associated with some impact categories, (2) differing classifications of LCI to impact categories and (3) differing definitions of impact categories.

There are genuine and deceptive instances when more than one LCIA methodology is used for a particular impact category. In the case of genuine instances, a practitioner might use different LCIA methodologies for a single impact category to confirm that the results are consistent; if the results are not consistent

then the practitioner might attempt to understand the reasons why the results are not consistent. For example, Weidema (Weidema, 2014a) noted that questionable assumptions, important omissions and flawed calculations were part of ReCiPe 2008 LCIA methodology, when compared to Eco-indicator99 (H) (Goedkoop et al., 2000) and Stepwise2006 (Weidema, 2009; Weidema et al., 2008). In the case of deceptive instances, a practitioner might use different LCIA methodologies for a single impact category to assess which characterization model provides comparatively smaller or smallest results, and then uses that characterization model (of that particular LCIA methodology) in the LCA while providing some other form of justification for the choice of the characterization model. Choice of characterization models or impact assessment methodologies results in uncertainty due to choices.

Goedkoop et al. (2009) highlights four missing midpoint categories (erosion, salination, noise, and light) and one missing endpoint category (damage to man-made environment) in ReCiPe 2008 impact assessment methodology. They also state that there are missing and incomplete links between midpoint categories and endpoint categories – a major source of uncertainty. For example, marine eutrophication is not linked to any endpoint. Goedkoop et al. (2009) cite uncertain and insufficient knowledge of the environmental mechanism as reasons for the above sources of uncertainty.

Laurin et al. (2016) argues that ISO does not provide sufficient guidance to select impact categories and therefore practitioners may omit important impact categories due to ignorance. Reap et al. (2008b) list the following reasons as to why LCA practitioners may omit impact categories: (1) lack of impact category in the selected LCIA methodology or LCA tool, (2) determining that the impact category is unnecessary for the case-study, (3) belief that the methodology is under-developed, (4) lack of data to facilitate the assessment of the specific impact category and so

on. If there exist impact categories in the LCIA methods, then there exists characterization models for those impact categories, that product impact category indicator results; unless the impact category is just a placeholder for future method updates.

Brent and Hietkamp (2003) compare five European LCIA methodologies (CML, Ecopoint, EPS, Eco-indicator 95 and Eco-indicator 99) to assess their applicability to a screening LCA with a geographical scope of South Africa. They conclude that some impact categories such as air pollution and mined abiotic resources are applicable, while other impact categories relating to ecosystem quality, water and land resources are not applicable. They also note that normalization and weighting maybe difficult to adapt due to differing reference data, and socio-cultural and political differences.

### **3.7.2 Characterization Models**

The characterization factors for each impact category are calculated using different highly specialized models developed in other disciplines. For example, the impact categories 'Acidification' and 'Eutrophication' utilizes different fate and effects models to calculate the characterization factors; for toxicity and ecotoxicity related impact categories, the harmoniously developed USETox model can be used to calculate characterization factors.

Midpoint (substance-specific) characterization factors are weighting factors for emissions and extractions that are characterized and quantified using highly complex multimedia fate, exposure, toxic effects, resources, ecosystem services and effects models (Goedkoop et al., 2009; Hauschild et al., 2008; O. Jolliet et al., 2016). The characterization factors of the substances are multiplied with the quantity of the inventory per functional unit to produce a midpoint indicator result.

Similar to the classification of inventories to one or more impact categories, impact categories may be classified into one or more endpoint categories. There are instances where a midpoint category is not assigned to a endpoint category – an example of which was presented in the previous section. To perform this conversion, the midpoint indicator result is multiplied by a midpoint-to-damage characterization factor (O. Jolliet et al., 2016).

Input data uncertainty is propagated through the characterization models and appear as output uncertainty in the characterization factors. Therefore, uncertainty exists in the characterization factor due to the propagation of various uncertainties such as (1) uncertainty due to the simplification of the characterization model, (2) uncertainty due to assumptions and choices in the characterization model, (3) uncertainty due to inaccurate input data, (4) uncertainty due to data gaps, et cetera. Jolliet et al. (2016) highlights the importance of quantifying uncertainty and spatial variability of characterization factors.

Hasuchild et al. (2012), on behalf of the Joint Research Center for the European Commission, performed a study that analyzed all existing characterization models at the midpoint (14 impact categories) and endpoint (3 damage categories) level, and other models with potential for use in LCIA. Using externally vetted criteria, some of which was general and others specific to each impact or damage category, ninety-one short listed models were assessed based on scientific qualities and stakeholder acceptance. The best characterization models were identified and they were classified based on their recommendations. They found that at the midpoint level, ten out of fourteen impact categories needed improvement in the best available characterization models. At the endpoint level, midpoint to endpoint characterization models for eleven out of fourteen impact categories were found to be weak.

### **3.7.3 Addressing Sources of Uncertainty and Variability in Impact Categories, LCIA Methodologies, and Characterization Models**

Rosalie et al. (2012) have found that use of quantification of uncertainty in LCIA is enhanced when the trade-off between various types of uncertainty is quantified. In 2003, the UNEP/SETAC Life Cycle Initiative facilitated the building of a toxicity model for life cycle impact assessment based on consensus building. This effort was propelled into motion after researchers identified large variations in various characterization models (CalTOx, Impact 2002+, USES-LCA, EDIP97), and at the same time recognized the value in the different modeling approaches. The resulting 'USEtox' model used parsimony as the guiding principle and was developed by an international group of LCIA characterization model developers (Hauschild et al., 2008; Rosenbaum et al., 2008).

This model, which is being used in ReCiPe 2008 and IMPACT World+, provides consistent characterization factors for numerous substances, as it relates to toxicity. Additionally, USEtox also fills data gaps in characterization factors. Thereby reducing some of the sources of uncertainty and variability across characterization models used in various LCIA methodologies.

Pinsonnault (2014) used enhanced structural path analysis to develop time-dependent characterization factors for climate change impact category, so as to quantify temporal variability in the characterization model. Given our limited knowledge of lifetime of substances as it relates to environmental impacts, specifically toxicity, Huijbregts et al. (2001b) performed scenario analysis to compare and understand the impacts of toxic substances over time horizons such as 20 years, 50 years, 100 years and infinite time horizon.

Uncertainty in the form of perspectives is integrated within ReCiPe 2008. Goedkoop et al. (2009) have consolidated different sources of uncertainty and



assumptions into three perspectives based on cultural theory (Thompson, Ellis, & Wildavsky, 1990): individualist, hierarchist, and egalitarian. While this is progress in terms of addressing uncertainty, the practitioner is now faced with uncertainty due to choices. De Schryver et al. (2012) compared the influence of the three value choices on human health damage score (midpoint categories: water scarcity, tropospheric ozone formation, particulate matter formation, human toxicity, ionizing radiation, stratospheric ozone depletion, and climate change) and found that there is an average difference of 1 order of magnitude between individualistic and hierarchist, and average difference of 2.5 orders (maximum of 4 orders) of magnitude between individualistic and egalitarian. They indicate that the sources for the differences are the time-horizons of the perspectives and the inclusion/exclusion of highly uncertain effects. They indicate that the ranking of product comparison can change based on the choice of the perspective.

IMPACT World+ (IMPACT World+, 2013) is the most recently released LCIA methodology with spatially focused characterization factors for the entire world and improved characterization modeling based on most up-to-date research. Rosenbaum and Jolliet (Rosenbaum & Jolliet, 2013) indicates the characterization factors for the LCIA methodology IMPACT World+ (IMPACT World+, 2013) comes with quantitative uncertainty and spatial variability estimates (Bourgault et al., 2013). This is accomplished using two semi-quantitative PM's for each impact category representing uncertainty and spatial variability, respectively, to calculate the squared geometric standard deviation for the CF. They indicate that this process is performed for the few CF's in some impact categories (e.g.: eutrophication) and for the thousands of CF's in other impact categories (e.g.: ecotoxicity). These spatially focused CF's work with geo-referenced inputs and outputs from the inventory (e.g.:

as made available in ecoinvent 3.0) to deliver results that are more accurate than existing methodologies.

As part of Phase 3 of the UNEP/SETAC Life Cycle Initiative, a flagship project was launched to administer guidance and build harmony towards LCIA indicators. The progress made by various task forces were discussed in a workshop in Valencia, Spain (Jan 24 – 29, 2016), and feedback was received on cross-cutting issues and key guidance issues (Frischknecht et al., 2016; O. Jolliet et al., 2014)

#### **3.7.4 Normalization**

The indicator scores of the impact categories and the damage categories are expressed using reference units that are different between categories, which can be hard to interpret and communicate (Hauschild & Huijbregts, 2015). The optional step of normalization in life cycle assessment calculates the indicator results with respect to some reference information that is available for categories so that the relative magnitude of the results is more meaningful to the practitioner and the decision maker.

In practice, the indicator result of each impact or damage category is divided by a corresponding impact or damage category indicator, thereby reflecting the relative performance with respect to the reference system (Hauschild & Huijbregts, 2015). Examples of reference information include: (1) total yearly emissions for reference year (Huijbregts et al., 2003), (2) emissions by population of a specific area in a certain year (Heijungs et al., 2007), (3) emissions by the world in a specific year (Heijungs et al., 2007), et cetera. Laurent and Hauschild (2015) argue that the scope of the normalization must align with the scope of the weighting.

For example, global supply chains might demand the use of global emissions as the normalization reference but use of national or regional weighting schemes will demand for the use of national or regional normalization references. Through

normalization, all impact categories and damage categories will have a single reference unit such as person equivalents or person years. Now, this enables practitioners and decision makers to compare the various impact or damage categories side-by-side. Additionally, normalization may help with checking for inconsistent results (Hauschild & Huijbregts, 2015; O. Jolliet et al., 2016).

The sources of uncertainty and variability in this step can be attributed to (1) accuracy of the normalization data (characterization factor, normalization factor, emissions data), (2) bias in normalization, and (3) limitations of the normalization methodology. Norris (2001) has identified two types of normalization: internal and external, based on whether the reference system is part of the study or not. According to Heijungs et al. (2007), ISO 14044 references the use of external reference information and therefore they are hesitant in considering internal normalization as a form of normalization.

The LCA advisory group of SETAC North America (2015) has published the benefits and drawbacks of a limited list of four normalization methods (external normalization to some reference material or process, external normalization to the total or per capita emissions/extractions, internal normalization to the highest impacting alternative, and internal normalization via outranking). It is evident from most studies that 'external normalization to the total or per capita emissions/extractions' is the most frequently used method of normalization, which Laurin et al. (2016) claims to have gained general acceptance. Laurin et al. (2016) go on to list out the drawbacks of this method that includes: data gaps in reference emissions (Heijungs et al., 2007), lack of consensus on the reference normalization data (Bare et al., 2006), unavailability of quantitative uncertainty and variability information for the reference normalization (Lautier et al., 2010), and spatial and

temporal variability in the reference normalization (Bare et al., 2006; Bare & Gloria, 2006; Finnveden et al., 2009).

Lautier et al. (2010) indicate that the main sources of uncertainty and variability in the Canadian normalization factors are due to data gaps (specifically with metal related emissions), and inventory assumptions, differing industrial activities in various regions. According to Benini et al. (2014), "normalization factors express the the total impact occurring in a reference region for a certain impact category". Laurent et al. (2011b) contend that normalization references for toxicity-associated impacts are more sensitive to inventory coverage and less sensitive to variation in emissions. Laurent et al. (2011a) provide guidance on how to extend normalization references from one region to another while minimizing uncertainty and inconsistency. They also quantify the variation associated with the normalization references.

Heijungs et al. (2007) has brought to light the existence of bias in normalization that can occur due to data gaps in the emissions data and the characterization factors. This results in some normalized midpoint or damage indicators being right, others being much lower or much higher. They state that this normalization bias affects the utility of the normalized results for the purposes of error-checking using anomalies, weighting based on value-choices, and independent presentation of normalized results. They conclude from their analysis that the best way to address normalization bias is to fill data gaps, attentively detect bias and then discuss its implications to the study. Sleeswijk et al. (2008) provide guidelines for prioritizing data sources and for data estimation, when it comes to addressing data gaps. Laurin et al. (2016) recommend development of additional methods for normalization to facilitate robust decision-making.

ISO 14044 (2006d) recommends the use of more than one reference system and using a sensitivity analysis to give decision makers a perspective on how different reference systems influence the category or damage indicators. Usually, normalization data is developed specifically for each impact assessment methodology. For example, ReCiPe LCIA methodology has two reference systems (1) Europe, 2000 and (2) World, 2000.

### **3.7.5 Grouping and Weighting**

Grouping is an optional process by which impact categories are grouped together for the purpose of sorting and/or ranking based on the goal and scope of the LCA study. Sorting can be performed on the basis of various factors such as spatial scales, emissions, elementary flows, et cetera. Ranking is based on value-choices (International Standards Organization, 2006d), and therefore is a source of uncertainty that can be addressed using sensitivity analysis, as mentioned in the previous sections.

Weighting is an optional process where indicators results are transformed by using numerical factors based on value-choices. For example, if the user believes that Global Warming Potential (GWP) is more important than Acidification, then the indicator result of GWP can be multiplied by a larger numerical factor than the Acidification result is multiplied by a smaller numerical factor. ISO 14044 (2006d) states that aggregation of weighted indicator results may be performed to obtain a single score. Itsubo (2015) states that weighting is important because trade-offs can be resolved in a definite and transparent manner, thereby facilitating easier decision making (European Commission Joint Research Centre, Institute for Environment and Sustainability, 2010b). The use of weighting makes it convenient to simplify and transmit complex environmental information in the form of a single score to the general consumer (Itsubo, 2015). Weighting factors are also referred to

as integration factors (Itsubo et al., 2012), when used to integrate multiple environmental impacts into single index.

Weighting has been a controversial issue as it deals with values relating to society at large, ethics and politics (Huppes & van Oers, 2011; Udo de Haes, 2000). Itsubo et al. (2012) states that results of weighting are influenced by age, sex, gender, religion, education and various other factors. Since this step is based on value-choices, different people or groups of people will make decisions that will lead to different sets of weighting factors – making it controversial. In other words, the weighting can mask the normalized impacts and can sometimes produce results that in contrast to the normalized results.

Itsubo (2015) indicates that there are three approaches to weighting based on the where it is applied in LCA: (1) proxy (inventory data), (2) midpoint, and (3) endpoint (type 1 and type 2). In the proxy approach, the weighting factor is to the inventory data. In the mid-point approach, the weighting factor is multiplied to the normalized midpoint indicator results. Type 1 endpoint approach requires the multiplication of the weighting factor with the normalized endpoint indicator results, whereas the type 2 endpoint approach requires multiplication with the characterized endpoint indicator results. Itsubo (2015) provides a comparison of pros and cons of these approaches, but makes it clear that only the midpoint approach is in conformance with ISO 14044. Jolliet et al. (O. Jolliet et al., 2016) recommend that weighting be performed only on the damage categories because there already exists a midpoint-damage factor based on natural science.

Weighting methods have been classified differently by many. Udo de Haes (2000) classifies it as (1) monetization methods, (2) panel methods, and (3) policy targets. Itsubo (2015) excludes policy targets from this classification for reasons that are unclear. Jolliet et al. (2016) refers to panel methods as surveys, but with roughly

the same meaning. Udo de Haes (2000) states that all these methods have their own disadvantages and advantages, which makes it uncertainty due to value choices. Seppälä and Hämäläinen (2001) note that these methods produce distinctive weighting factors based on diverse factors. Johnsen and Løkke (2012) have reviewed eight criteria (published between 1994 and 2011) available to evaluate weighting methods. The evaluation criteria were grouped into general criteria and environmental damage related criteria. They observed that the criteria emphasized comprehensiveness and transparency. Johnsen and Løkke (2012) note that a major proportion of the criteria was scientifically based, even though ISO 14044 states that weighting is not scientifically based.

Often weighting factors are developed in a generalized manner, without respect to the product being assessed, the people using the product, and so on. The lack of representativeness in the weighting factors with respect to the goal and scope of the LCA is a source of uncertainty. Itsubo et al. (2012) contends that weighting should be representative of societal preferences (e.g.: national averages) as opposed to smaller samples, such as those obtained from panel methods. For implementation in the LIME2 LCIA methodology, they used conjoint analysis and surveys to determine the weighting factors representing the Japanese public. In 2015, Itsubo et al. (2015) expanded their methodology which was used to develop weighting factors for Japan, to include all G20 member states.

Through the use of visiting surveys, interviews, internet surveys, and statistical analysis, they were able to produce two types of statistically significant weighting factors: (1) dimensionless and (2) monetary (willingness to pay). They developed weighting factors for each of the G20 countries, and for the eight developed countries in the G20, and for the twelve developing countries in the G20. The study indicated that there is relatively significant difference in weighting factors

and coefficient of variation between areas of protection in developing countries, and minimal difference in developed countries.

Environmental preferences of people change spatially and temporally, as with other factors such as economics, culture, social conditions, and so on (Itsubo et al., 2015). Itsubo (2015) highlights the importance of understanding the variability of individual environmental preferences and emphasizes the need to made explicit the transparency into the weighting factors. To that end, they used random parameter logit model to quantify and visualize the variability of individual preferences, for implementation in the LIME2 LCIA methodology.

ISO 14044 (2006d) recommends the use of several weighting factors and weighting methods and performing a sensitivity analysis so that the decision maker can understand the consequences of different value choices and weighting methods.

### **3.8. Sources of uncertainty and variability: Interpretation & communication**

The interpretation phase is where the practitioner analyzes the results, identifies hot-spots for environmental intervention, makes conclusions, provides recommendations, explains limitations and so on using the results of the life cycle inventory analysis and/or the life cycle impact assessment (O. Jolliet et al., 2016). Uncertainty can occur in how the LCA results are analyzed and interpreted by the practitioner, for the specific end-use, and for the specific study.

Communication of results from life cycle assessment is crucial, since the decision makers need to understand the various results from different types of analysis performed in the LCA. The various analyses performed in an LCA include inventory analysis, impact analysis (characterized results, normalized results, weighted results), sensitivity analysis, scenario analysis, data quality analysis, gravity analysis (e.g.: pareto analysis), uncertainty analysis, contribution analysis, dominance analysis, influence analysis, anomaly assessment, completeness check,



consistency check, et cetera. Results can be communicated in the form of statements or through visual means. The results can be misleading if it is not communicated effectively to the decision-maker. Table 7 provides a consolidated list of the sources of uncertainty and variability in interpretation and communication.

Table 7: Sources of uncertainty in Interpretation phase and methods to address them.

<b>Sources of uncertainty, as provided by various scientific articles, reports, and books</b>	<b>Methods and guidance to address uncertainty, as provided by various scientific articles, reports, and books</b>
<ul style="list-style-type: none"> <li>• Improper use of interpretation methods</li> <li>• Inability to easily and effectively track all steps, processes, assumptions of an LCA</li> </ul>	(Heijungs & Kleijn, 2001), (Heijungs et al., 2005), (Mutel & Muller, 2013), (O. Jolliet et al., 2016)
<ul style="list-style-type: none"> <li>• Inconsistency in names of elementary flows in the LCI datasets and the LCIA methods (O. Jolliet et al., 2016)</li> </ul>	(O. Jolliet et al., 2016)
<ul style="list-style-type: none"> <li>• Insufficient visualization of data</li> <li>• Linguistic imprecision (Morgan et al., 1990)</li> <li>• Use of deterministic mean to communicate results (Sekar et al., 2013)</li> </ul>	(Sekar et al., 2013), (Mastrandrea et al., 2010), (Intergovernmental Panel on Climate Change (IPCC), 2004), (Moss & Schneider, 2000), (Morgan et al., 2009), (A. C. Petersen et al., 2013), (van der Sluijs et al., 2010), (van der Sluijs et al., 2004), (Visser, Petersen, Beusen, Heuberger, & Janssen, 2006), (PBL Netherlands Environmental Assessment Agency, 2014), (Kloprogge, van der Sluijs, & Wardekker, 2007), (Fischhoff & Davis, 2014), (Wardekker, Kloprogge, Petersen, Janssen, & van der Sluijs, 2013)
<ul style="list-style-type: none"> <li>• Difficulty comparing products based on relative trade-offs between alternatives (Prado-López et al., 2015)</li> </ul>	(Prado-López et al., 2015)

### **3.8.1 Interpretation**

There are three elements to interpretation, according to ISO 14044 (2006d), with the intention of providing clear and usable information to the decision-maker (O. Jolliet et al., 2016). There are several methods recommended for the first two elements: identify significant issues and evaluation. In order to determine significant issues in LCA, ISO 14044 recommends the use of the following methods: (1) structuring of LCI inputs and outputs into various aspects of an LCA such as life cycle stages, relevant groups of processes, et cetera, (2) contribution analysis, (3) dominance analysis, (4) influence analysis, and (5) anomaly assessment. In order to evaluate the LCA, the following methods are proposed by ISO 14044: (1) completeness check, (2) sensitivity check for allocation rules, cut-off criteria, system boundary, judgement and assumptions, selection of impact category, classification of inventory results to impact categories, calculation of impact category results, normalized data, weighted data, weighting method, and data quality, and (3) consistency check on differences in data sources, differences in data accuracy, differences in technology coverage, differences in time-related coverage, differences in data age, and differences in geographical coverage. The standard also states that the results of data quality analysis and uncertainty analysis should supplement these three evaluation checks. The final element of interpretation is the provision of conclusions, limitations and recommendations.

Often, interpretation is often performed rapidly and superficially (O. Jolliet et al., 2016), which can affect the quality of the LCA outcome that the decision-maker is going to rely on. Jolliet et al. (2016) states that the interpretation should be performed systematically with each of the other three phases to (1) audit different opportunities to reduce environmental impacts, and (2) establish priorities for the actionable opportunities.

In 2001, five years after the first version of ISO 14044 was released, Heijungs and Kleijn (2001) proposed five numerical methods to interpretation that can help with the evaluation element of interpretation. These methods are (1) contribution analysis, (2) perturbation analysis, (3) uncertainty analysis, (4) comparative analysis, and (5) discernibility analysis. Heijungs et al. (2005) include another method to interpretation proposed by Heijungs and Suh (2002) in addition to the already proposed five methods, which is (6) key issue analysis. Now, one might wonder, how are these methods different from the ones already suggested in the ISO 14044:2006. It is evident that other contribution analysis, perturbation analysis (referred to as sensitivity analysis in ISO 14044), and uncertainty analysis, the other three methods explored in Heijungs et al. (2005) adds to the list of tools to interpret LCA results. Uncertainty analysis is recommended by ISO 14044 but Heijungs et al. (2005) provides guidance which is lacking in ISO 14044:2006. In other words, comparative analysis, discernibility analysis, and key issue analysis provide LCA practitioners with tools in addition to what is recommended in ISO 14044.

Uncertainty in interpretation can occur in the following cases: (1) Inputs and outputs are not structured adequately, (2) apparent mistakes, (3) not delving deeper into the results and finding the key issues, (4) lack of consideration for any and all sources of uncertainty, variability, data quality and model quality (5) inability to identify influential parameters, (6) insufficient understanding of the implications of assumptions and choices, et cetera.

There are no new methods to address these issues. It just requires careful calculation, verification, balance checks, keeping an eye out for anomalies, double checking LCA software results with hand calculations, comparing results with other studies, use of several different LCIA methodologies for comparison of toxicity

impacts, looking out for errors relating to mismatch in nomenclature between inventory and impact assessment methods, use of spread sheets to keep track of the data, assumptions and calculations, maintain a consistent process to document all files created and changes made. Mutel and Muller (2013) recommend the use of online scientific notebooks to annotate each step of the LCA model building, akin to a lab notebook, thereby making it easy to reproduce the same study at a later time, without any deviations.

Many challenges have been reported with respect to comparing product alternatives. Prado-Lopez et al. (2015) propose the use of a overlapping area of probability distributions of characterized results of alternatives to assess the trade-offs relative to data uncertainty quantified using the PM method. They indicate greater overlapping area between the distributions refer to similar performance and trade-off is insignificant. This method is very similar to the one proposed by Sekar et al. (2013) that has been discussed in the Life Cycle Inventory section.

Nicholson (2014) advises that practitioners to be careful of Type I, Type II and Type III errors when comparing product systems. She suggests the use of statistical analysis (Monte Carlo analysis, 95% confidence interval, p-value) to determine if the compared products are meaningfully different. Sekar et al. (Sekar et al., 2013) inform us that the use of "difference thresholds" for product comparison may not be statistically valid in all cases (for example: Is a 10% difference in overall environmental score sufficient to confidently state that one product is better than its comparison).

A good example of describing the implications of uncertainty analysis is from Gregory et al. (2013), who states that they did not include uncertainty in the model or in the characterization factors and therefore their method of quantifying uncertainty (stochastic parametric uncertainty analysis and probabilistic scenario

analysis) “underestimates the actual uncertainty and overestimates the ability to resolve differences between alternatives”.

### **3.8.2 Communication of uncertainty**

The Netherlands Environmental Assessment Agency (PBL) states that the authors of policy reports find the communication of uncertainty awkward (Wardekker et al., 2013). The communication of uncertainty is important because decision makers can be provided with all the information necessary to make informed decisions that addresses their short term and long term objectives (Patt & Weber, 2014). Fischhoff and Davis (2014) state that if uncertainty is not communicated effectively, then decision-makers may either put too much faith or too little faith in the information provided. In this regard, the International Panel on Climate Change (Intergovernmental Panel on Climate Change (IPCC), 2004; Mastrandrea et al., 2010; Moss & Schneider, 2000), the government of the United States of America (National Oceanic and Atmospheric Administration, Department of Energy, Department of Transportation, Environmental Protection Agency, National Aeronautics and Space Administration, and National Science Foundation) (Morgan et al., 2009) and the government of the Netherlands (PBL Netherlands Environmental Assessment Agency and Dutch National Institute for Public Health and Environment (RIVM)) (Kloprogge et al., 2007; A. C. Petersen et al., 2013; van der Sluijs et al., 2004; 2010; Visser et al., 2006; Wardekker et al., 2013) have published guidance documents.

J Arjan et al. (2013) identifies five crucial aspects to communication of uncertainty: (1) determine the target audience, (2) determine what uncertainty information is to be communicated, and when (3) understand how the target audience processes the information and how they use it, (4) how and where to

communicate uncertainty information, and (5) presentation of uncertainty information.

Differing target audiences such as scientists, policy makers, general public, et cetera, have different sets of knowledge, therefore their understanding of various topics is different, and so are the questions that they have. Once the target audience is determined, their requirements such as what information they need, the amount of information they need, the types of uncertainties pertinent to them, and time at which they need it, should be carefully determined. Since different audiences react differently to the same information, it is pertinent that the communicator understands how information is digested and used. For example, careful attention should be paid to the framing of the issue, the context in which the issue is presented, to uncertainty issues that are subject to debate, et cetera. Uncertainty information located in one place in the report often gets ignored, especially if it is in the appendix. Therefore, uncertainty information should be spread evenly throughout the report in line with the relevant topics. It is also important to ensure that the core messages with respect to uncertainties are short, consistent with the previous message, sufficient reasoning is provided, et cetera. Uncertainty information can be presented in the form of verbal descriptions, numerical tabulations, and graphical arts. These three forms of presentation may be combined in some form or the other to compensate for their drawbacks (Wardekker et al., 2013).

Many people are more comfortable at understanding, using and remembering verbal communications. At the same time, verbal information can also be vague (Wardekker et al., 2013). Suggestions for improved verbal communication of uncertainty include the use of (1) consistent and specific terms for various aspects of uncertainty (Fischhoff & Davis, 2014) and (2) consistent and specific qualifiers or summary terms used to describe the uncertainty terms. Examples of terms include

likelihood, level of understanding, level of confidence (Intergovernmental Panel on Climate Change (IPCC), 2004), scales of likelihood (Wardekker et al., 2013).

Examples of summary terms used to describe consistency of evidence is 'limited', 'medium' and 'robust', and of summary terms used to express the level of confidence include 'very low', 'low', 'medium', 'high', and 'very high' (Mastrandrea et al., 2010). Some people prefer numbers to serve their informational needs, as it is more specific. On the other hand, numbers can be difficult to comprehend and remember (Wardekker et al., 2013). Suggestions for improved numerical communications include the abstinence of pseudo accuracy (results conveyed more accurately than can be justified) and pseudo inaccuracy (results conveyed too vaguely), clearly defining what the numerical uncertainty information is, clearly describing what the numerical information means, and why it is important or unimportant, and the use of ranges, probability distributions (International Standards Organization, 2006d), likelihood, comparisons, et cetera (Wardekker et al., 2013). Sekar et al. (2013) offer two options to communicate results of an LCA. First, they suggest practitioners to communicate the variability of the mean, as opposed to the deterministic mean. For example, the global warming potential (GWP) varies between 8.13 kgCO<sub>2</sub> eq. Second, they suggest the use of upper confidence interval (UCI) mean for a conservative estimate as opposed to using the deterministic mean. Both options were suggested in relation to the use of the bootstrapping method to quantify the variability around the mean.

Laurin et al. (2016) state that the current visualization techniques used in LCA can be difficult to interpret and misleading, especially in the case of characterized results. They observe the need for better visualization techniques as it relates to trade-offs and uncertainty, in order to enable better decision making. Graphical images provide considerable information and variety, but may be difficult

to understand. Suggestions for improved graphical communication include minimizing the number of issues covered in the graph, the need for graphs to easily communicate the uncertainty information, use naming in the graphs, the ability of the title and the graph to communicate what needs to be communicated, use of the best presentation method based on the information to be communicated and the target audience, et cetera (Wardekker et al., 2013). Manning et al. (2004) states that standard graphical probability distribution functions should be used only when there is high level of confidence in the science that it is based on.

In 2015, The Guardian newspaper of Britain published an article titled "The communication of uncertainty is hindering climate change action" (Corner, 2014). The article highlighted that policymakers and the public did not trust the climate change researchers on the basis that the results were uncertain. The article referenced the work of Patt and Weber (2014) to indicate the people are the most unmanageable form of uncertainty, not climate change, and that our daily experiences and current political views influence humans much more than statistical learning. Patt and Weber (2014) further note that the perception of the reality and intensity of climate is less affected by the improved communication of uncertainty and more affected by the feasible solutions that are provided. When applying this learning within LCA, it would sensible that LCA practitioners communicate uncertainty effectively using which they can examine and prioritize opportunities for reduction in environmental impacts. In other words, communication of uncertainty used as a process to determine executable solutions to mitigate environmental impacts.

Lastly, there are uncertainties that are applicable to all aspects of LCA. These sources of uncertainties are listed in Table 8.



Table 8: Sources of uncertainty in LCA, in general, and methods to address them.

<b>Sources of uncertainty, as provided by various scientific articles, reports, and books</b>	<b>Methods and guidance to address uncertainty, as provided by various scientific articles, reports, and books</b>
Estimation of uncertainty (Björklund, 2002; Huijbregts, 1998a)	n/a
Ignorance, also referred to as epistemological uncertainty (Björklund, 2002)	n/a
Mistakes (Björklund, 2002)	n/a
Cognitive bias such as anchoring (Intergovernmental Panel on Climate Change (IPCC), 2004)	(Intergovernmental Panel on Climate Change (IPCC), 2004)

### 3.9. Discussion

In order to perform a life cycle assessment, a practitioner needs to refer to the ISO standards (ISO 14040, ISO 14044, ISO 14047, ISO 14049), which are behind a paywall. Most practitioners have access to ISO 14040 and ISO 14044, but may not have access to ISO 14047 and ISO 14049. The two latter standards provide additional technical guidance to performing an LCA using the former two standards. The lack of ISO 14047 and ISO 14049 may or may not impact an LCA practitioner, which can be hard to determine. In order to supplement the ISO standards, there are fifteen or more guides (some free and some behind a paywall), peer-reviewed journal articles (mostly behind a paywall), LCA software tutorial manuals, and LCA studies published on the internet. The wide array of supplementary documents provides inconsistent instructions, which leads an LCA practitioner to make a selected set of choices and assumptions on his/her own or make it by consulting with one or more experts. At the same time, there are researchers referencing expired standards (ISO 14040: 1997, ISO 14041:1998, ISO 14042:2000, ISO 14043:2000,

ISO 14047:2003, ISO 14049:2000), and guidance documents that were created with references to the expired standards, the implications of which are not clear. This situation relating to standards and guides leads to one question: *Is it feasible to expect one or more documents to provide consistent instructions regarding the performance of life cycle assessment?*

Based on numerous studies, it is evident that 'attributional' LCA in its current form is incapable of support complex real-world life cycle assessments. This has led various forms and suggested-forms of LCA: back casting LCA, consequential LCA, decision LCA, dynamic LCA, economic input-output LCA, explorative LCA, normative LCA, predictive LCA (Guinée & Heijungs, 2011), fire LCA, hybrid LCA, and so on. Udo de Haes et al. (2004) argue that one should not expect LCA to evolve into as super tool to do everything required for the analysis of a particular case, as the developments may come in conflict with the core structure of the LCA. Instead they propose three strategies that supplement LCA: (1) LCA extension (one model used in conjunction with the LCA) (2) toolbox (separate models used in conjunction with the LCA), and (3) hybrid analysis (combination of models used in conjunction with the LCA). This lead us to the question: *Is there demand to formalize the extension of LCA, within the framework of ISO 14040 and ISO 14044?*

For any LCA practitioner interested in performing uncertainty analysis as part of the LCA, as recommended by ISO standards, there does not exist a clear foundation. There are many uncertainty-related terms that are utilized in LCA studies, which leave readers confused due to the lack of clear and consistent definitions. Heijungs (2013) highlights that LCA practitioners borrow many terms from other disciplines and use them incorrectly. In order to address the issue of inconsistent uncertainty terminology in climate change, the National Research Programme Knowledge for Climate (Kwakkel et al., 2011), published an uncertainty

terminology document for use within the Knowledge for Climate research program. Similarly, in order to avoid confusion when discussing about uncertainty and variability, the National Research Council's Committee on Models in the Regulatory Decision Process (2015) has compiled the definitions of key uncertainty terms. If such a document is to be created for use by the LCA community, then it needs to occur through a multi-stakeholder process. Traditionally, such efforts are led by the UNEP/SETAC Life Cycle Initiative. Examples of such efforts include: 'Global Guidance Principles for LCA databases' (Sonnemann & Vigon, 2011), and the ongoing 'Global Guidance on environmental life cycle assessment indicators' (Frischknecht et al., 2016; O. Jolliet et al., 2014). The UNEP/SETAC Life Cycle Initiative is quite slow in decision making and it is unclear if they can be persuaded to take up this project. On the other hand, the Product Category Rule Guidance Development Initiative was created as an offshoot of the American Center for Life Cycle Assessment's Product Category Rule (PCR) sub-committee, brought together a multi-stakeholder group and successfully created a guidance document for PCR development. This proves that if there is demand, then supply will find its way. This leads us to the question: *Is there demand for a uncertainty terminology document for use in the LCA community?*

There are roughly thirty typologies of uncertainty and variability published across various disciplines, and roughly eight typologies in LCA. The advantage of a robust typology of uncertainty in LCA is that it helps identify and classify various sources of uncertainties and variabilities. Given that uncertainty typology is an important aspect of uncertainty characterization, the need for uncertainty typology is unquestionable for uncertainty analysis. This leads us to the question: *Is there demand for uncertainty analysis within the LCA community?*

There are numerous sources of uncertainties – some of which we are aware of and some which we aren't aware of. Rosalie et al. (2012) states that uncertainties

can be included within the analysis only when one is aware of the uncertainty and only when one can quantify the uncertainty. While there are roughly thirty typologies for the sources of uncertainties and variabilities, which may vary from one discipline to another, and one researcher to another, a productive outcome towards consistency would be to consolidate all such typologies in order to identify all plausible sources of uncertainty and variability (Intergovernmental Panel on Climate Change (IPCC), 2004) in life cycle assessment. This leads us to the question: *Is there a demand to identify all sources of uncertainty within 'attributional' LCA and, possibly, other related extension models?*

Lopez et al. (2015) states that they use the PM approach to quantify parametric uncertainty due to convenience of it being part of LCA software packages. Llyod and Ries (2007) states that performing any quantitative uncertainty analysis does not guarantee reliable results. From their analysis, they state that "analytical uncertainty propagation, interval calculations, and fuzzy datasets may lead to less accurate approximations of LCA". They, further, state that existing approaches to quantifying uncertainty may not incorporate all sources of uncertainty due to limitations of the approaches. In other words, one must figure out the most appropriate method of uncertainty analysis. In order to determine the most appropriate method, there is a need to understand the purpose, benefits, limitations, and scope of all the existing methods to address uncertainty and variability. This leads us to the question: *Is there a demand to identify, assess the purpose, assess the benefits, and assess the limitations of existing methods to address uncertainty and variability?* With this information, practitioners can assess the adequacy of methods to address the sources of uncertainty that is pertinent to them. If the methods are insufficient, then there exists clear direction for research into new and innovative research methods.

Webster (2003) states that it is generally accepted the outcomes of all models should be a distribution and not a single point value. Contrastingly, a quick review of LCA studies that are published in peer-reviewed journals and over the internet, indicates that large number of studies are published without performing uncertainty analysis and through the use of single point values. In 2013, The Journal of Industrial Ecology (*J. Ind. Ecol.*) upped the criteria for the publication of case studies in its journal, based on evolution of novelty in research, and the improvement of overall expertise (Lifset, 2013). In the same year, The International Journal of Life Cycle Assessment (*Int. J. Life Cycle Assess.*) proposed the adoption of similar criteria, wherein manuscripts failing to meet the criteria will not be accepted for peer review (Klöpffer & Curran, 2013). While there has been an editorial redressal of how many and if case studies should be published in *Int. J. Life Cycle Assess.*, there has been non regarding point estimates or uncertainty analysis. Ultimately, it would be an excellent idea to improve the quality of manuscripts, at least in part, if journals established criteria regarding point estimates and uncertainty analysis. This leads us to the question: *Is the LCA community willing to make a stand for itself to ensure the credibility and reliability of LCA?* If so, the LCA community could adopt a set of principles regarding uncertainty assessment.

The authors have hereby proposed principles of uncertainty assessment in LCA (adapted from Heinemeyer et al. (2008)):

- Uncertainty analysis shall be part of every life cycle assessment
- LCA results shall not be expressed as a single point value.
- The level of detail of every uncertainty analysis should be based on a tiered approach and consistent with the overall goal and scope of the life cycle assessment

- Sources of uncertainty and variability shall be systematically identified and evaluated
- The presence and absence of moderate to strong dependencies between model inputs shall be discussed and appropriately accounted for in the life cycle assessment
- Data, expert judgement or both shall be used to inform the specification of uncertainties for scenarios, models and model parameters.
- Sensitivity analysis shall be an integral component in uncertainty analysis in order to identify key sources of uncertainties and variabilities.
- Uncertainty analysis shall be systematically documented in a comprehensive and transparent manner, including both qualitative and quantitative aspects.
- Uncertainty analysis shall be subject an evaluation process, once performed

Effectively communication of uncertainty information to the relevant end-users is equally important as the uncertainty quantification. Various forms of graphs (box- and whisker plot, histogram, error bars, et cetera) are used to communicate uncertainty. Other ways to communicate uncertainty also include comparison indicators, contribution to uncertainty and so on (Lloyd & Ries, 2007). However, it is not clear why one graph form or communication method is better than the other or why authors choose one approach of communication over another. This leads to the question: *Is the LCA community genuinely interested in effectively communicating the LCA results based on the target audience?* If so, then there is a need to create a guidance document for LCA practitioners on how to communicate LCA results to their target audience.

### **3.10 Concluding Remarks**

In the recent past, and the present, the LCA community has come together to collectively establish documents such as the Global Guidance Principles for Life Cycle Assessment Databases (Sonnemann et al., 2013), Guidance for Product Category Development (Ingwersen et al., 2013), and Global Guidance on Environmental Life Cycle Impact Assessment Indicators (Frischknecht et al., 2016; O. Jolliet et al., 2014). Such a time has come again.

Despite the overwhelming issues of concern relating to LCA results, uncertainty is still being used to express how much one is unsure about the results, in ways that people think is best – not consistently, and maybe not even robustly. Since Heijungs (1996) – the first of many articles about uncertainty in LCA, there is a growing number of documents (reports, books, peer-reviewed journal articles, et cetera) about uncertainty (terms, types, characterization, quantification and communication) being produced, but it is inconsistent and is causing confusion among LCA practitioners. If we are to ensure reliability of LCA as a decision making tool, then we need to coalesce towards consistency in how we deal with uncertainty and variability.

The author recommends the following using multi-stakeholder initiatives and a focused attention on 'attributional LCA': (1) develop consistent guidance that extends the information provided in ISO 14044, ISO 1447, and ISO 14047, (2) identify and guide the use of external tools along with LCA to analyze complex problems, (3) establish a terminology document, especially as it relates to uncertainty and variability, (4) comprehensively identify all sources of uncertainty and variability, (5) establish a robust typology for uncertainty and variability, (6) provide methodological guidance on how to address uncertainty and variability, (7) develop guidance on how to communicate uncertainty, (8) reject the validity of LCA

studies that are published without considering uncertainty and variability in methods and communication, (9) facilitate additional research towards ensuring that LCA information is credible and reliable, and (10) ensure open-access to all documents supporting credible and reliable LCA's.



### 4.1 Introduction

The growing awareness of environmental impacts of consumer goods and services has propelled the use of Life Cycle Assessment (LCA) as a decision-support tool. LCA can be thought of to consist of three modules: data, methods, and software, all of which are integral to the operation of the tool. The demand for advancement of these three modules has turned LCA into a field, with a global community of users, researchers, consultants and businesses. This community is actively engaged in developing methods, creating case studies, collecting data, and developing software (Williams et al., 2009).

LCA requires life cycle inventory (LCI) information, which is data intensive, in order to perform an environmental assessment of a product or process (Finnveden et al., 2009). As exemplified in the field of information and communication technology, the phrase "Garbage In, Garbage Out" (Lidwell et al., 2010) applies to the input LCI data and the output results (Coulon et al., 1997). The lack of appropriate data for a product system under study is often more challenging than the limited choice of LCA characterization methodology or the restricted user-experience of the software platform (Coulon et al., 1997). At present, there are ten national and international environmental life cycle inventory databases, that include Agribalyse, ProBas, USDA, Ecoinvent, GaBi, ÖkobaDat, LC-Inventories.ch, NEEDS, ELCD, and Bioenergiedat (OpenLCA Nexus, 2015). Other non-public databases include those from industry and industry consortia, regional entities, and consultants. Not all of the available databases are readily accessible due to (1) lack of a single/directed store(s) to purchase the datasets for the various available software tools, (2) incompatibility of certain database formats with the software tools and (3) bias created from the

bundling of a limited number of databases (Finnveden et al., 2009) to certain software tools. Most databases owned by consultants are often proprietary in nature. While public databases can address some data needs, and the proprietary databases addresses furthermore, there is not sufficient data collected and standardized to address all the data needs of the broader LCA community.

Chemicals form an important component of most man-made products. Given the growing demand to use LCA results to innovate in and improve the value chain, there is a need to fill LCI data gaps so that manufacturers and suppliers can make decisions that positively affect the environment. While there are more than 84,000 chemical substances used in consumer products and processes (U.S. EPA, 2011), existing LCI databases (public and proprietary) house a conservative 1500 chemical substances. The lack of sufficient chemical inventory data in publicly available databases can be attributed to three reasons: (1) collecting chemical inventory data is complex, time consuming and expensive, (2) production data is highly valuable and often proprietary (Jimenez- Gonzalez et al., 2000) and, (3) the number of chemicals for which data must be collected is prohibitive (Wernet et al., 2008, 2009).

Existing procedures to fill chemical LCI data gaps include a molecular structure based neural network model (Wernet et al., 2008), estimating input-output scheme for mass and energy flows in a chemical production process using heuristics and small amount of on-site data (Geisler et al., 2004), estimating gate-to-gate life cycle information using chemical engineering process design techniques (Jimenez- Gonzalez et al., 2000), estimating the chemical LCIs using the inherent burden approach (Bretz and Frankhauser, 1996), and estimating inventory data using stoichiometric equations from technical literature (Hischier et al., 2004). One method that is widely used to fill data gaps but that which is rarely discussed in research literature is the use of substitute or proxy LCI data in lieu of a non-existent

dataset(s). Although the Pedigree Matrix approach (Weidema and Wesnaes, 1996) seeks to address proxy data by quantifying the associated uncertainty through qualitative attributes, it is primarily limited to technological and geographical differences of the product or process and it does not extend to a completely different product altogether.

There is increasing evidence that substitution is used as a convenient option to fill LCI data gaps, and that data gaps are just omitted as an alternative (Wernet et al., 2008). The use of generic proxies, such as “chemicals, organic” and “chemicals, inorganic” from the Ecoinvent database, is questionable as its impacts is almost always not representative of all the missing chemicals that it is replacing; additionally, the inherent uncertainty in the generic proxies (un-weighted average mixture of the top 20 available and inventoried chemicals, based on worldwide production volumes) increases the questionability of representativeness. If a proxy makes up a major part of the quantitative burden of a process, prior literature suggests that the LCA researcher should invest some work using other established data collection/modeling methods to make a more detailed inventory (Hischier et al., 2004). Additionally, there is always the risk that a proxy underestimates or overestimates the burdens, especially, in product comparisons. Even with this understanding, many LCA practitioners believe that using any proxy is better than to leave a data gap unaddressed (Wernet et al., 2008).

The major unresolved problem with proxy selection is the associated subjectivity of choices (lack of repeatability) and its impact on the LCA results. This paper explores the quantification of uncertainty associated with the use of the substitute/proxy dataset and attempts to formalize a robust systematic process for the selection of proxies through a case study of laundry detergents.

## **4.2 Case study of Laundry Detergents**

Most home and personal care goods are the resultant of production and processing of chemicals. Thus, a case study of laundry detergents can be considered representative of products in the household chemical products sector, as it shares a very similar supply chain and manufacturing process. Van Hoof et al. (2003) indicates that ingredient data gaps could affect the conclusions of the cradle-to-gate LCA (excluding use and post-use phase) of laundry detergents. Additionally, there are numerous other case studies based on laundry detergents that exemplify different issues in LCA (available in Appendix). These case studies indicate that laundry detergents are not just convenient but a good product platform to explore methods and analyze issues in life cycle assessment.

## **4.3 Methods**

Expert elicitation is a method that is traditionally used when confronted with the lack of data. It is a systematic approach that synthesizes the subjective judgments of experts (Slottje et al., 2008). The use of expert knowledge and choices is not uncommon in life cycle assessment. Given that any and all LCA practitioners perform proxy selections, the authors decided to crowd source the proxy selections from experts based on the hypothesis that some experts make better choices and that the criteria that they use could guide proxy selections by novices. Expert elicitation was performed through Institutional Review Board (IRB) approved (via Arizona State University) web surveys, with participants located around the world, over a period of two months.

### **4.3.1 Selection of Experts**

Four areas of expertise were identified to be valuable for selecting the most suitable proxy for a chemical ingredient used in laundry detergents: (1) life cycle

assessment, (2) chemistry, (3) chemical engineering, and (4) toxicology. Based on conversations with industry experts, it was determined that the knowledge of life cycle assessment was critical, and therefore was made a prerequisite criterion to be a participant in the survey. One or more of the other expertise areas such as chemistry, chemical engineering, and toxicology was considered an added benefit.

#### **4.3.2 Data & LCA Methodology**

The following eight databases that were bundled within SimaPro 7.3 were utilized in this study: (1) Ecoinvent 2.2, (2) ELCD, (3) USLCI, (4) ETH-ESU 96, (5) BUWAL250, (6) IDEMAT 2001, (7) LCA Food DK and (8) Industry data 2.0. The cradle-to-gate Cumulative Energy Demand (CED) for all chemicals in Ecoinvent was calculated using the methodology "Cumulative Energy Demand V 1.08" using the LCA software SimaPro 7.3 (Frischknecht et al., 2007a). Infrastructure processes were included based on the results from the study performed by Frischknecht et al. (2007b) which specifically states that capital goods must be included in the energy analyses of agricultural products and processes, that are commonly used in the manufacture of chemical-based home and personal care products. The choice of CED as an impact was undertaken due to its simplicity and reduced uncertainty, as opposed to using an end-point indicator such as Eco-indicator 99 methodology. Additionally, Huijbregts et al. (2005) indicate that fossil fuels are an important driver for most environmental problems.

#### **4.3.3 Classification of Chemicals by Functional Chemical Groups**

All chemical-based consumer products have ingredient-chemicals that perform certain functions. While there are some chemicals that perform more than one function, there are also others that perform better in the presence of other

chemicals. Irrespective, all chemicals can be generally classified based on their functions, otherwise known as functional chemical groups.

The functional chemical groups for laundry detergents, roughly twenty-five in number, were determined from product formulation books (Smulders et al., 2003; Zoller, 2008; Showell, 2005). All chemicals in above stated databases, bundled with SimaPro 7.3, were sorted based on the functional chemical groups of laundry detergents. Chemicals that did not fit into a pre-defined functional chemical group were classified as either organic or inorganic chemicals. The classification of chemicals by functional chemical groups serves three important reasons: (1) to ensure functional substitution in a detergent formulation, (2) to get specific with the proxy selection criteria and (3) to get specific with the quantification of the uncertainty associated with proxy selection, also referred to as proxy deviation parameter (PDP).

While there are twenty-five functional chemical groups, only select number functional chemical groups were used in the survey in order to prevent survey fatigue and to prioritize the time of the experts. The authors also sought to ensure that the functional chemical groups selected for the survey encompassed the majority of the data substitution needs. For example, anionic surfactants comprise a large portion, by weight, in the detergent formulation. Additionally, there are many chemicals that are used as anionic surfactants, but few of which have LCI data. Therefore, it was determined that anionic surfactants be one of the functional chemical groups in the survey. The functional chemical groups that were to be part of the survey were also required to have sufficient number of chemicals with LCI data, so that a target chemical (one that requires a proxy) has sufficient number of functionally equivalent substitute-options for the experts to choose from. A target chemical, in other words, is one that is used as a target for substitution, or proxy.

#### **4.3.4 Survey Design & Process**

The IRB approved web survey consisted of four blocks of information: 1) cover letter, 2) instructions, 3) experience and, 4) proxy questions. The cover letter communicated the background and purpose of the survey, the voluntary and anonymous nature of the survey, and the benefits of participation in the survey. The instructions block provided basic information and rules to survey respondents, such as the number of functional chemical groups/ substitutions (five), the need to avoid using LCA tools when answering the survey, the basis of proxy selection be CED, the need for substitution criteria to be clear and concise, and the geographical scope of the substitutions be the United States of America. The experience block sought to obtain the time-span of experience in the four areas of expertise. The questions block provided the core substitution questions, shown in Table 9, for each of the following five functional chemical groups: (1) Anionic surfactants, (2) Non-ionic surfactants, (3) Complexing/sequestering agents, (4) Thickening agents/processing aids, and (5) Inorganic builders. The following three categories of options were provided to survey respondents to select proxies from: 1) chemicals with the same functional purpose, 2) other organic chemicals and, 3) other inorganic chemicals.

A preliminary survey was conducted using a non-probability convenient sample of 10 people from the laundry care committee of the Home & Personal Care Sector of the Sustainability Consortium. A revised second survey was conducted using a snowball sampling methodology through the open-access PRé LCA listserv (Pré, 2011). Based on responses from the second survey and the assessment of complexity in replicating proxy choices, the ability to choose a combination of chemicals as a substitute for a single given chemical was eliminated from the final version of the survey.

Table 9. List of survey questions for each of the five selected functional chemical groups.

1	Select a chemical that best represents the Cumulative Energy Demand (CED) of the "target chemical" over its cradle-to-gate life cycle.
2	List the criteria used in the selection of the proxy chemical.
3	How much confidence do you have in your selection of the proxy for the given chemical?
4	If you did not make the above proxy selection solely based on scientific criteria, what amount of intuition did you use?
5	If you were to choose a proxy for the same chemical given above, but based on its total environmental impact, would you choose a different proxy?

Conferences are considered to be a congregation of experts, with varying levels and areas of expertise from all over the world. The sampling frame was created by gathering contacts from the three LCA conferences organized by different entities, in different countries, and different years. A random sample of 300 individuals was chosen for the survey from a list of 479. The polls were open for sixty days with one reminder sent after the first 30 days. Due to the anonymous nature of the survey, the global distribution of the experts could not be ascertained.

#### **4.3.5 Analysis**

Once the surveys were returned, the following actions were performed: (1) the criteria provided by experts were sorted and standardized with consistent wording so that it can be analyzed when results are grouped, (2) the proxy selections were separated into the following three categories: best proxy, majority proxy, and other proxies. For each functional chemical group, the proxy selection that which was the closest in CED impact to the target chemical was categorized as best proxy. For each functional chemical group, the proxy selected by majority of the



respondents was categorized as majority proxy. The majority proxy may be the same as the best proxy, in which case it is referred to as best-majority proxy. Other proxy choices that do not fall under these two categories are categorized as other proxies.

If the CED of the majority proxy and the best proxy are sufficiently close, then the criteria provided for both can be potentially utilized to arrive at the same proxy selections e the name of the proxy chemical is less important than the CED of proxy chemical with minimal deviation from the target chemical. If the CED of the majority proxy and the best proxy are not sufficiently close, then the criteria provided for the best proxy alone is utilized to arrive at the proxy selection.

Provided that criteria can be sufficiently distinguished between the best proxy (including majority proxy, if CED is sufficiently close) and other proxies, then, for each functional chemical group, the difference in CED between the target chemical and the best proxy (or average of best proxy and majority proxy, if the CED is sufficiently close) is defined as least PDP. For users, this criterion is used to guide the selection of the best proxy for the specific functional chemical group, and the least PDP is added to the CED of the user-selected proxy to address the uncertainty due to the proxy use, for that specific functional chemical group.

In case that the criteria for the best/best-majority proxy and the other proxies are not sufficiently distinguishable, then, for each functional chemical group, the difference between the CED of the target chemical and the average CED of all the expert selected proxies is known as the average PDP. For users, all expert provided criterion is used to guide the proxy selection and the average PDP is added to the CED of the user-selected proxy to addresses the uncertainty associated with proxy use, for that specific functional chemical group.

The criterion associated with the least PDP is more specific to the selection of the best proxy while that of the average deviation parameter is less specific.

The influence of independent variables such as expertise profile and total experience years on the dependent variables such as proxy type (best/majority/best-majority/other) (based on survey question 1), amount of confidence (survey question 3), amount of intuition used (survey question 4), and the user-choice of selecting an alternate proxy when environmental impact is concerned (survey question 5), was analyzed using a Bootstrap Chi-square test. The authors chose to use this test, as the assumptions for the Pearson's Chi-square test were not met (more than 20% of the cells had an expected frequency of less than 5). The statistical significance of the association between the two nominal variables is determined from the p-value.

#### **4.4 Results**

A response/return rate of 10.7% was achieved with 32 responses and a sampling error of 16.4%. The expertise profile and summary of experience years of the survey respondents are shown in Table 10. In terms of individual expertise, there were 32 people with knowledge of LCA, 20 people with the knowledge of chemistry, 11 people with knowledge of chemical engineering, and 9 people with knowledge of toxicology, participating in the survey. On average, survey respondents had the least experience (with respect to years) in toxicology and the most in life cycle assessment.

Table 10: Expertise Profile of Survey Respondents.

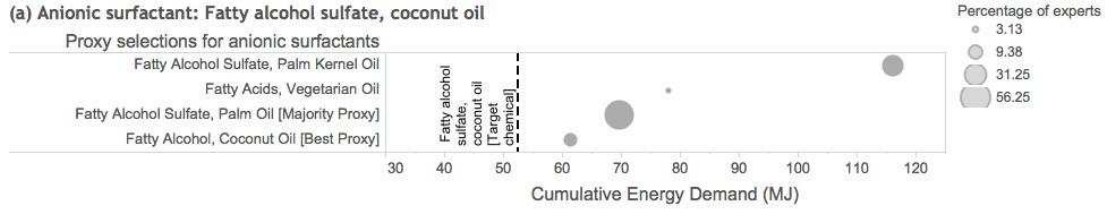
Expertise profiles	No. of experts	Experience years				
		Mean	Std. Dev.	Min	Max	Mode
LCA	10	5.8	5.3	2.0	18.0	3.0
LCA + Chemistry	8	21.1	16.4	3.0	43.0	n/a
LCA + Chemical Engg.	1	11.0	n/a	11.0	11.0	n/a
LCA + Toxicology	0	n/a	n/a	n/a	n/a	n/a
LCA + Chemical Engg. + Chemistry	4	29.5	35.9	9.0	83.0	9.0
LCA + Chemical Engg. + Toxicology	1	22.0	n/a	22.0	22.0	n/a
LCA + Chemistry + Toxicology	3	33.3	27.5	15.0	65.0	n/a
LCA + Chemical Engg. + Chemistry + Toxicology	5	23.2	13.4	10.0	40.0	n/a

#### 4.4.1 Expert selected proxies

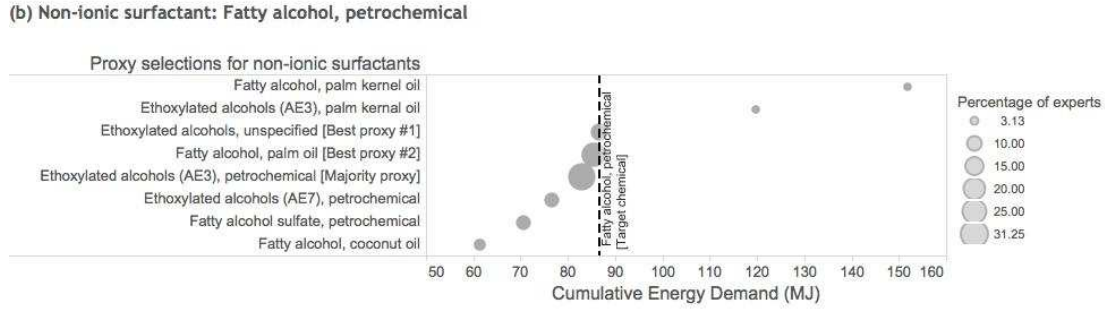
It is evident from Figure. 4 that, for certain target chemicals/functional chemical groups, experts converge or diverge in the number of selected proxies. In this study, the number of expert-selected proxies for a target chemical varies from four (Anionic surfactants: Fatty alcohol sulfate, coconut oil) to nine (Thickening agent/ process aid: Sodium formate). The largest group of experts to select one proxy, as in the case of fatty alcohol sulfate from palm oil, is 56%, that which is roughly 10 MJ more impactful than the best proxy and 20 MJ more impactful than the target chemical.

Figure 4. Selection of proxies by experts; the dotted line represents the CED of the target chemical; the location of the bubbles in the graph represent the CED of the chemicals inline; the large bubble size indicates that more experts have chosen that particular chemical as a proxy for the target chemical, and the small bubble size represents the contrary.

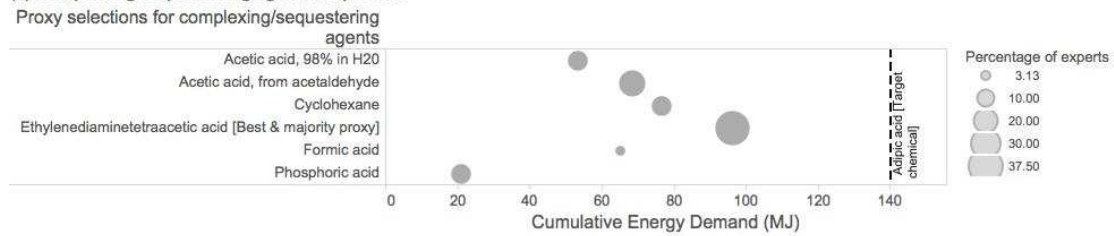
**(a) Anionic surfactant: Fatty alcohol sulfate, coconut oil**



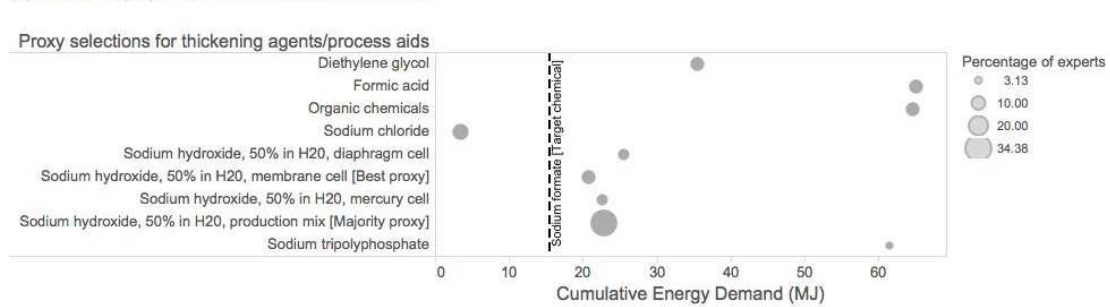
**(b) Non-ionic surfactant: Fatty alcohol, petrochemical**



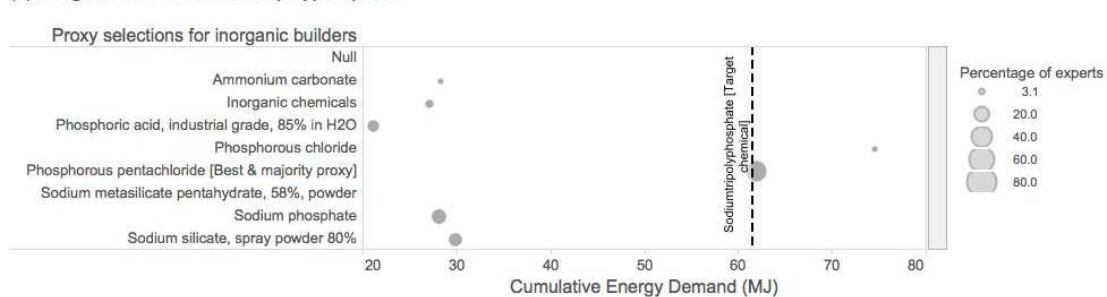
**(c) Complexing/sequestering agent: Adipic acid**



**(d) Thickening agent/process aid: Sodium formate**



**(e) Inorganic Builder: Sodiumtripolyphosphate**



The best proxy and majority proxy can be the same chemical, as in the cases of the inorganic builder and complexing/sequestering agents. The best proxy and majority proxy selected for thickening agents offers an interesting complexity, in that, it is the same chemical (Sodium Hydroxide), but from different manufacturing methods and different CED. The best proxy is Sodium Hydroxide (50% in water) that is manufactured using a membrane cell, whereas the majority proxy is Sodium Hydroxide (50% in water) that is a production mix of three manufacturing methods: diaphragm cell, membrane cell and mercury cell. Due to the minimal difference in CED, the selection criteria were merged and the CED's averaged to create the least PDP.

The difference in CED of the best-majority proxy and the target chemical can be very small, as in the case of inorganic builder and non-ionic surfactant. Specifically, in the case of non-ionic surfactants, the two best proxies and the majority proxy are sufficiently close enough that they can be merged to form a best-majority proxy whose CED marginally differs from the CED of the target chemical. The difference in CED of the best-majority proxy and the target chemical can be as large as 40 MJ, as in the case of complexing/sequestering agent: EDTA. The CED of all the proxies, for a given target chemical, are almost always lower than the CED of the target chemical or higher than the CED of the target chemical - which means, experts collectively and consistently underestimate or overestimate the CED impact of the target chemical. Amongst all functional chemical groups, the proxies for the non-ionic surfactant have the least spread in CED with respect to the proxies themselves and with respect to the target chemical. As with the number of selected proxies, the difference in CED between various proxies for a given functional chemical group showed a spread as large as 100% and as small as roughly 0.5%.

It is evident from the criteria provided that experts recommend the substitution of petrochemicals with petrochemicals and oleo chemicals with oleo chemicals. This is substantiated by Souter (2003), who indicates that carbon chains of synthetic feedstock's may be branched and include even and odd carbon atoms, whereas natural feedstock's are always linear and even numbered.

#### **4.4.2 Selection Criteria**

The selection criteria that the experts provided were the only possible way of understanding the potentially repeatable basis behind why experts made the specific proxy choices. Although experts were asked to provide concise and crisp reasoning for their choices, sometimes they were to the contrary. The criteria provided were sorted and standardized so that they can be assessed and compared when analyzing proxy choices. The authors sought out to identify unique criteria that would differentiate best proxy, majority proxy and other proxies.

In the case of anionic surfactants, where the best proxy and the majority proxy differ by a CED of roughly 10 MJ, the three criteria provided by experts who selected the best proxy overlaps with criteria for other proxy and majority proxy. In other words, there were no unique criteria to distinguish the best proxy from the majority proxy or other proxies.

In the case of non-ionic surfactants, there were two best proxies (unspecified Ethoxylated alcohols and fatty alcohol from palm oil) based on their minimal difference in CED (1.2 MJ). The best proxies have only three criteria (similar function, similar nomenclature, and similar production technology) that do not overlap with other proxy and one criterion that does not overlap with majority proxy (similar production technology). Since the majority proxy differs by only 3.82 MJ from the CED of the target chemical, the criteria for majority proxy and best proxy

were combined. Thereby creating a set of six unique criteria to select one of the two best proxies or the majority proxy.

In the case of complexing/sequestering agents, the best-majority proxy differs in CED from the target chemical by about 44 MJ. Of the two criteria provided by experts for the selection of best-majority proxy, one criteria (similar energy profile) is unique.

In the case of thickening agents/process aids, the best proxy and the majority proxy differ by roughly 2 MJ. Therefore, the criteria for both can be combined and compared with the criteria for other proxies. Of the six criteria provided, two were unique to selection of the best-majority proxy.

In the case of inorganic builders, the best-majority proxy differs with the target chemical by a CED of less than 1 MJ. The only unique criterion here was similar price.

Based on the identification of unique criteria for each chemical functional group, as applicable, it is evident that the unique criteria alone may not help one select the best/majority proxy. It is a combination of unique and repeated criteria that the experts themselves used to come up with the best/best-majority proxy selections. Criteria related figures are available in the Appendix.

Table 11 provides the consolidated criteria for each functional chemical group along with the proxy deviation parameter. As previously stated, the consolidated criteria can be used to guide proxy selections and the proxy deviation parameter be used to address the uncertainty caused by the use of proxy. Anionic surfactant is the only group that uses an average PDP, as there were no unique criteria utilized to make the proxy selection. All other functional chemical groups use the least PDP, as there were unique criteria utilized to make the proxy selection. The distinguishing factor between the average PDP and the least PDP is not the size of the parameter

but the basis in which it was quantified: all criteria provided by experts for all proxies vs. specific criteria provided by experts for the best/best-majority proxy choice

#### **4.4.3 Representativeness of impacts**

While CED was chosen as the impact quantification methodology for this study, for reasons mentioned previously, in reality, most LCA studies focus more on the broader range of environmental impacts. In order to gauge expert opinion on whether they would choose the same proxy when it came to selection based on environmental impact, a question was posed as part of the survey.

It is evident from Figure 5 that more than 50% of experts consistently state that they will choose a different proxy if the selection was based on environmental impact as opposed to cumulative energy demand. This information aligns with a recent study published by Laurent et al. (2010), which indicates that carbon footprints are not a good representation of the overall environmental impacts; especially with the case of chemical production.

#### **4.4.4 Statistical association**

Statistical testing was performed to test the association of the independent and dependent factors. The p-value for all the associations was greater than 0.05, thus failing to reject the null hypothesis that there is no association between the two pairs of variables (Thisted, 2010; Vickers, 2009). Therefore, the relationship between the selection of best/best-majority proxy and expertise profile, the level of confidence of the experts in their choices, the level of intuition used by experts in their choices, and the representativeness of impacts could not be statistically proven due to a small sample size.

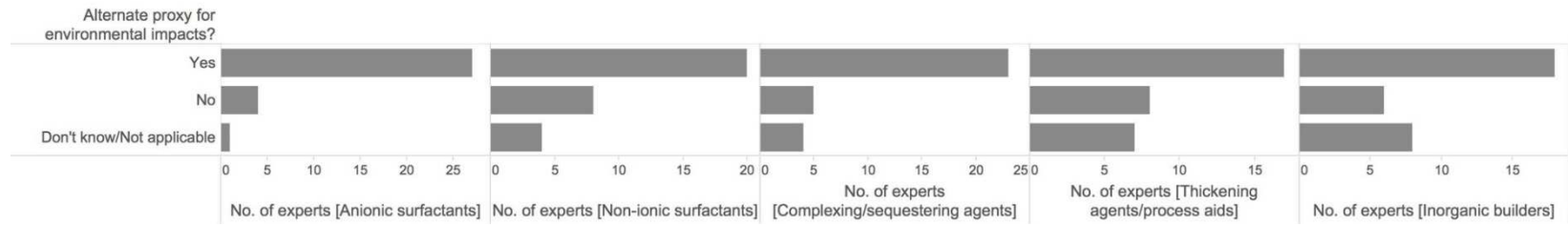


Table 11: Guide to selecting proxies for five functional chemical groups; definitions for *least PDP* and *average PDP* are provided in section 4.5.

<b>Functional chemical groups</b>	<b>Proxy selection criteria</b>	<b>PDP type</b>	<b>PDP</b>
<b>Anionic surfactants</b>	Similar chemical structure	Average	53.7%
	Material sourcing: oleo chemicals have high energy usage; therefore choose another oleo chemical		
	Material sourcing: palm and coconut as a source in very comparable; perennial crops		
	Material sourcing: choose same chemical with different oleo chemical source		
	Similar life cycles		
	Similar function		
	Similar nomenclature		
	Similar price		
	Composition of fatty acids is similar to fatty alcohol sulfate described in Journal of the American Oil Chemists' Society / Volume 34, Number 4, 175-178, DOI: 10.1007/BF02670946		
	Material sourcing: choose a different chemical from the same source		
	Similar raw material processing		
	Material sourcing: oleo chemicals can only be replaced by another oleo chemical		
	Material sourcing: choose same chemical with vegetable oil as source		
	Similar chemical transformations		
	Material sourcing: palm kernel and coconut kernel as source are very similar		
Similar technological processes used			

<b>Functional chemical groups</b>	<b>Proxy selection criteria</b>	<b>PDP type</b>	<b>PDP</b>
<b>Non-ionic</b>	Similar precursor chemical	Least	2%
	Similar chemical structure		
	Similar lifecycle		
	Similar function		
	Similar energy profiles		
	Same chemical, different feedstock		
	Similar feedstock		
	Similar precursor chemical		
	Similar price		
	Similar nomenclature		
	Similar production technology		
	Petrochemicals can only be replaced by petrochemicals		
<b>Complexing/sequestering agents</b>	Similar energy profile	Least	31.4%
	Similar function		
<b>Thickening agents/processing aids</b>	One of two precursors	Least	41.6%
	Similar nomenclature		
	Similar energy profile		
	Similar production process		
	Similar function		
<b>Inorganic builders</b>	Similar nomenclature	Least	0.6%
	Similar supply chain		
	Similar energy profile		
	Similar function		
	Similar production technology		
	Similar price		

Figure 5. The willingness of an expert to use a different proxy when environmental impact is concerned, for each of the five functional chemical groups.



## 4.5 Discussion

There are two primary limitations to this study: (1) sample size of experts, and (2) number of target chemicals per functional chemical group and number of functional chemical groups.

The advantage of establishing statistical association between expertise profile/total experience years and proxy types serves to filter out low performing experts and obtain a comprehensive understanding of the criteria, skills and tools used by better performing experts to make the best proxy choices. Additionally, these better performing experts can be used to check and improve the robustness of this methodology. The failure to prove the statistical association between the independent and dependent variables, due to small sample size, prevented the authors from getting a better understanding of the profile of experts that can be targeted for robust selection criteria and uncertainty parameters.

Given that there are many chemicals that could be used as ingredients in laundry detergents, it was pertinent that this study addressed as many of them in each functional chemical group to get a better understanding of the trends involved and the characteristic generalizations that can be made. Based on the feedback obtained from the preliminary surveys, the authors reduced the number of target chemicals in each functional chemical group from three to one, and also reduce the number of functional chemical groups from ten to five. The lack of sufficient or appropriate incentives for the experts led to reduction in the reduction in the number of target chemicals and the number of functional chemical groups in the study. The absence of more than one target chemical per functional group prevented the authors from (1) understanding trends in the selection of best/best-majority proxies, (2) understand trends in the spread of CED with respect to the target chemical CED,

and (3) understand trend in the selection criteria and the proxy deviation parameter types.

Finally, one cannot expect any user of this methodology to select the best proxy just because they have access to the expert-provided criteria. It is incumbent on the user to research further into those specific criteria to get a better understanding of the target chemical and the proxy chemical under consideration.

Errors exist in expert elicitation, which must be addressed as this method is improved. Errors can occur when making decidedly strong conclusions using limited number of chemicals per functional chemical group, and when this method is incapable of being applied to other functional chemical groups due to the lack of LCI data. The sorting of selection criteria involves standardization of the wording used, so that categorizing the criteria will be convenient. Inconsistent interpretation of the criteria during the standardization process will lead to unreliable results. It is important to note that some criteria provided by experts may be incorrect and therefore must be eliminated, despite convergence, during the sorting and categorizing process. When performing this criteria elimination process, it is pertinent that the users have sufficient expertise in chemistry and LCA.

Despite these caveats, this study has provided valuable insights and proof of concept for a methodology to fill LCI data gaps using expert elicitation.

#### **4.6 Conclusion**

In summary, guidance criteria for proxy selection for five functional chemical groups used in laundry detergents, has been established. The uncertainty associated with proxy selection, referred to as PDP, has been quantified to be used with the proxies selected using the guidance criteria provided for the respective functional chemical groups in laundry detergents. More than 50% of experts consistently

indicated that they would choose a different proxy if total environmental impact were considered as opposed to cumulative energy demand.

This study has attempted to formalize a robust and systematic process for the selection of proxies using expert elicitation. The method provides a pathway to for LCA practitioners to obtain guidance from experts for the selection of proxies and quantify the uncertainty associated with its use. The results of the study imply the following: First, this method of proxy selection to address data gaps is feasible. Second, this method is more robust and transparent than existing methods of selecting proxies since it provides expert guidance for selecting proxies, and enables the quantification of the associated uncertainty. Finally, this methodology adds to a host of other methodologies that provide options for LCA practitioners to use to fill data gaps.

## CHAPTER 5

### SENSITIVITY OF PRODUCT-EVOLUTION ON LCA RESULTS

#### **5.1 Introduction**

It is generally accepted that the life cycle assessment of any product is valid for a period of three to five years, based on the life of published environmental product declarations (EPDs) (International EPD System, 2015; NSF NCSS, 2015; EPD Norge, 2015). However, what if the product under consideration evolves into one or more variations in that period? If this product-evolution is not duly reflected in the life cycle assessment (LCA), implications exist for decision-makers, both institutional and consumers, based on the use of the out-of-date information.

Commercial and industrial products based on chemical formulations evolve over time in a frequent manner due to internal forces (e.g.: better performance, stability, processability) and external forces (e.g.: new legislation, supply chain variability, raw material availability). Given that the frequency of evolution is not publicly available and cannot be generalized, the authors choose to refer to it as non-uniform. Internal forces refer to activities performed by the manufacturer towards innovation and formula improvements to achieve either better performance, better stability, better processability, better economics or combinations thereof. External forces refer to activities that affect the production which includes new legislation, shortage or unavailability of raw materials, cost fluctuations of raw materials and customers demanding changes.

Manufacturers are not required to communicate formulation changes to the consumers unless they have an impact on the labelling and classification. At the same time, most manufacturers frequently update their declaration of simplified ingredients on their brand homepage. Additionally, frequent changes in product branding (Elliot and Yannopoulou, 2007), as a result of product-evolution, may

confuse consumers and hamper sales. While product-evolution may-not affect product-functionality, it has the potential to affect LCA's, labeling (Golden et al., 2010b, 2011) and EPDs. McKinnon (2010) indicates that manufacturer's fail to recalculate the LCAs of their products as often as products evolve, due to limited resources and the general uncertainty in what percentage change in formulation composition necessitates a new LCA. Presently, LCA's are performed without accounting for the evolution of products, and thus will generate LCA results with un-quantified temporal uncertainty.

Despite the growing demand for the use of LCA as a decision making tool (Guinée et al., 2011; White and Golden, 2008), there still exists many unresolved issues that hamper the confidence of LCA results and the reliability of the interpretation of the LCA results. Reap et al. (2008a, 2008b) and Zamagni et al. (2009) provide a detailed list of some of the unresolved problems in goal and scope, life cycle inventory analysis, life cycle impact assessment, and interpretation stages of LCA. It has been long reported that LCA is a snapshot methodology that cannot yet account for the dynamic nature of the environment and supply chains (Reap et al., 2008a, 2008b; Williams et al., 2009). The unresolved problem that is relevant to this paper is the lack of temporal-resolution in the Life Cycle Inventory (LCI) data, modeling and results of cradle-to-gate and cradle-to-grave assessments of chemicals-based commercial and industrial products. Temporal-resolution refers to the ability to accommodate changes in the product or process over time within the life cycle assessment model. Temporal uncertainty is the quantified outcome of variation of LCA results that was not accommodated within the static LCA model for the chosen product or process.

Levasseur et al. (2010) calls for the use of "dynamic LCA" to address the temporal divergence in impacts – a formal generalized methodology for which does



not exist. Williams et al. (2009) state three points to define an ideal LCI, of which two are highly relevant to variable supply chains. First, LCI should consider product aggregating through spatial and temporal averaging. Second, the supply chain model of the target product or process must reflect the actual inputs and outputs. While the recently published "Global Guidance Principles for Life Cycle Assessment Databases" (UNEP-SETAC, 2011) provides detailed steps for horizontal spatial averaging and vertical spatial aggregating of LCI data, they do not attempt to address temporal aggregation.

Williams et al. (2009) were one of the first to identify product-evolution to be part of temporal-uncertainty, as they attempted to address it using Hybrid LCA. Deng and Williams (2011) address technological change of Intel desktop microprocessors using "typical product" as a functional unit. Krishnan et al. (2008) highlight the impact of rapid product change, using the case of increase in ultra-pure water requirements (total silica 3ppb — 0.5ppb; aluminum 10ppt — 1ppt; particles 350cts/l —100cts/l) for increasingly smaller transistor gate lengths (250nm — 65nm).

In recognizing that product formulations can often change due to either altering the chemical structures of formulations or even by acquiring similar feedstocks and formulations but from different suppliers in different geographies the question arises as to: (1) what percentage of change in the environmental impact should necessitate the LCA result to be updated? (2) should non-uniform product evolutions be represented by a temporal-uncertainty parameter that is added to the LCA results and, (3) when a product evolves and its functionality changes, is it acceptable for the temporal-uncertainty parameter to address the change in the reference flow (amount of product needed to fulfill the function)? (4) How can one effectively compare the product-footprints of two competing products from the same

product category, if one or more of the products are varying in a non-uniform manner?

The authors argue that the inability to account for product-evolution within an existing LCA can hide the true assessment of environmental burdens and impact the use of LCA as a reliable tool to perform environmental accounting of the supply chain. Therefore, the authors seek to address this important issue in LCAs by using a case study of commercial heavy-duty liquid (HDL) laundry detergents to: (1) identifying and generalizing causes of product-evolution, (2) exemplify the sensitivity of causes of product-evolution with respect to environmental impacts, and attempt to identify if one cause is more important than the other, and (3) estimate the temporal-uncertainty associated with product-evolution.

The authors believe that better understanding these causes can enable LCA practitioners to integrate these variabilities into the modeling, and thereby address the uncertainty in the results and in the interpretation of the results. The authors use a case study of consumer laundry detergents, building on prior works (Golden et al., 2010a) with a cradle-to-gate scope to demonstrate the sensitivity of product-evolution on the LCA results.

## **5.2. Causes of Product-evolution in Heavy-Duty Liquid (HDL) Laundry Detergents**

Variability is described as a spread of quantitative values that is evident when there is heterogeneity in spatial, temporal and population scales (US EPA, 2011). From the supply chain of HDL laundry detergents (Sachdev et al., 2005), we can identify four broad categories of variability that are associated with product change in chemical-based products. They are (1) *formulation composition variability*, (2) *formulation attribute variability*, (3) *facility variability* and, (4) *spatial variability* (Table 12). Formulation composition variability refers to the change in the chemical

composition in the detergent formulation. Formulation composition variability addresses the core product-evolution, and is propagated upward from the supply chain in the form of facility variability and spatial variability. Formulation attribute variability addresses core product-evolution at the next higher level. Facility variability is associated with possible differences that can occur with production technology and production process. Spatial variability is a result of supply chain complexity that locates suppliers in different parts of the globe, and the associated potential differences in transportation modes utilized to move the chemical components.

Table 12: Types of variability in liquid laundry detergents.

<b>Variability classification</b>	<b>Variability type</b>	<b>Explored in this study</b>
<b>Formulation composition variability</b>	Carbon-chain length	Yes, analytically
	Ethoxylation	Yes, analytically
	Homologue mixture	Yes, analytically
	Salt	Yes, analytically
	Feedstock	Yes, analytically
	Active-matter	Yes, analytically
	Surfactant-used	Yes, analytically
	Enzyme	Yes, discussed
	Enzyme-used	Yes, discussed
<b>Formulation attribute variability</b>	Concentration	Yes, discussed
	Dose size	Yes, discussed
<b>Facility variability</b>	Production process	No
	Production technology	No
<b>Spatial variability</b>	Distance variability	No
	Transportation mode	No

*Formulation composition variability* occurs as one or more of the following: (1) carbon-chain length variability, (2) ethoxylation variability, (3) homologue variability, (4) salt variability, (5) feedstock variability, (6) active-matter variability, (7) surfactant-used variability, (8) enzyme variability, (9) enzyme used variability.

Each types of formulation composition variability may occur one or more times in a given formulation, either alone or coupled with others.

*Carbon-chain length variability* refers to the change in the carbon-chain length or average carbon-chain length of one or more chemical components in the detergent formulation. It also occurs when new chemistry or technologies are available. Surfactants are the only group of detergent chemicals that exemplify carbon-chain length variability. Surfactants are usually manufactured as mixtures of homologues, whose production volumes, availability and use are different in different regions and with different manufacturers, and therefore are referred to with their average alkyl chain lengths. For example, European linear alkyl benzene sulfonate (LAS) is a mixture of C<sub>10</sub>, C<sub>11</sub>, C<sub>12</sub>, and C<sub>13</sub> homologues of alkyl chains, which is either referred to as C<sub>10</sub>-C<sub>13</sub> LAS or C<sub>11.65</sub> LAS (OECD, 2010; Zah and Hischer, 2007). The average alkyl chain length of 11.65 is the weighted average of the homologues (C<sub>10</sub>, C<sub>11</sub>, C<sub>12</sub>, and C<sub>13</sub>) that are used in the mixture, as stated in Berna et al. (1995). While commercially manufactured LAS are available mostly as mixtures, there are formulations (Flick 1986, 1994) that use a single homologue of surfactant.

The number of ethylene oxides (EO), also referred to as moles of ethoxylation or polyether groups or ethoxylation degree or degree of ethylene oxide polymerization, is the parameter of concern for *ethoxylation variability*. This variability is also evidenced only in detergent chemical components that are surfactants. The appropriate levels of ethoxylation tend to improve detergency (Zah and Hischer, 2007). Watson (2006) states that a proper balance of alkyl chain length with a wide range of ethoxy groups can produce surfactants with varied properties. For example, the number of ethoxy groups in alcohol ether sulfate (AES) ranges from 0 to 8 (P&G, 2012; OECD, 2010). OECD (2012) indicates that the number of moles of EO is one of the many parameters that vary in different grades

of AES that are commercially produced. P&G (2012) indicates that AES with an average of 2.7 moles of ethoxylation is used for products that have household applications.

A homologue is a compound that belongs to a series of compounds that differs by the number of repeating units. Carbon-chain length variability and ethoxylation variability contain homologues. The ratio of different homologues enables the calculation of weighted average carbon-chain or the average moles of ethoxylation. The ratio depends on the production volume of the individual homologues (HERA, 2002, 2003, 2004, 2009, 2012). While this is the case, *homologue mixture variability* is based on the fact that C<sub>8-16</sub> AS may occur as one of two options: (1) inclusion of all homologues (C<sub>8</sub>, C<sub>9</sub>, C<sub>10</sub>, C<sub>11</sub>, C<sub>12</sub>, C<sub>13</sub>, C<sub>14</sub>, C<sub>15</sub>, C<sub>16</sub>) or (2) inclusion of only even number homologues (C<sub>8</sub>, C<sub>10</sub>, C<sub>12</sub>, C<sub>14</sub>, C<sub>16</sub>). This type of variability is based on (1) the differing production volumes of homologues by chemical manufacturers and (2) the region of production. Note that there is more than one ratio of the given homologues to obtain a single average carbon-chain length or a single average ethoxylation degree.

*Salt variability* refers to change in salt to which different chemicals are neutralized. These salts include sodium, potassium, ammonium, calcium, mono ethanolamine (MEA) and triethanolamine (TEA). While the availability of sodium salt of various chemicals is predominant, chemicals neutralized to other salts are also found in the market place (Chemical Land 21, 2012).

*Feedstock variability* refers to the difference in feedstock(s) used to produce a single chemical component. Stahlmans et al. (1995) provides detailed scoping for establishing the inventories for surfactants using petrochemcially-sourced surfactants and oleochemcially-sourced surfactants. For example, fatty alcohol sulfate from

petroleum can be replaced by fatty alcohol sulfate from coconut oil, palm oil, or palm kernel oil, as the chemical properties of the end product are the same.

*Active-matter variability* refers to the change in the active chemicals present in the chemical component. In other words, some chemical components are available or used in certain concentrations given their dilution in water or other aqueous substances. For example, citric acid (50% in water) could potentially be changed to citric acid (90% in water), in a certain detergent formulation. OECD (2010) refers to 50% active Linear Alkylbenzene Sulfonate (LAS) as half strength LAS, with the remaining 50% as water. In the active 50%, pure LAS ranges from 87-98%, while impurities such as iso-branched LAS and Dialkyltetralin sulfonates make up for the rest. There are other instances where the active-matter can only be presented in ranges. For example, sodium lauryl ether sulfate (3EO) is an anionic surfactant that is available as a mixture of 58-62% of sodium lauryl ether sulfate, 24-28% water and 12-16% ethyl alcohol (Ashland Chemical Company, 1999).

Most HDL detergents have both anionic surfactants and non-ionic surfactants. There are instances when the non-ionic surfactant can be replaced by anionic surfactant. For example, Alcohol Ethoxylate (non-ionic) can be replaced by Alcohol Ethoxy Sulfate (anionic). This variability, referred to as *surfactant-used variability*, would enable us to estimate the impact of sulphonation on Alcohol Ethoxylate in the detergent formulation.

*Enzymes variability* refers to change in the specification of particular enzymes used in the detergent formulation. For example, when using amylase enzymes for the removal of starch containing stains in laundry detergents, options include Stainzyme or Stainzume plus, and Termamyl or Termammyl ultra. Or when using Lipase enzyme for the removal of greasy stains, one can use Lipex or Lipolase or one of the various options provided by the supplier (Novozyme, 2012a, 2012b).

*Enzyme-used variability* refers to the addition or phasing out of one particular enzyme in the formulation (Novozyme, 2012a, 2012b; Nielsen, 2010).

Formulation attribute variability occurs as (1) concentration variability, (2) dose size variability in liquid laundry detergents. *Concentration variability* refers to the change in concentration of the chemical component with respect to the dose size of the detergent. Concentrations of chemical components in publicly available detergent formulations are expressed as *weight/weight percent (w/w%)*. In attempting to balance the formulation, either in batch or continuous production process, the concentration of chemical components tends to sway on either sides, within acceptable limits. The concentration of chemical components in many publicly available formulations appear as ranges to potentially accommodate changes in concentration of chemical components and to prevent complete disclosure of the formulation in order to protect the intellectual property of the manufacturer (Ash and Ash, 1980; Lange, 1994).

All formulations are designed based on the dose size, which differs based on concentration and/or brand – this is referred to as *dose size variability*. This variability is multiplicative in nature since the proportions of the individual chemical components increase or decrease based on the increase or decrease of the dose size. For example, it was identified through the market analysis that premium detergents were also found in a dose size of 2 fl.oz. In effect, this would mean that the impact seen in 1.6 fl.oz. will be appropriately multiplied to obtain the impact for 2 fl.oz., which would be 25% higher than what is actually seen. At the same time, the impact of consumer behavior results in over dosing of twice or thrice the recommended dose size, which results in the impacts being twice or thrice the base impacts.

*Facility variability* occurs as production process variability and production technology, and they might be intertwined at times. Chemical production plants,

almost always, utilize multi-product/multi-purpose batch, continuous, and semi-continuous process systems to produce different products. The flexible operation is made possible by sharing different pieces of equipment through same or different operational sequence, intermediate products and other resources. Based on the production quantity, production process and demand pattern, the flexible nature of the production plant allows it to maintain a flexible production schedule and therefore create monetary savings (Floudas and Lin, 2004). This variability, referred to as *production process variability*, is not just applicable to the production of precursor chemicals, but also to the production of detergents (Watson, 2005).

Another aspect of facility variability is the *production technology variability*. As the name suggests, different methods are used to produce the same output product. For example, sodium hydroxide can be produced via diaphragm cell, membrane cell, or mercury cell. Bewley and Coons (2010) note that the difference in production technology employed in developing and developed countries, for the manufacture of detergents components, is reducing.

*Spatial variability* occurs due to the propagation of the detergent formulation changes along the supply chain, and due to the variable nature of the supply chain. *Distance variability* is associated with the identity and location of supplier(s) of the chemical component that has changed in the formulation, as a consequence of formulation composition variability. *Transportation mode variability* refers to the different transportation modes using in different geographic locations to transport chemical components from suppliers. Spatial variability can get complicated when venturing beyond level I suppliers (w.r.t. manufacturers), as we may not know how many levels further must we proceed, as it is also difficult to trace suppliers beyond level I. In this study, we limit spatial variability to level I suppliers.



As mentioned in section 5.2, the amount and frequency of formulation composition variability, facility variability, and spatial variability varies from manufacturer to manufacturer based on the reasons stated.

### **5.3 Methods**

ISO 14040 and 14044 (ISO, 2006a, 2006b) serve as the core reference documents for LCA methodology. In order to assess the implications of product-evolution on static LCA results, sensitivity analysis was performed for each of the identified variability types (Table 1). This was done so by choosing a base-case formulation (Table 13), and applying the appropriate variability on the base-case and quantifying the deviation in LCA impacts of the formulation to quantify the temporal-uncertainty. In order to attempt to understand market implications, we chose one formulation from each of the three price-tiers (value, mid, premium) to be base-formulations. The LCA impacts of the three chosen base-case formulations were calculated, and are referred to as base-impacts. The sensitivity of each variability type was assessed separately by making one-on-one substitutions to the base-case formulation and recording the change in environmental impacts. This analysis enabled the authors to (1) assess the relevance of the various variability types, (2) estimate the temporal-uncertainty ranges associated with each variability type and for coupled variability, for the chosen base-case formulations.

While the stated method provides an assessment of implications of different individual variability types on the base-case formulations, the random nature of variability dictates that there exists potential for more than one variability type to affect a formulation, at a time. To explore this, individual variability in each formulation is coupled together to quantify the temporal-uncertainty. All quantified uncertainties due to the variability are expressed as scalar ranges of impacts, as there is no reasonable or logical backing to choose means and standard deviations.

The complex nature of this problem requires that the quantified uncertainty be best represented in ranges, as the probability of impacts occurring, due to one or more variability, at any point in the scalar range is equal. If a particular variability type was evidenced in more than one chemical component in the formulation, then the extremes values of the impact associated with the variability was considered to be the uncertainty range.

### **5.3.1 Scope**

The reference unit for this study is one recommended dose size of an isotropic HDL detergent (Sachdev et al., 2005) that belongs to value, mid, and premium price-tiers, for use in top-loader washing machine. We chose to use a reference unit as opposed to a functional unit, as the functional performance of the detergents is not of concern to this study, but assessing the environmental implications of product change is of importance. The reference flow is a dose size of 1.6 fl.oz. (50.6 g) of a value-tier, mid-tier, and premium-tier isotropic HDL detergents.

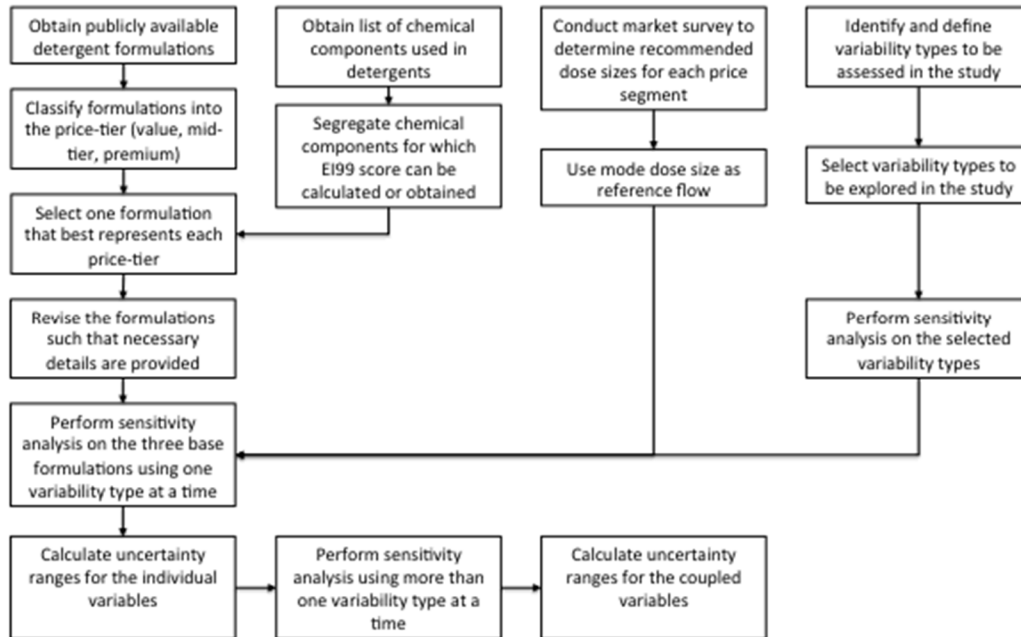
The cradle-to-gate (infrastructure included) impacts of each chemical component in the detergent formulation are part of the system boundary for this study. Geographic scope of the study is Europe, based on use of European LCIA methodology and the use of European inventory data. The formulations sourced from the publicly available literature are not attributed to geographic locations

Due to insufficient information on certain variability types, the lack of LCI to explore certain variability, and lack of prior studies on certain variables, the following variables were not included in the analysis: production process variability, production technology variability, distance variability and transportation mode variability (Table 13). Figure 6 provides a step-by-step description of the method utilized to assess the individual and coupled variables to calculate the resultant temporal-uncertainty ranges.

Table 13: Base-case HDL detergent formulations for the three price tiers (value, mid, and premium).

<b>Chemical components</b>	<b>Value-tier</b>	<b>Mid-tier</b>	<b>Premium-tier</b>
C <sub>12</sub> Sodium dodecylbenzenesulfonate			18%
C <sub>11-13</sub> Linear alkyl benzene sulfonate		12%	
C <sub>12-13</sub> Alcohol ethoxylate (7EO)	1%	3%	
C <sub>12-15</sub> Alcohol ethoxylate (6-9EO)			14%
C <sub>12-14</sub> Fatty acids (Coconut oil)		2%	
C <sub>12-18</sub> Fatty acids (Vegetable oil)			11%
C <sub>12</sub> Alcohol ether sulfate (2EO)	5%		
C <sub>14-15</sub> Alkyl Ethoxy (2.25 EO) sulfate		12%	
C <sub>12</sub> Alkyl sulfate	5%		
Citric acid (50%)	0.75%		
Citric acid (100%)		3%	5%
Diethylenetriaminepentaacetic acid, DTPA			1%
Monoethanolamine	0.32%	3%	11%
Sodium hydroxide (50%), production mix	1.40%		
Sodium hydroxide (90%), production mix		6%	1%
Propylene glycol	0.28%	3%	12.70%
Ethanol			1.80%
Sodium formate (36%)	1.25%		
Sodium xylene sulfonate		4%	
Amylase enzyme: Termamyl			0.10%
Lipase enzyme: Liquinase			0.15%
Protease enzyme: Ovozyme	0.24%	0.80%	0.50%
Cellulase enzymes: Endo-A glucanase			0.05%
Cellulase enzyme: Carezyme			0.09%
Polyester-based soil release polymer: Sulfonated polyethylene terephthalate		0.20%	0.50%
Borax (38%)	0.60%		
Boric acid			2.40%
Suds suppressor: Silicone product	0.02%	0.50%	1%
Fluorescent whitening agent: Triazinylaminostilben type	0.10%	0.15%	0.20%
Water	84.04%	51%	19.71%

Figure 6: Flowchart of method to assess the sensitivity of product-evolution.



### 5.3.2 LCIA methodology

In order to capture the environmental impacts associated with product-evolution in a comprehensive manner, the authors chose to select an impact assessment methodology that provides an endpoint indicator. Limitations in data availability for chemical components used on detergent formulations forced the authors to seek other avenues to obtain data, and therefore there was a need to align with those avenues that had relevant environmental-impact data. Ecoindicator 99 (EI99) methodology (Goedkoop et al., 2000) satisfied the demands of the endpoint impact assessment methodology and aligned with additional data sources that provided endpoint impact assessment data. SimaPro 7.3 was used as an LCA tool to obtain impact assessment results for detergent components using Ecoinvent 2.2 database (Frischknecht et al., 2007; Althus et al., 2007).

### 5.3.3 Data

In order to supplement our data needs, we used the Finechem tool (Wernet et al., 2008, 2009; ETH Zurich, 2011), that was designed to predict resource use and environmental impacts of petroleum based organic chemicals, using neural networks to learn from the association of molecular structure of chemicals from Ecoinvent and other internal databases, to resource use and environmental impacts. We limit ourselves to the use of EI99 (H/A) score in this tool, so that it is compatible with LCA results of chemicals from SimaPro, and estimated impacts of chemicals found in household products from Koehler and Wildbolz (2009). FineChem tool is limited to inputs of molecular weight in the range of 30–1400 g/mol, number of functional groups in the range of 0–30, and organic petrochemicals. Therefore, impact data for all desired chemicals could not be obtained using the tool. While the tool provided predicted mean and standard deviation, we chose to use the upper bounds of the data due to the predicted nature of the data and the relative model errors of 10–30% (Wernet et al., 2009). Additionally, the upper bounds of most duplicate chemicals that were also found in Ecoinvent 2.2 were numerically close.

Geographical considerations in the Ecoinvent data were disregarded in order to maintain a variety of choices in different variability scenarios. European average data (RER) was used as much as possible. Geographical considerations in the data from the Finechem tool and from Koehler and Wildbolz (2009) could not be identified, but was assumed to be Europe, since that was the location of both studies. Uncertainty associated with geographically substituted data was hard to quantify since there was no consistent difference in impact data of Ecoinvent chemicals from different countries.

Given that the base detergent formulations are sourced from publicly available literature (Flick, 1994), they lack sufficient detail necessary for good

modeling. Therefore, assumptions are made in the choice of datasets, with respect to production technology, carbon-chain length, number of moles of ethoxylation, salt, feedstock, et cetera. Scenario uncertainty exists in the form of alternate choices made in the selection of chemical components for the base-case formulations.

#### **5.4 Analysis**

Sensitivity analysis involves systematically varying the inputs and determining the level of sensitivity of the outputs. The authors assessed the sensitivity of the identified variables using three selected base-case formulations (Table 12), representing each of the three price segments of regular laundry detergents (See Appendix).

When an existing detergent component is replaced with a new component in the base-case formulation, the associated LCI is also replaced in the LCA model and the endpoint impact recalculated. The percentage increase or decrease provides the level of sensitivity of that particular variability to the particular base-case formulation. The percentage range of variation in endpoint (EI99 Pts) impacts is captured as temporal-uncertainty.

#### **5.5 Results**

All selected variables in this study are exemplified only in the surfactants present in the base-case formulations. These may also be exemplified in other functional chemical components, such as inorganic builders, organic builders, bleaching agents, and other compounds found in other detergent formulations.

##### **5.5.1 Individual Variability**

There are two aspects to assessing the magnitude of change due to the individual variability types: (1) without respect to a detergent formulation, and (2)

with respect to a detergent formulation. Figure S2, S3, S4, S5, S6, and S7 shows the sensitivity ranges for various detergent chemical components that fall under the selected seven types of formulation composition variability (Table 1). Based on the sensitivity analysis of detergent chemical components for which data was available, the ranges of endpoint impacts (EI99 points) per kilogram are shown in Table 13.

In order to get a comprehensive understanding of the sensitivity implications, the individual variables were assessed with respect to the base-case formulations, which mimic a weighting system (Table 14). Chemical components that have a higher percentage weight per dose size, have the potential to have more influence on the formulation than chemicals with a lower percentage weight per dose size.

Table 14: Sensitivity ranges for selected variables from formulation composition variability, shown in Appendix C.

<b>Selected variables from formulation composition variability</b>	<b>Sensitivity ranges (%)</b>
Carbon-chain	7.79 – 18
Ethoxylation	4.68 – 84.74
Homologue	0.85 – 11.43
Feedstock	26.37 – 150.09
Salt	17.54 – 129.43
Active-matter	137.85 – 144.27
Surfactant-used	Applicable only with respect to base-case formulations

First, it is evident from Figure 7 that not all variability types are exemplified in the three base-case formulations. The value-tier formulation exemplifies all seven variability types, while mid-tier exemplifies five variability types (with the exception of feedstock and active-matter) and the premium-tier exemplifies four variability

types (with the exception of homologue, feedstock and active-matter). This occurs not just because of the lack of chemical components exemplifying the variability type, but also because of the lack of LCI or EI99 impact data for the alternative components.

Secondly, the recurrence of the single variability type more than once in the base-case formulation is not uncommon (examples include carbon-chain variability, ethoxylation variability, and homologue variability). Again, it is dependent on the presence of the chemicals exemplifying such variability and the presence of alternate chemicals with LCI or EI99 impact data. While it may seem that product-evolution (except salt and surfactant-used) in value-tier and mid-tier detergents almost always consistently increase the product-footprint of the base-case formulation, is not necessarily the case. The factors that influence the product-footprint include the presence of chemicals exemplifying the variables and their alternatives, and their concentrations in the base-case formulation. In other words, it is possible for the product-footprints to fall below that of the base-case, as well.

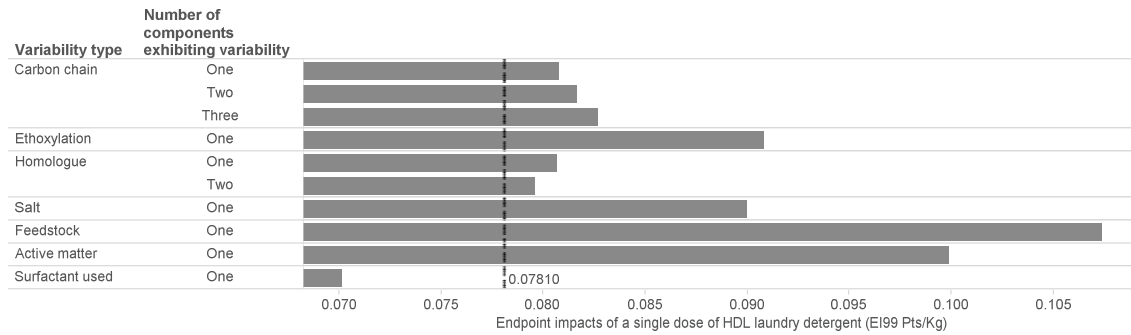
Sensitivity analysis was performed on the base-case formulation using the selected variables indicate that the product-footprint varies from -10%—37% for value-tier HDL detergents, -12%—19% for mid-tier HDL detergents, and -24%—133% for premium-tier HDL detergents.

Carbon-chain variability was often evident in more than one component in the base-case formulations. The product-footprint varied by 3%—6% for value-tier detergents, 4%—5% for mid-tier detergents, and 1%—133% for premium detergents, due to carbon-chain variability on the selected base-case formulations. Across tiers, the product-footprint varied by 1%—133%, due to carbon-chain variability.

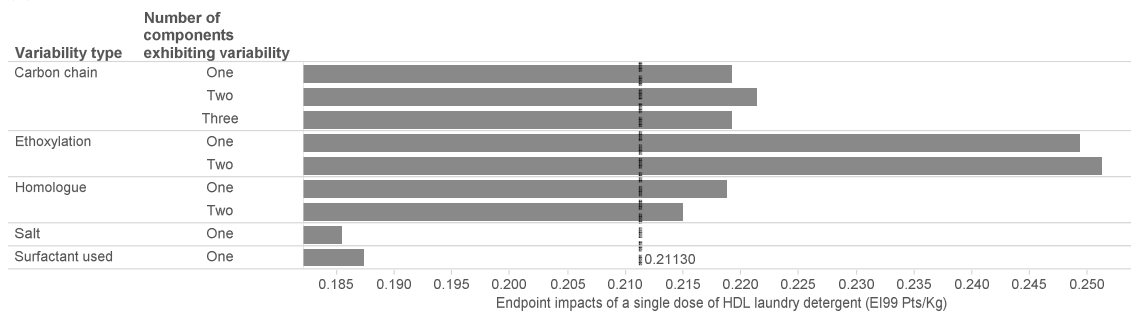


Figure 7: Sensitivity of relevant formulation composition variabilities on the base formulations for the three price tiers (value, mid, premium); dash lines indicate the base-case impact respectively.

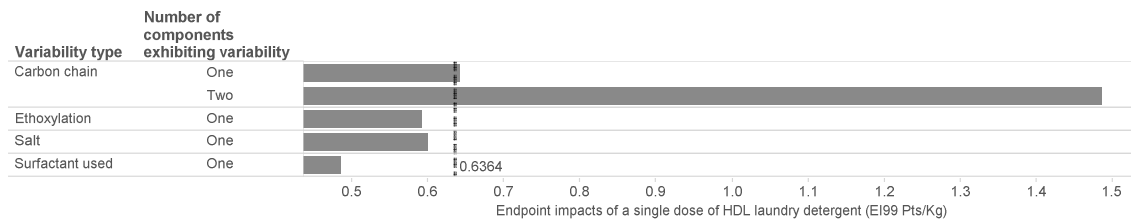
(a) Value-tier



(b) Mid-tier



(c) Premium-tier



Ethoxylation variability was also evident in more than one component in the base-case formulations. The product-footprint varied by 16% for value-tier detergents, 19%–18% for mid-tier detergents, and -7% for premium detergents, due to ethoxylation variability on the selected base-case formulations. Across tiers, the product-footprint varied by -7%–19%, due to ethoxylation variability.

Homologue variability was also evident in more than one component in the value-tier and mid-tier base-case formulations, and absent in the premium-tier base-case formulation. The product-footprint varied by 2%—3% for value-tier detergents, and 2%—4% for mid-tier detergents, due to homologue variability on the selected value-tier and mid-tier base-case formulations. Across tiers, the product-footprint varied by 2%—4%, due to homologue variability.

Salt variability was also evident in one component in all the base-case formulations. The product-footprint varied by 15% for value-tier detergents, -12% for mid-tier detergents, and -6% for premium detergents, due to ethoxylation variability on the selected base-case formulations. Across tiers, the product-footprint varied by -6%—15%, due to salt variability.

Feedstock variability was only evident in one component in value-tier base-case formulation, and absent in the mid-tier and premium-tier base-case formulations. The product-footprint varied by 37% for value-tier detergents.

Active-matter variability was only evident in one component in value-tier base-case formulation, and absent in the mid-tier and premium-tier base-case formulations. The product-footprint varied by 28% for value-tier detergents.

Surfactant-used variability was evident in one component in all the base-case formulations. The product-footprint varied by -10% for value-tier detergents, -11% for mid-tier detergents, and -24% for premium detergents, due to surfactant-used variability on the selected base-case formulations. Across tiers, the product-footprint varied by -10%—-24%, due to surfactant-used variability.

### **5.5.2 Coupled Variability**

The results discussed so far were based on individual variables, whose sensitivities are measured one at a time, in order to calculate the temporal uncertainty ranges for the three price-tier formulations. In reality, there is high

degree of probability that these variables do not appear individually but together in a single formulation as coupled variables. Impacts associated with coupled variables are additive in nature, and therefore have the potential to increase the ranges of temporal-uncertainty. When performing sensitivity analysis for coupled variables in a consistent manner across the three base-case formulations, it is evident that the product footprint varies by 44% for value-tier HDL detergents, 23% for mid-tier HDL detergents, and 145% for premium HDL detergents. Based on industry knowledge, it can be interpreted that (1) the 44% of temporal-uncertainty in the value-tier base-case formulation is associated with frequent fluctuations in the formulation composition in order for the manufacturer to consistently provide the most cost-efficient product, and (2) the 145% of temporal uncertainty in the premium-tier base-case formulation is associated with vast list of ingredients used.

## **5.6 Discussion and Conclusion**

The scope of expressing the implications of the identified variables is limited by the data availability and by the formulations used in this analysis. It is important not to dismiss some variables that have less than 5% impact on the formulation, as with cut off error. It is imperative to be highly detailed when it comes to process accounting, so that all impacts are accounted for and discounting impacts for methodological or analytical reasons is eliminated.

There are several ways to move forward, while actively recognizing that products vary at random rates and percentages. The first option is to create a product profile life cycle assessment that represents the product related impacts over a defined period of time. This product profile would capture detailed temporal, geographical and technological information that could be used to review the product development and use, and provide relevance to the decisions made from LCA results. The second option is to use LCA software's that provide capabilities for suppliers to

provide live/up-to-date life cycle inventory data, such that the manufacturer can calculate product-footprints more accurately. Enterprise Resource Planning (ERP) software's, that are already designed to capture dynamic facility data, can be integrated with the LCA tool for additional convenience. Additionally, the Sustainable Apparel Coalition building upon the Material Sustainability Index (MSI) have developed the Higg Index which in design will allow for multi-tier suppliers to update LCA inventory data at a frequency greater than is done in proprietary inventory databases. The third option is to develop a prediction model that predicts formulation composition changes based on the internal and external forces such that the associated temporal-certainty can be used to address product evolution.

Based on the consistent methods to calculate and incorporate an established set of uncertainties into the LCA results, the authors propose that industry and LCA experts come together and address the four questions raised by the authors in the Introduction. In the meantime, the authors propose that a public list of ingredients along with their end-point environmental impacts be created, so that formulators and LCA experts can use it to obtain guidance on which composition change might necessitate a new LCA.

Product-evolution applies to all man-made products, where in the rate and percentage change varies. It is critical that all LCA practitioners acknowledge product-evolution and implications when calculating product-footprints, and actively seek ways to address it. Product-evolution and the related temporal-uncertainty can be reduced through improved data collection and reporting, and dynamic modeling of data.

## CHAPTER 6

### DISCUSSION

In the third chapter, the author reviewed the current state of knowledge and application of uncertainty and variability and concluded that there is an immediate need for several multi-stakeholder actions and individual primary research actions to improve the reliability and credibility of 'attributional' LCA. These multi-stakeholder actions were based on questions that were raised towards the need for across-the-board consistency, when performing LCA and uncertainty assessment in LCA. The individual primary research actions were based on the need to address various sources of uncertainty in the methodology or the application of the methodology in practical situations. Based on the recommendations from chapter three, the author took upon the task of addressing two individual primary research actions: (1) addressing one source of uncertainty, and (2) addressing one source of variability.

Chapter four addresses the uncertainty due to the use of surrogate data in place of missing LCI data by proposing an expert-elicitation based method to perform surrogate selection in a robust manner and to quantify the associated uncertainty. Chapter five addresses the variability in bill-of-materials due to product-evolution. Sensitivity analysis was used to analyze the different causes of product-evolution (sources of variability) and quantify the uncertainty ranges.

In all cases, the quantified uncertainty is to be interpreted along with the LCA results, with respect to the goal and scope, in order to provide credence to the conclusions and recommendations of an LCA.

It is important to note that the author chose to limit scientific exploration of this thesis within the scope of 'attributional' LCA as it is most well established form of LCA, and which undeniably conforms to ISO 14040 and ISO 14044. There are many sources of uncertainty and variability that demand addressment either because they

have not been addressed before or because they can be addressed better through different methodologies. Additionally, it is common sense to expect that the number of sources of uncertainty and variability will grow as LCA is applied into newer areas and more complex situations.

### **6.1 Novelty in Research**

Data gaps in LCI databases are not uncommon, and are frequently encountered when performing LCA's of chemical-based products. There are more than 84,000 chemical substances used in consumer goods and processes (U.S. EPA, 2011). On the other hand, existing LCI databases (public and proprietary) house a conservative 1500 chemical substances. The least resource intensive method to fill LCI data gaps is to use surrogate data, which can either be based on the practitioner's knowledge or based on consultation with another expert or resource. As exemplified in the field of information and communication technology, the phrase "Garbage In, Garbage Out" (Lidwell et al., 2010) applies to the input LCI data and the output results (Coulon et al., 1997). The major unresolved problem with proxy selection is the associated subjectivity of choices (lack of repeatability) and its impact on the LCA results. Therefore, the author has proposed a novel method for surrogate selection and the quantification of associated uncertainty using expert elicitation. The use of 'expert elicitation' is not new in LCA, but it has never been used to establish a formal method for surrogate selection to address LCI data gaps.

Life cycle assessment is performed on a product or process, with the explicit understanding that the selected product or process is established (does not change in the study). In reality, products evolve over time, sometimes in a non-uniform manner. In other words, a product or process for which an LCA is being performed might change before the LCA is completed. In such a case, the LCA impacts are representative of an outdated product, and therefore does not provide the intended

value. The author demonstrates this complication through a novel approach using sensitivity analysis. Given that static nature of LCA, the author proposes various solutions that can incorporate this dynamic issue and address this complication, within the scope of the ISO 14040 and 14044 standards.

## **6.2 Limitations in Research**

Despite the core focus on uncertainty and variability in this thesis, uncertainty analysis has not been applied in the case studies. Notwithstanding the existence of numerous sources of uncertainty and methodologies to address them, the most commonly addressed source of uncertainty is LCI data uncertainty, also referred to as parameter uncertainty. Other sources of uncertainty are often not addressed to lack of sufficient knowledge or data about the uncertainty. Therefore, if at all, any uncertainty analysis had to be performed, then it would have been performing Monte Carlo analysis using Pedigree Matrix (PM) – to quantify the uncertainty associated with LCI data. If such an analysis would have been performed, then, the results would appear as geometric mean and geometric standard deviation as opposed to just the mean if no uncertainty analysis was conducted. The PM takes two types of uncertainties into consideration: basic uncertainty (based on expert judgment) and additional uncertainty (based on data quality assigned by expert judgment). In the following two paragraphs, the author explains why Monte Carlo analysis using PM was not performed in the two case studies in this thesis.

In the case study associated with patching data gaps using expert elicitation (Chapter 4), it must be noted that the author does not perform an LCA. For experts to identify the best surrogate LCI, the names of numerous surrogates and their cumulative energy demand (CED) impacts for the cradle-to-manufacturing gate are calculated and provided. The main reason why uncertainty analysis was not performed for this case study is as follows. This study uses data from the following

eight LCI databases: (1) Ecoinvent 2.2, (2) ELCD, (3) USLCI, (4) ETH-ESU 96, (5) BUWAL250, (6) IDEMAT 2001, (7) LCA Food DK and (8) Industry data 2.0. Amongst these databases, only ecoinvent 2.2 has PM associated with the data. Therefore, the author would not be able to consistently use PM to quantify the uncertainty associated with each of the surrogates.

In the case study associated with assessing the sensitivity of product evolution (Chapter 5), it must be noted that the author performs cradle-to-manufacturing gate LCAs using publicly available formulations. Given the limitations in LCI data availability of chemical components of laundry detergents, additional data was sourced from (1) FineChem prediction tool and (2) Koehler and Wildbolz (2009). While the FineChem tool provided predicted mean and standard deviation, we chose to use the upper bounds of the data due to the predicted nature of the data and the relative model errors of 10–30% (Wernet et al., 2009). Additionally, it was found that the upper bound impacts from the FineChem tool were numerically close to the mean impact in Ecoinvent 2.2, for most of the chemicals found in both. Standard deviations were not provided for Ecoindicator 99 scores by Koehler and Wildbolz (2009). As a result, in order to maintain consistency in the data, uncertainty analysis was not performed on the ecoinvent data.

When performing an actual LCA, it is pertinent that LCA practitioners attempt to address as many sources of uncertainty and variability as possible. It is recommended that all sources of uncertainty and variability be addressed individually and double checked by addressing it in a consolidated manner, or vice-versa. This thesis work has maintained transparency in the analysis by providing all necessary additional information in the appendix.



## CHAPTER 7

### CONCLUSION

We are at a critical juncture, where the demand for the use of 'attributional' LCA is increasing at a rapid pace, but the effort (multi-stakeholder and individual research) to address uncertainty and variability has not kept up with the demand in terms of consistency, quantity, and rigor. We can either continue to build on the existing research on uncertainty and variability in LCA, without questioning its basis, or we can delve deeper into the foundation of the existing research and assess how we got here, and then build research only on the more robust foundations.

This study attempts to set the basis for future research and multi-stakeholder activity within the LCA community, as it relates to improving the reliability of LCA studies by addressing uncertainty and variability in attributional LCA. It re-establishes the fact that there is still no agreed-upon definition and established typologies for uncertainty and variability, within the field of LCA and in other fields as well. The vagueness of ISO standards for LCA, result in differential interpretations and consequently inconsistent LCA's, and therefore are also a source of uncertainty and variability. Several guidance documents exist to supplement ISO standards, but they are inconsistent in the guidance that they provide, which leads to further uncertainty and variability in the LCA's performed using them.

The only consistent aspect of uncertainty and variability in LCA are the sources of uncertainty, not all of which have been identified. Therefore, the sources of uncertainty and variability in LCA and proposed methods to address them have been consolidated, so that any LCA practitioner can use it as guide. The sources of uncertainty and variability were categorized into (1) Standards, (2) LCA software tool, (3) Goal and scope definition, (4) Inventory analysis, (5) Impact assessment, and (6) Interpretation and communication. It is clear that various reasons exist as to

why uncertainty and variability are often not addressed in LCA studies, one of which being the difficulty to comprehend and use the methods proposed by researchers. As a result, one easy-to-use method to quantify uncertainty associated with the use of surrogate data to fill data gaps has been proposed. Using this method, practitioners can identify the best proxy for the missing data and quantify the uncertainty associated with it. Sensitivity analysis has been utilized to demonstrate the variability associated with product-evolution, for which multiple solutions have been proposed.

Based on the review of the current status of assessment of uncertainty and variability and relevant arguments, the following questions have been raised:

1. Is it feasible to expect one or more documents to provide consistent instructions regarding the performance of life cycle assessment?
2. Is there demand to formalize the extension of LCA, within the framework of ISO 14040 and ISO 14044?
3. Is there demand for an uncertainty terminology document for use in the LCA community?
4. Is there demand for uncertainty analysis within the LCA community?
5. Is there a demand to identify all sources of uncertainty within LCA and, possibly, other related extension modelling tools?
6. Is there a demand to identify, assess the purpose, assess the benefits, and assess the limitations of existing methods to address uncertainty and variability?
7. Is the LCA community genuinely interested in effectively communicating the LCA results based on the target audience?
8. Is the LCA community willing to make a stand for itself to ensure the credibility and reliability of LCA?

In conclusion, it is clearly evident that there is a need for individual efforts and group efforts to address various issues of uncertainty and variability that affect the reliability and credibility of LCA. Individual efforts include the identification of the sources of uncertainty and variability and proposals for methods to address them. Multi-stakeholder efforts include those that form the foundation of LCA and of uncertainty and variability in LCA, and guidance that which facilitates the performance of robust uncertainty assessments for all LCA's.

## CHAPTER 8

### FUTURE WORK

Despite the fact that a large amount of research effort has gone into uncertainty and variability in life cycle assessment, the research is disorganized, inconsistent, confusing, and does not facilitate the dependable application of uncertainty and variability assessments by LCA practitioners. This weak foundation is clearly evident in many research papers, LCA reports, and other documents at a time where demand for LCA in various sectors of the economy and policy making are booming. There is much work, especially multi-stakeholder work, to be done to robustly deal with uncertainty and variability in LCA, in a consistent manner. Here is the work that the author is going to undertake in the near term:

- Expand the identification of the sources of uncertainty and variability, beyond what has been done in Chapter 3, by applying the more than thirty identified typologies of uncertainty on published LCA case studies. In this process, establish all the typologies that relevant to LCA and compare them with already proposed typologies.
- Bring clarity towards methodological issues in LCA, such as inadequate functional unit and reference flows (already in progress).
- Assess proposed uncertainty assessment methodologies in LCA through replication and propose step-by-step guidance for methodology usage.
- Explore the interpretation of uncertainty information amongst different stakeholders in different geographies.

Here is a list of work that needs to be undertaken by a multi-stakeholder group, and needs to be addressed in the near term:

- Clearly establishing uncertainty theory as it relates to life cycle assessment. This includes definition for uncertainty and variability, terminologies and typologies for uncertainty and variability, et cetera.
- Creating consistent guidance for performing LCA that supplements the ISO standards.
- Establishing consistent guidance to perform qualitative and quantitative assessment of uncertainty and variability in LCA.
- Providing guidance on the use of extension models with LCA to address complex problems.
- Providing clarity on credibility of the various other forms of LCA, and how the established guidance on uncertainty and variability is applicable to those forms.

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APPENDIX A

CHAPTER 2: SUPPORTING INFORMATION FOR CONSOLIDATING ADRESSMENT OF  
UNCERTAINTY AND VARIABILITY IN ATTRIBUTIONAL LCA

## **Typologies of Uncertainty**

Van der Sluijs (1997) has created a list of twelve typologies of uncertainty published from the year 1984 to 1994. Heijungs (2004) has created a list of six typologies of uncertainty published from the year 1989 to 2001. Excluding the overlaps, Heijungs (2004) adds four typologies of uncertainty published from the year 1989 to 2001. When comparing the two overlapping typologies between Heijungs (2004) and van der Sluijs (1997), it is evident that they both aren't identical, when it supposed to be. Firstly, Heijungs (2004) did not include one uncertainty type with the label "uncertainty about model form" from Morgan et al. (1990), which van der Sluijs (1997) included. If there was a specific reason for the omission, it wasn't stated by Heijungs (2004).

Secondly, Heijungs (2004) details the uncertainty typology from (Funtowicz & Ravetz, 1990) as: (1) data uncertainty, (2) model uncertainty and (3) completeness uncertainty. In contrast, van der Sluijs (1997) details the uncertainty typology from Funtowicz and Ravetz (1990) as (1) inexactness (significant digits/error bars), (2) unreliability, and (3) border with ignorance. When analyzing why the reason for why the typology was not identical, it was evident that Heijungs (2004) mistakenly cites Funtowicz and Ravetz (1990) as the source, when in fact, the actual source is Vesely and Rasmuson (1984), which is also included in the list by (van der Sluijs, 1997). For reasons unknown, Heijungs (2004) did not include the different types of variability (spatial variability, temporal variability, inter-individual variability) in the uncertainty typology as stated in U.S. Environmental Protection Agency (1989), even though other variability types were included in other typologies in the list.

Table A1: Typologies of uncertainty and variability (adapted from Heijungs & Huijbregts (2004) and van der Sluijs (1997))

(Vesely & Rasmuson, 1984)	<ul style="list-style-type: none"> <li>• Data uncertainties (arise from the quality or appropriateness of the data used as inputs to models)</li> <li>• Modelling uncertainties: <ul style="list-style-type: none"> <li>○ Incomplete understanding of the modelled phenomena</li> <li>○ Numeral approximations used in mathematical representation</li> </ul> </li> <li>• Completeness uncertainties (all omissions due to lack of knowledge)</li> </ul>
(Environmental Resources Limited, 1985)	<p>Errors in modelling:</p> <ul style="list-style-type: none"> <li>• process error (due to model simplification)</li> <li>• functional error (uncertainty about the nature of the functional relations)</li> <li>• resolution error</li> <li>• numerical error</li> </ul>
Hall, 1985	<ul style="list-style-type: none"> <li>• Process uncertainty</li> <li>• Model uncertainty</li> <li>• Statistical uncertainty</li> <li>• Forcing uncertainty (involved in predictions which presuppose values that are unknowable)</li> </ul>
Alcamo and Bartnicki, 1987	<ul style="list-style-type: none"> <li>• Model structure <ul style="list-style-type: none"> <li>○ Diagnostic</li> <li>○ Prognostic</li> </ul> </li> <li>• Parameters <ul style="list-style-type: none"> <li>○ Diagnostic</li> <li>○ Prognostic</li> </ul> </li> <li>• Forcing functions <ul style="list-style-type: none"> <li>○ Diagnostic</li> <li>○ Prognostic</li> </ul> </li> <li>• Initial state <ul style="list-style-type: none"> <li>○ Diagnostic</li> <li>○ Prognostic</li> </ul> </li> <li>• Model operation <ul style="list-style-type: none"> <li>○ Diagnostic</li> <li>○ Prognostic</li> </ul> </li> </ul>
Beck, 1987	<ul style="list-style-type: none"> <li>• Uncertainty in internal description of the system: <ul style="list-style-type: none"> <li>○ Errors of aggregation (temporal, spatial, ecological)</li> <li>○ Numerical errors of solution</li> <li>○ Errors of model structure</li> <li>○ Errors in parameter and state estimation</li> </ul> </li> </ul>

	<ul style="list-style-type: none"> <li>• Uncertainty in external description of the system: <ul style="list-style-type: none"> <li>○ Uncertainty (natural variability) due to unobserved</li> <li>○ system input disturbances</li> <li>○ Measurement errors</li> </ul> </li> <li>• Uncertainty in initial state of the system</li> <li>• Propagation of state and parameter errors</li> </ul>
(U.S. Environmental Protection Agency, 1989)	<ul style="list-style-type: none"> <li>• Uncertainty <ul style="list-style-type: none"> <li>○ Scenario uncertainty</li> <li>○ Parameter uncertainty</li> <li>○ Model uncertainty</li> </ul> </li> <li>• Variability <ul style="list-style-type: none"> <li>○ Spatial variability</li> <li>○ Temporal variability</li> <li>○ Inter-individual variability</li> </ul> </li> </ul>
Morgan and Henrion, 1990	<ul style="list-style-type: none"> <li>• Sources of uncertainty in empirical quantities <ul style="list-style-type: none"> <li>○ Statistical variation and random error</li> <li>○ Subjective judgement and systematic error</li> <li>○ Linguistic imprecision</li> <li>○ Variability</li> <li>○ Inherent randomness and unpredictability</li> <li>○ Disagreement</li> <li>○ Approximation</li> </ul> </li> <li>• Uncertainty about model form</li> </ul>
(Funtowicz & Ravetz, 1990)	<ul style="list-style-type: none"> <li>• Inexactness (significant digits/error bars)</li> <li>• Unreliability</li> <li>• Border with ignorance</li> </ul>
Wallsten, 1990	<ul style="list-style-type: none"> <li>• Ambiguity (confusion in communication, avoidable)</li> <li>• Vagueness (imprecision in meaning)</li> <li>• Precise uncertainties (objective and subjective probability)</li> </ul>
(Wynne, 1992)	<ul style="list-style-type: none"> <li>• Risk (probabilities are known and quantifiable)</li> <li>• Uncertainty (probabilities are unknown; important parameters maybe known, uncertainty maybe reducible but with increase in ignorance)</li> <li>• Ignorance (don't know what we don't know; ignorance increases with increased commitments based on completeness and validity of knowledge)</li> </ul>

	<ul style="list-style-type: none"> <li>• Indeterminacy (uncertainty due to causal chains or open networks)</li> </ul>
Helton, 1994	<ul style="list-style-type: none"> <li>• Stochastic uncertainty (arises because the system under study can behave in many different ways; it is a property of the system)</li> <li>• Subjective uncertainty (arises from a lack of knowledge about the system; it is a property of the analysts performing the study)</li> </ul>
Hoffman and Hammonds, 1994	<ul style="list-style-type: none"> <li>• Uncertainty due to lack of knowledge</li> <li>• Uncertainty due to variability</li> </ul>
Rowe, 1994	<ul style="list-style-type: none"> <li>• Four dimensions of uncertainty: <ul style="list-style-type: none"> <li>○ Temporal (uncertainty in future states/ past states)</li> <li>○ Structural (uncertainty due to complexity)</li> <li>○ Metrical (uncertainty in measurement)</li> <li>○ Translational (uncertainty in explaining uncertain results)</li> </ul> </li> <li>• Variability is a contributor to uncertainty in all dimensions Sources of variability: <ul style="list-style-type: none"> <li>○ Underlying variants - inherent to nature - that contribute to the spread of parameter values: <ul style="list-style-type: none"> <li>▪ apparent inherent randomness of nature</li> <li>▪ inconsistent human behaviour</li> <li>▪ nonlinear dynamic systems (chaotic) behaviour</li> </ul> </li> <li>○ Collective / individual membership assignment</li> <li>○ Value diversity</li> </ul> </li> </ul>
(Huijbregts, 1998)	<ul style="list-style-type: none"> <li>• Parameter uncertainty</li> <li>• Model uncertainty</li> <li>• Uncertainty due to choices</li> <li>• Spatial variability</li> <li>• Temporal variability</li> <li>• Variability between sources and objects</li> </ul>
(Bedford & Cooke, 2001)	<ul style="list-style-type: none"> <li>• Aleatory uncertainty</li> <li>• Epistemic uncertainty</li> <li>• Parameter uncertainty</li> <li>• Data uncertainty</li> <li>• Model uncertainty</li> <li>• Ambiguity</li> <li>• Volitional uncertainty</li> </ul>
(Regan, Colyvan, & Burgman, 2002)	<ul style="list-style-type: none"> <li>• Epistemic uncertainty <ul style="list-style-type: none"> <li>○ Measurement error</li> <li>○ Systematic error</li> </ul> </li> </ul>

	<ul style="list-style-type: none"> <li>○ Natural variation</li> <li>○ Inherent randomness</li> <li>○ Model uncertainty</li> <li>○ Subjective judgement</li> <li>• Linguistic uncertainty <ul style="list-style-type: none"> <li>○ Vagueness</li> <li>○ Context dependence</li> <li>○ Ambiguity</li> <li>○ Interdeterminacy of theoretical terms</li> </ul> </li> <li>• Underspecificity</li> </ul>
(Webster, 2003)	<ul style="list-style-type: none"> <li>• Empirical uncertainty (data gaps)</li> <li>• Methodological uncertainty (bias, expert opinions, model assumptions)</li> <li>• Institutional uncertainty</li> <li>• Philosophical uncertainty</li> </ul>
(Walker et al., 2003)	<ul style="list-style-type: none"> <li>• Locations of uncertainty <ul style="list-style-type: none"> <li>○ Context uncertainty</li> <li>○ Model uncertainty <ul style="list-style-type: none"> <li>▪ Model structure uncertainty</li> <li>▪ Model technical uncertainty</li> </ul> </li> <li>○ Input uncertainty</li> <li>○ Parameter uncertainty</li> <li>○ Model outcome uncertainty</li> </ul> </li> <li>• Levels of uncertainty <ul style="list-style-type: none"> <li>○ Statistical uncertainty</li> <li>○ Scenario uncertainty</li> <li>○ Recognized ignorance</li> <li>○ Total ignorance</li> </ul> </li> <li>• Nature of uncertainty <ul style="list-style-type: none"> <li>○ Epistemic uncertainty</li> <li>○ Variability uncertainty</li> </ul> </li> </ul>
(Loucks, van Beek, Stedinger, Dijkman, & Villars, 2005)	<ul style="list-style-type: none"> <li>• Knowledge uncertainty <ul style="list-style-type: none"> <li>○ Model/Structural uncertainty (imperfect representation of processes)</li> <li>○ Parameter uncertainty (imperfect knowledge of values)</li> </ul> </li> <li>• Natural variability <ul style="list-style-type: none"> <li>○ Temporal variability</li> <li>○ Spatial variability</li> </ul> </li> <li>• Decision uncertainty (inability to predict future decisions or goals, and its relative importance) <ul style="list-style-type: none"> <li>○ Goals – Objectives</li> <li>○ Values – Preferences</li> </ul> </li> </ul>
(Loucks et al., 2005)	<ul style="list-style-type: none"> <li>• Informational uncertainty <ul style="list-style-type: none"> <li>○ Imprecision in specifying boundary and initial conditions</li> <li>○ Imprecision in measuring output values</li> </ul> </li> <li>• Model uncertainty</li> </ul>

	<ul style="list-style-type: none"> <li>○ Uncertain model structure and parameter values</li> <li>○ Variability of input and output values over spatial scale smaller than scope</li> <li>○ Variability of input and output values over temporal scale smaller than scope</li> <li>○ Errors in linking models with differing spatial and temporal scales</li> <li>• Numerical errors (model solution algorithm)</li> </ul>
(Krupnick et al., 2006)	<ul style="list-style-type: none"> <li>• Variability (moral choices, et cetera)</li> <li>• Parameter uncertainty <ul style="list-style-type: none"> <li>○ Measurement errors (random errors and statistical variation, systemic bias)</li> <li>○ Unpredictability (inherent randomness)</li> <li>○ Conflicting data and lack of data</li> <li>○ Extrapolation errors (random sampling errors, temporal prediction errors, surrogate data, non-representativeness)</li> <li>○ Misclassification</li> </ul> </li> <li>• Model uncertainty <ul style="list-style-type: none"> <li>○ Structural choices</li> <li>○ Simplification</li> <li>○ Incompleteness</li> <li>○ Choice of probability distributions</li> <li>○ Correlation and dependencies</li> <li>○ System resolution</li> </ul> </li> <li>• Decision uncertainty (ambiguity or controversy on how to quantify) <ul style="list-style-type: none"> <li>○ Choice of risk measure and summary statistics</li> <li>○ Choice of discount rate</li> <li>○ Decision about Risk Tolerance</li> <li>○ Utility Functions</li> <li>○ Distributional Considerations</li> </ul> </li> <li>• Linguistic Uncertainty (applies to variability, parameter uncertainty, model uncertainty and decision uncertainty)</li> </ul>
(Heinemeyer et al., 2008)	<ul style="list-style-type: none"> <li>• Scenario uncertainty (choice of model and model parameters, descriptive errors, aggregation errors, errors of assessment, errors of incomplete analysis)</li> <li>• Model uncertainty (model assumptions, boundaries,</li> </ul>

	<p>dependencies, detail, extrapolation, implementation, technical model aspects)</p> <ul style="list-style-type: none"> <li>• Parameter uncertainty (measurement errors, sample uncertainty, data type, extrapolation uncertainty, statistical distribution used)</li> </ul>
(Kiureghian & Ditlevsen, 2009)	<ul style="list-style-type: none"> <li>• Uncertainty in basic variables (measured values and constants) <ul style="list-style-type: none"> <li>○ Aleatory uncertainty</li> <li>○ Epistemic uncertainty</li> </ul> </li> <li>• Model uncertainty <ul style="list-style-type: none"> <li>○ Aleatory uncertainty</li> <li>○ Epistemic uncertainty</li> </ul> </li> <li>• Parameter uncertainty <ul style="list-style-type: none"> <li>○ Aleatory uncertainty</li> <li>○ Epistemic uncertainty</li> </ul> </li> </ul>
(Spiegelhalter & Riesch, 2011)	<ul style="list-style-type: none"> <li>• Future events (essential unpredictability)</li> <li>• Parameters within models (limitation in information)</li> <li>• Alternative model structures (limitation in formalized knowledge)</li> <li>• Effects of model inadequacy from recognized sources (known limitation in understanding and modeling ability)</li> <li>• Effects of model inadequacy from unspecified sources (unknown limitation in understanding)</li> </ul>
(O'Reilly, Brysse, Oppenheimer, & Oreskes, 2011)	<ul style="list-style-type: none"> <li>• Model Uncertainty <ul style="list-style-type: none"> <li>○ Structural (code used in the model)</li> <li>○ Parameter (data inputs)</li> </ul> </li> <li>• Conflict uncertainty (disagreement on how to interpret information)</li> <li>• Judgement uncertainty (act of judging the study by the assessors – extension of conflict uncertainty)</li> </ul>

### Uncertainty Definition

The term 'Uncertainty' has varied definitions based on its field of origin (Williams, Weber, & Hawkins, 2009). Tallacchini (2005), who focuses on science and law, states that 'scientific uncertainty' is generally referred to the various forms of lack of information in science (knowledge complexity, partial/full unavailability of



data, unpredictable results, stochastic nature of predictions). In physical sciences, uncertainty is used interchangeably with error, and is defined as the difference between the analyst's knowledge and the true value (Taylor, 1997) . In risk assessment, the World Health Organization defines uncertainty as imperfect knowledge with respect to time and the system under consideration (World Health Organization, 2004). In exposure assessment, U.S. Environmental Protection Agency (2011) defines uncertainty "as the lack of knowledge about factors affecting exposure and risk". In statistics, uncertainty is the "degree of precision with which a quantity is measured" (van Belle, 2008). Gifford et al. (1979) have listed out several definitions of uncertainty with respect to measures (low uncertainty, high uncertainty) from a psychological and organizational research point of view. Spiegelhalter and Riesch (2011) suggests that uncertainty should be best thought of as a relationship between (1) objects of uncertainty (future events, model parameters, model structures, model adequacy types), (2) forms of expression of uncertainty (full explicit probability distribution function, list of possibilities, informal qualitative and/or qualifying statements, incompletely specified probability, informal acknowledgment of existence of uncertainty, explicit denial of the existence of uncertainty, no mention of uncertainty, (3) sources of uncertainty (e.g.: variability, ignorance, chance, computational limitations), (4) subject (e.g.: individual, decision makers, public, risk-assessor), and (5) affect (e.g.: fear, excitement, dread, et cetera). According to Wynne (1992), indeterminacy, when recognized, is large-scale uncertainty and is the basis of construction of scientific knowledge. While there are many definitions of uncertainty, most often, peer-reviewed journal articles don't spend enough time/words discussing what they mean by uncertainty but more on how to address the uncertainty under consideration.

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APPENDIX B

CHAPTER 3: SUPPORTING INFORMATION FOR ADDRESSING DATA GAPS IN LIFE  
CYCLE INVENTORY

## IRB Approval



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### Office of Research Integrity and Assurance

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**To:** Eric Williams  
ERC

**From:** *for*  
*GD* Mark Roosa, Chair  
Soc Beh IRB

**Date:** 10/13/2010

**Committee Action:** **Exemption Granted**

**IRB Action Date:** 10/13/2010

**IRB Protocol #:** 1010005591

**Study Title:** Patching Data Gaps Through Expert Elicitation

The above-referenced protocol is considered exempt after review by the Institutional Review Board pursuant to Federal regulations, 45 CFR Part 46.101(b)(2) .

This part of the federal regulations requires that the information be recorded by investigators in such a manner that subjects cannot be identified, directly or through identifiers linked to the subjects. It is necessary that the information obtained not be such that if disclosed outside the research, it could reasonably place the subjects at risk of criminal or civil liability, or be damaging to the subjects' financial standing, employability, or reputation.

You should retain a copy of this letter for your records.

**Justin Ford**

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**From:** Justin Ford  
**Sent:** Wednesday, October 13, 2010 4:01 PM  
**To:** Eric Williams (Professor); Vairavan Subramanian  
**Subject:** IRB Exempt Approval: 1010005591  
**Attachments:** Williams.pdf; image001.gif; image002.gif

Dear Dr. Williams,

The IRB has determined that your study qualifies as exempt pursuant to Federal regulation, 45 CFR, Part 46.101(b)(2).

Your approval notice has been attached to this e-mail, please retain a copy for your records.

Good luck with the research and please let me know if I can be of any further assistance.

All the best,  
Justin

**Justin T. Ford**

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IRB Specialist

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## Additional Tables

Table B1: Expertise profile, years of experience with respect to individual area of expertise, and total (range) experience years of each survey respondent

Respondent	Chemistry	Toxicology	Chemical Engineering	Life Cycle Assessment	Expertise profile	Total experience years
R1	5	1	5	6	LCA + Chemical Engg. + Chemistry + Toxicology	11 to 20
R2	40	10	0	15	LCA + Chemistry + Toxicology	61 to 70
R3	2	1	0	12	LCA + Chemistry + Toxicology	11 to 20
R4	40	0	40	3	LCA + Chemical Engg. + Chemistry	81 to 90
R5	35	0	0	3	LCA + Chemistry	31 to 40
R6	3	0	3	3	LCA + Chemical Engg. + Chemistry	1 to 10
R7	6	3	0	11	LCA + Chemistry + Toxicology	11 to 20
R8	26	0	0	17	LCA + Chemistry	41 to 50
R9	2	1	2	5	LCA + Chemical Engg. + Chemistry + Toxicology	1 to 10
R10	0	0	0	5	LCA	1 to 10
R11	1	0	5	11	LCA + Chemical Engg. + Chemistry	11 to 20
R12	25	0	0	14	LCA + Chemistry	31 to 40
R13	0	3	12	7	LCA + Chemical Engg. + Toxicology	21 to 30
R14	0	0	0	18	LCA	11 to 20
R15	0	0	0	13	LCA	11 to 20
R16	4	0	0	2.5	LCA + Chemistry	1 to 10
R17	0	0	0	3	LCA	1 to 10
R18	2	0	0	5	LCA + Chemistry	1 to 10
R19	0	0	8	3	LCA + Chemical Engg.	11 to 20
R20	10	10	10	10	LCA + Chemical Engg. + Chemistry + Toxicology	31 to 40
R21	15	0	0	3	LCA + Chemistry	11 to 20
R22	0	0	0	3	LCA	1 to 10
R23	0	0	0	5	LCA	1 to 10
R24	1	0	0	2	LCA + Chemistry	1 to 10
R25	0	0	0	2	LCA	1 to 10
R26	0	0	0	2	LCA	1 to 10
R27	1	1	6	6	LCA + Chemical Engg. + Chemistry + Toxicology	11 to 20
R28	0	0	0	3	LCA	1 to 10
R29	0	0	0	4	LCA	1 to 10
R30	10	0	0	4	LCA + Chemistry	11 to 20
R31	3	0	3	3	LCA + Chemical Engg. + Chemistry	1 to 10
R32	12	3	12	8	LCA + Chemical Engg. + Chemistry + Toxicology	31 to 40

Table B2: Results of the statistical testing of the association between expertise profile and proxy type

	Likelihood ratio	Degrees of freedom	p-value
<b>Anionic surfactants</b>	19.315	12	0.081
<b>Non-ionic surfactants</b>	9.723	12	0.640
<b>Complexing/sequestering agents</b>	6.216	6	0.399
<b>Thickening agents/process aids</b>	20.536	12	0.058
<b>Inorganic builders</b>	6.838	6	0.336

Table B3: Results of the statistical testing of the association between total experience years and proxy type

	<b>Likelihood ratio</b>	<b>Degrees of freedom</b>	<b>p-value</b>
<b>Anionic surfactants</b>	48.503	26	0.05
<b>Non-ionic surfactants</b>	12.241	12	0.427
<b>Complexing/sequestering agents</b>	10.035	6	0.123
<b>Thickening agents/process aids</b>	9.755	12	0.637
<b>Inorganic builders</b>	7.375	6	0.288

Table B4: Results of the statistical testing of the association between total expertise profile and confidence

	<b>Likelihood ratio</b>	<b>Degrees of freedom</b>	<b>p-value</b>
<b>Anionic surfactants</b>	28.421	30	0.312
<b>Non-ionic surfactants</b>	23.765	24	0.475
<b>Complexing/sequestering agents</b>	23.765	24	0.475
<b>Thickening agents/process aids</b>	19.4	24	0.730
<b>Inorganic builders</b>	18.066	24	0.800

Table B5: Results of the statistical testing of the association between total experience years and confidence

	<b>Likelihood ratio</b>	<b>Degrees of freedom</b>	<b>p-value</b>
<b>Anionic surfactants</b>	53.476	65	0.58
<b>Non-ionic surfactants</b>	21.923	24	0.584
<b>Complexing/sequestering agents</b>	21.923	24	0.584
<b>Thickening agents/process aids</b>	22.964	24	0.522
<b>Inorganic builders</b>	24.175	24	0.452



Table B6: Results of the statistical testing of the association between expertise profile and intuition

	<b>Likelihood ratio</b>	<b>Degrees of freedom</b>	<b>p-value</b>
<b>Anionic surfactants</b>	20.472	24	0.670
<b>Non-ionic surfactants</b>	29.726	24	0.194
<b>Complexing/sequestering agents</b>	29.726	24	0.194
<b>Thickening agents/process aids</b>	16.962	24	0.850
<b>Inorganic builders</b>	27.888	24	0.265

Table B7: Results of the statistical testing of the association between total experience years and intuition

	<b>Likelihood ratio</b>	<b>Degrees of freedom</b>	<b>p-value</b>
<b>Anionic surfactants</b>	49.347	52	0.344
<b>Non-ionic surfactants</b>	21.154	24	0.630
<b>Complexing/sequestering agents</b>	21.154	24	0.630
<b>Thickening agents/process aids</b>	19.985	24	0.698
<b>Inorganic builders</b>	26.725	24	0.317

Table B8: Results of the statistical testing of the association between expertise profile and alternate proxy

	<b>Likelihood ratio</b>	<b>Degrees of freedom</b>	<b>p-value</b>
<b>Anionic surfactants</b>	9.662	12	0.501
<b>Non-ionic surfactants</b>	14.191	18	0.717
<b>Complexing/sequestering agents</b>	14.191	18	0.717
<b>Thickening agents/process aids</b>	15.460	12	0.217
<b>Inorganic builders</b>	8.870	12	0.731

Table B9: Results of the statistical testing of the association between experience years and alternate proxy

	<b>Likelihood ratio</b>	<b>Degrees of freedom</b>	<b>p-value</b>
<b>Anionic surfactants</b>	20.605	26	0.762
<b>Non-ionic surfactants</b>	13.028	18	0.790
<b>Complexing/sequestering agents</b>	13.028	18	0.790
<b>Thickening agents/process aids</b>	10.903	12	0.537
<b>Inorganic builders</b>	6.493	12	0.889

Table B10: Proxy type of each response provided each survey respondent for each of the five functional chemical groups, along with their respective expertise profile and total experience years

Respondent	Expertise profile	Total experience years	Anionic surfactants proxy type	Non-ionic surfactants proxy type	Complexing/seques-tering agents proxy type	Thickening agents/processing aids proxy type	Inorganic builder proxy type
R1	LCA + Chemical Engg. + Chemistry + Toxicology	11 to 20	Best proxy	Other	Other	Other	Other
R2	LCA + Chemistry + Toxicology	61 to 70	Other	Best proxy	Best & majority pr	Other	Other
R3	LCA + Chemistry + Toxicology	11 to 20	Majority proxy	Majority proxy	Best & majority pr	Other	Best & majority pr
R4	LCA + Chemical Engg. + Chemistry	81 to 90	Best proxy	Other	Best & majority pr	Majority proxy	Other
R5	LCA + Chemistry	31 to 40	Majority proxy	Other	Other	Majority proxy	Other
R6	LCA + Chemical Engg. + Chemistry	1 to 10	Other	Majority proxy	Other	Majority proxy	Other
R7	LCA + Chemistry + Toxicology	11 to 20	Majority proxy	Other	Other	Other	Other
R8	LCA + Chemistry	41 to 50	Majority proxy	Other	Best & majority pr	Other	Best & majority pr
R9	LCA + Chemical Engg. + Chemistry + Toxicology	1 to 10	Majority proxy	Other	Other	Other	Other
R10	LCA	1 to 10	Majority proxy	Majority proxy	Other	Other	Best & majority pr
R11	LCA + Chemical Engg. + Chemistry	11 to 20	Other	Best proxy	Other	Majority proxy	Other
R12	LCA + Chemistry	31 to 40	Majority proxy	Other	Best & majority pr	Other	Best & majority pr
R13	LCA + Chemical Engg. + Toxicology	21 to 30	Majority proxy	Majority proxy	Best & majority pr	Majority proxy	Other
R14	LCA	11 to 20	Majority proxy	Majority proxy	Other	Other	Other
R15	LCA	11 to 20	Other	Best proxy	Other	Best proxy	Other
R16	LCA + Chemistry	1 to 10	Other	Other	Other	Other	Other
R17	LCA	1 to 10	Other	Majority proxy	Other	Best proxy	Best & majority pr
R18	LCA + Chemistry	1 to 10	Majority proxy	Majority proxy	Other	Best proxy	Other
R19	LCA + Chemical Engg.	11 to 20	Majority proxy	Best proxy	Best & majority pr	Other	Other
R20	LCA + Chemical Engg. + Chemistry + Toxicology	31 to 40	Majority proxy	Best proxy	Other	Other	Best & majority pr
R21	LCA + Chemistry	11 to 20	Other	Best proxy	Other	Other	Best & majority pr
R22	LCA	1 to 10	Other	Other	Best & majority pr	Majority proxy	Best & majority pr
R23	LCA	1 to 10	Majority proxy	Best proxy	Other	Majority proxy	Best & majority pr
R24	LCA + Chemistry	1 to 10	Majority proxy	Best proxy	Best & majority pr	Other	Other
R25	LCA	1 to 10	Majority proxy	Majority proxy	Best & majority pr	Other	Other
R26	LCA	1 to 10	Majority proxy	Other	Other	Other	Best & majority pr
R27	LCA + Chemical Engg. + Chemistry + Toxicology	11 to 20	Majority proxy	Majority proxy	Other	Majority proxy	Other
R28	LCA	1 to 10	Other	Best proxy	Other	Majority proxy	Other
R29	LCA	1 to 10	Majority proxy	Majority proxy	Best & majority pr	Majority proxy	Other
R30	LCA + Chemistry	11 to 20	Other	Best proxy	Other	Other	Best & majority pr
R31	LCA + Chemical Engg. + Chemistry	1 to 10	Other	Best proxy	Other	Majority proxy	Other
R32	LCA + Chemical Engg. + Chemistry + Toxicology	31 to 40	Best proxy	Best proxy	Best & majority pr	Other	Best & majority pr

## Additional Figures

Figure B1: Criteria utilized by experts to select the best proxy, majority proxy, and other proxies for anionic surfactant, fatty alcohol sulfate from coconut oil

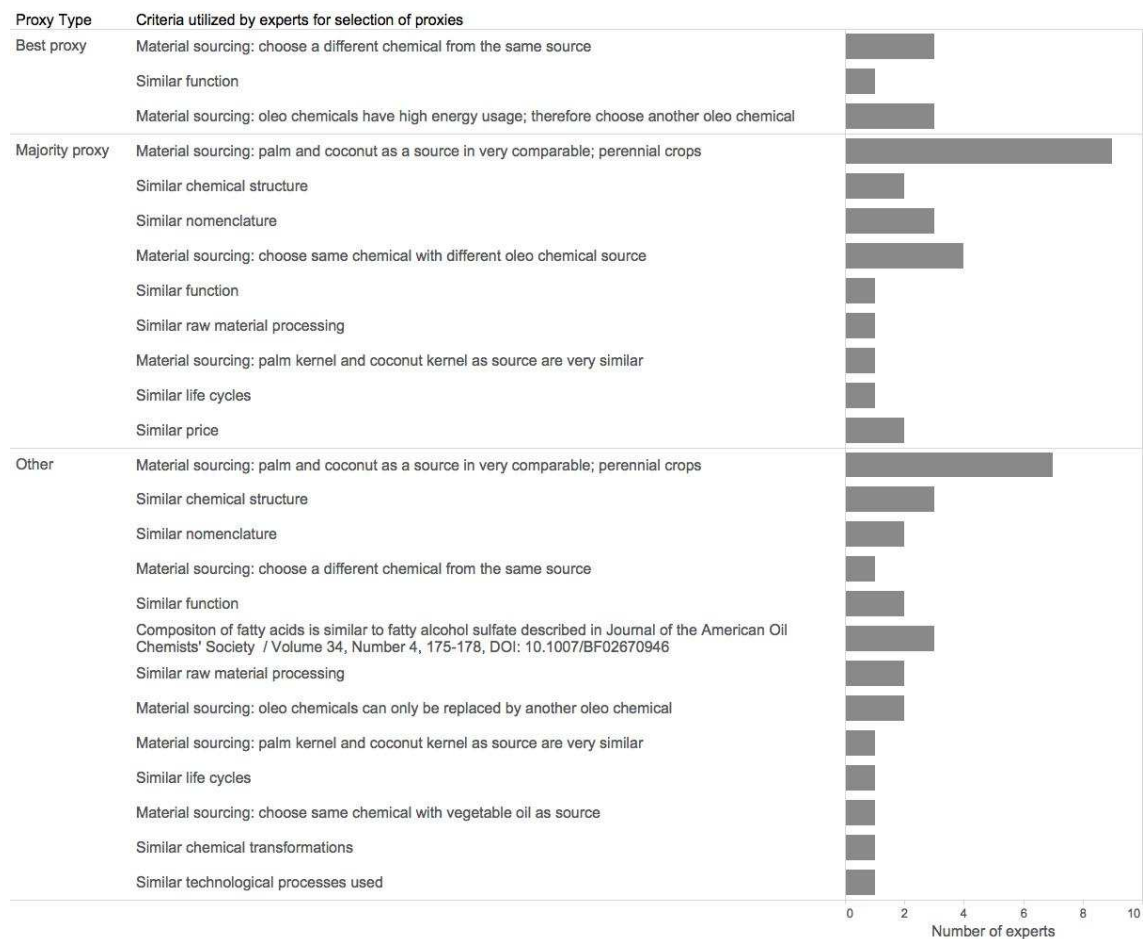


Figure B2: Criteria utilized by experts to select the best proxy, majority proxy, and other proxies for nonionic surfactant, fatty alcohol from petrochemicals

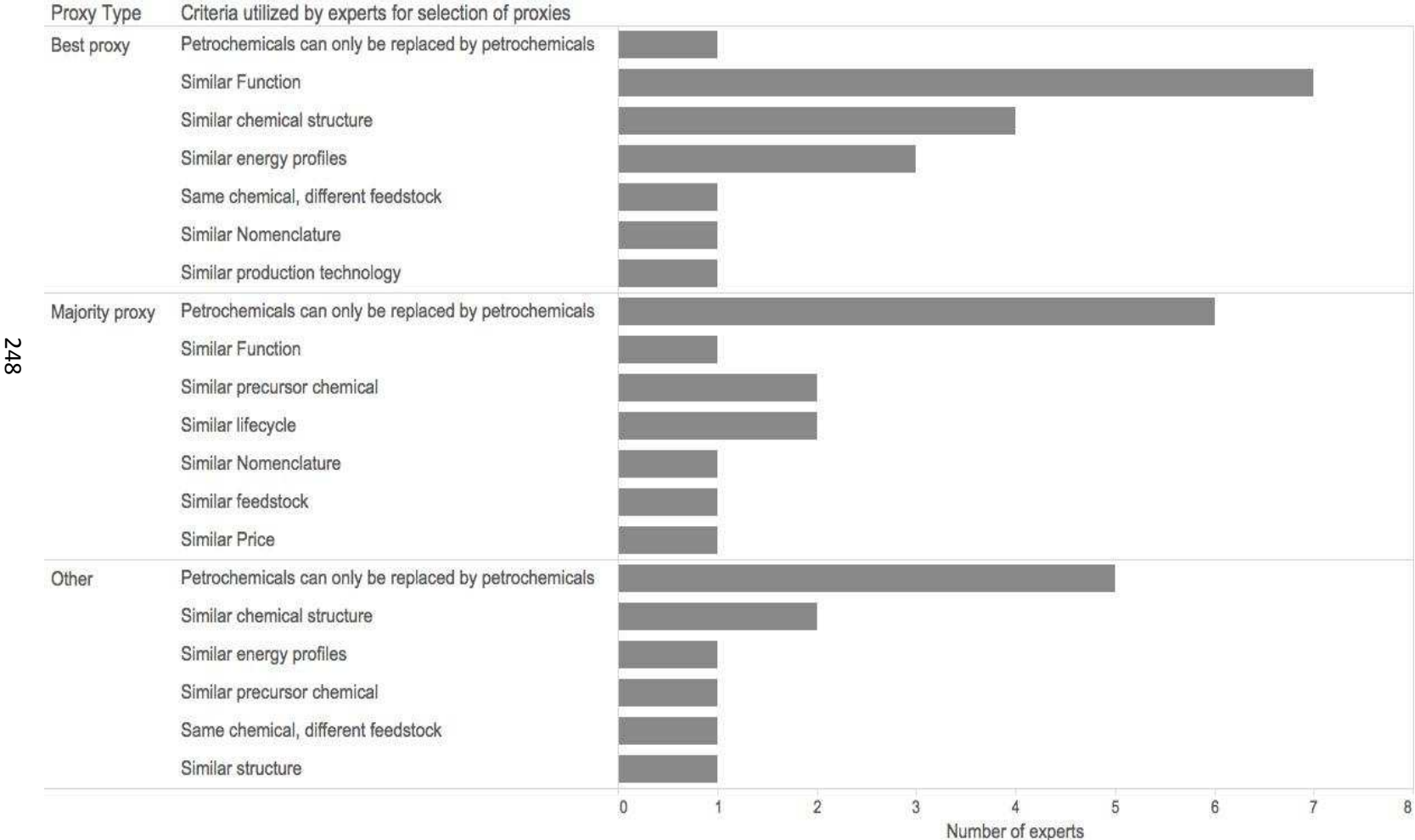


Figure B3: Criteria utilized by experts to select the best proxy, majority proxy, and other proxies for nonionic surfactant, fatty alcohol from petrochemicals; where best proxy and majority proxy are merge

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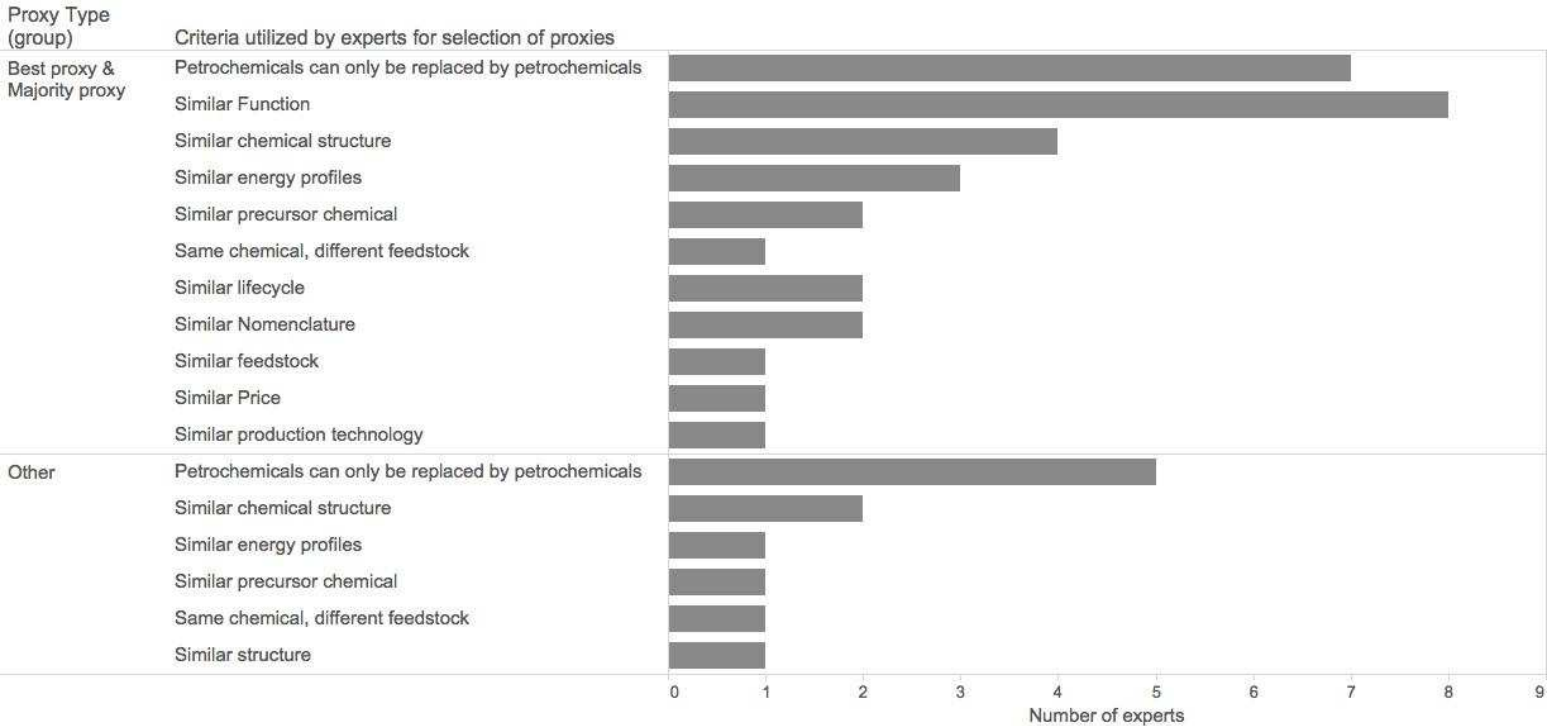


Figure B4: Criteria utilized by experts to select the best proxy, majority proxy, and other proxies for complexing/sequestering agents, adipic acid

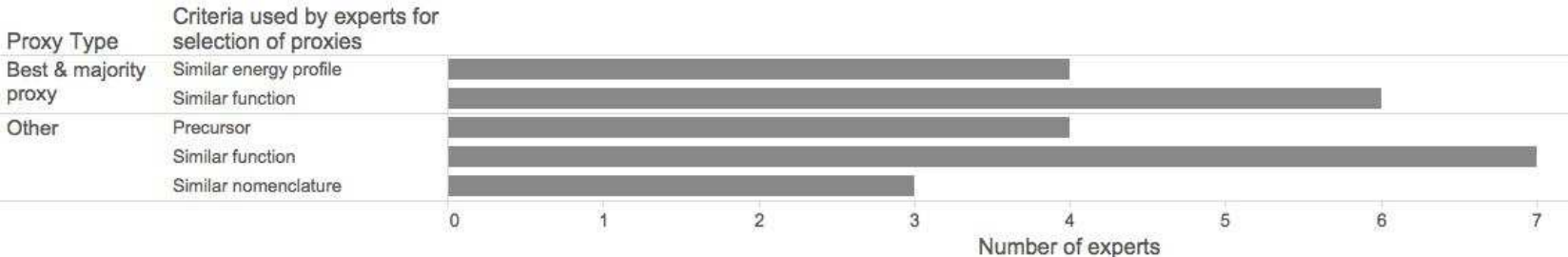


Figure B5: Criteria utilized by experts to select the best proxy, majority proxy, and other proxies for thickening agents/processing aids, sodium formate

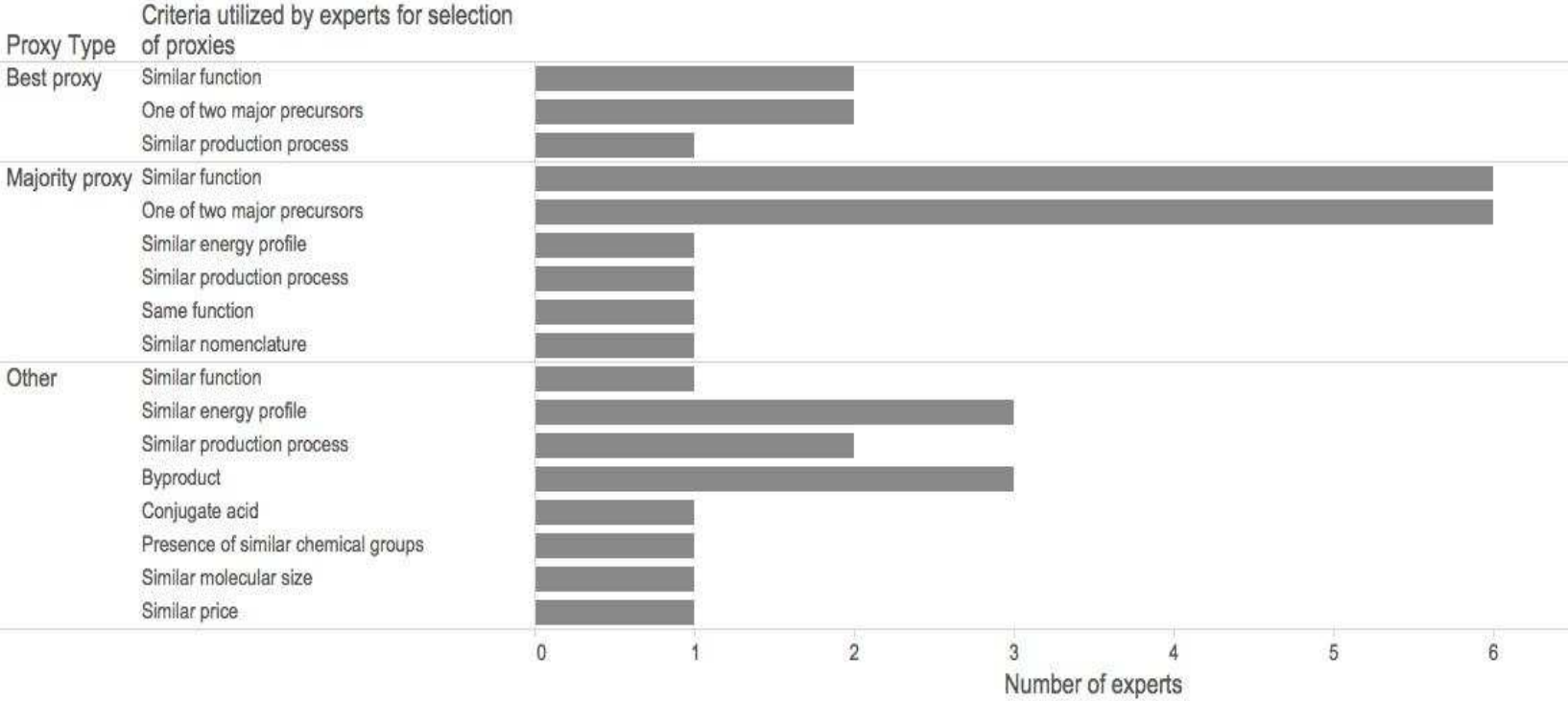




Figure B6: Criteria utilized by experts to select the best proxy, majority proxy, and other proxies for thickening agents/processing aids, sodium formate; where best proxy and majority proxy are merged

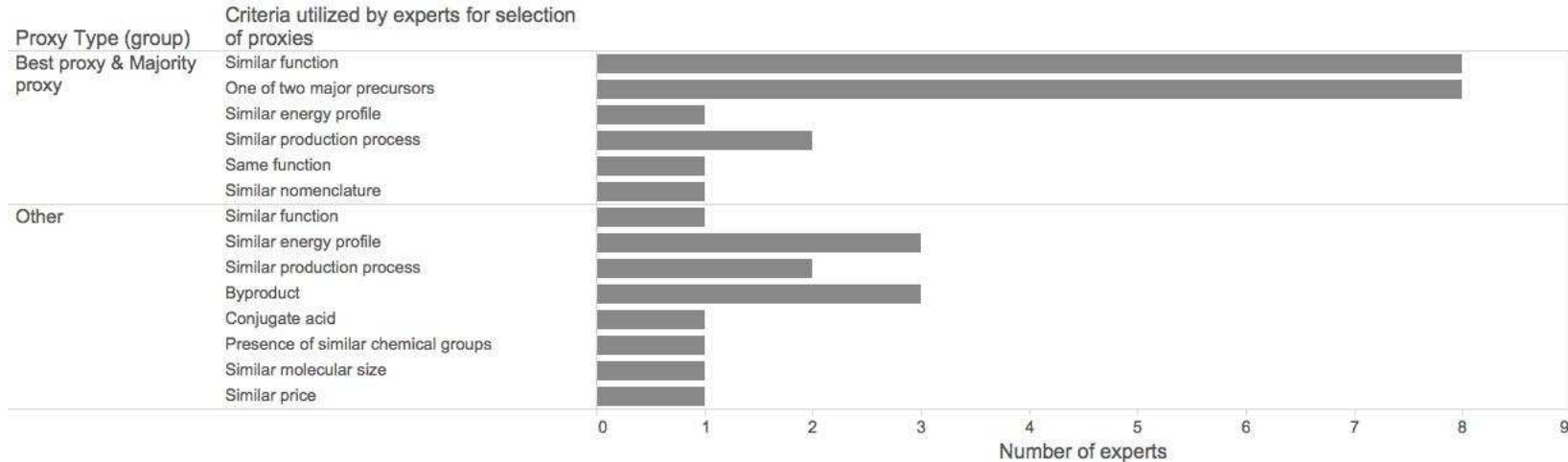
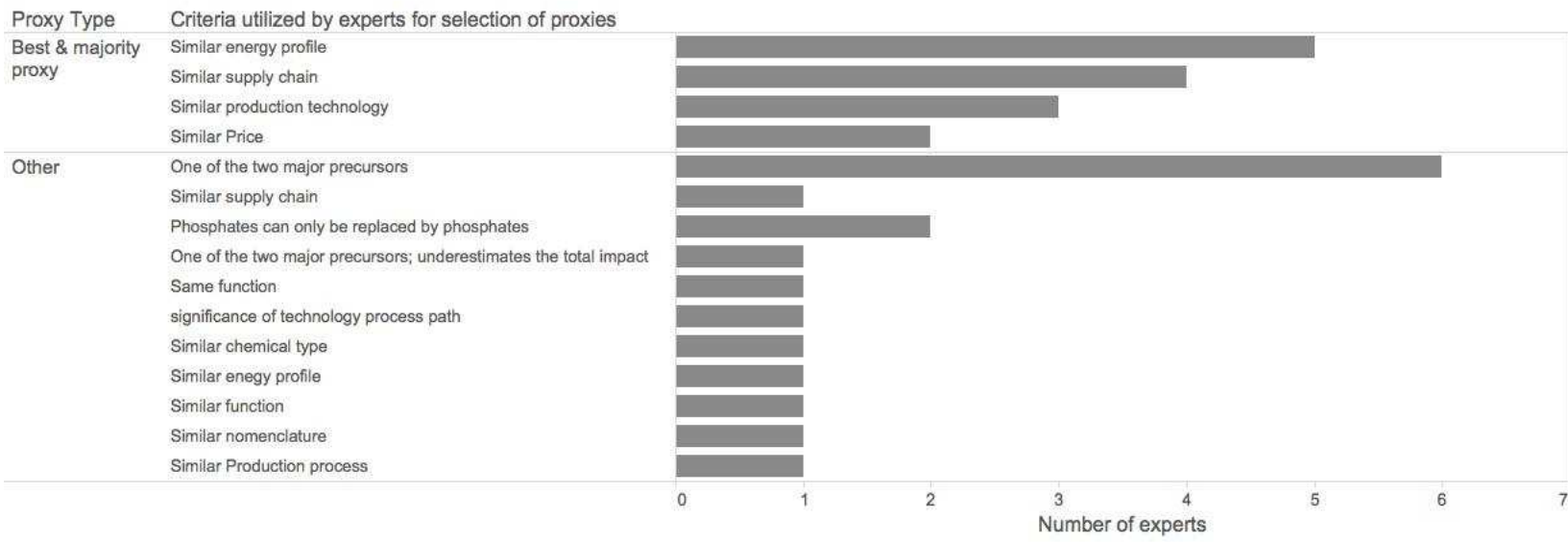


Figure B7: Criteria utilized by experts to select the best proxy, majority proxy, and other proxies for inorganic builders, sodiumtripolyphosphate



## **Limitations of Pedigree Matrix Approach**

The Pedigree Matrix can address the use of a dataset on the production of acetic acid from process y instead of the dataset on the production of acetic acid from process x, but cannot address the use of a dataset on the production of citric acid instead of the use a dataset on the production of acetic acid. Other problems with the pedigree approach include: (1) the lack of a method to select the supposed proxies and, (2) availability of data quality indicators (DQI) only in the LCI database Ecoinvent. In the absence of a method to select supposed proxies, there can be many proxies that could be assigned the same DQI values. Thus any variability in impact due to the data is not sufficiently addressed. For example, if there are three datasets for a single product that differ spatially from each other due to their sourcing, all three datasets will have the same DQI, with respect to the United States. While these three datasets might have different overall environmental impacts, the user has an option to choose the dataset with the lowest impact and calculate the associated uncertainty using the same DQI's. This variability in choice of proxy selection reduces the credibility of LCA. It must be noted that the pedigree matrix approach provides only a qualitative assessment of data uncertainty (measurement errors and data quality) (Weidema et al., 1996).

## **Case studies on Laundry Detergents**

- Cullen and Allwood (2009) demonstrated the double counting problems associated with aggregated LCA studies,
- Edwards and DeCarvalho (1998) assessed the impacts of unused household cleaning products on microbial wastewater treatment systems,
- Golden et al. (2010) analyzed the systemic implications of the consumer use phase,

- Koehler and Wildbolz (2009) assessed the relevance of different life cycle phases and,
- Misra and Sivongxay (2009) evaluated the reuse of laundry grey-water for residential irrigation.
- Paloviita and Järvi (2008) evaluated the importance of the use phase in environmental value chain management,
- Schulze et al. (2001) compared different life cycle impact assessment methodologies for aquatic toxicity, and
- De Koning et al. (2010) estimated the uncertainty associated with varying product systems for carbon footprint comparisons.

### **Influence of expertise on proxy choices**

Given that expert elicitation is the primary tool used in this study, it is important to understand the influence of the experts on the choices made. This was done by statistically analyzing the association between the expertise profile (table 2) and the associated total years of experience with that of the type of proxy choices.

When statistically testing the association between expertise profile (listed in table 2) and proxy type (best/majority/best-majority/other) for each functional chemical group, the authors considered the null hypothesis (H<sub>0</sub>) to be that there is no association between the two variables and the alternative hypothesis (H<sub>a</sub>) to be that there is an association between the two variables. In all cases, the p-value was found of be greater than or equal to 0.05 (anionic surfactant p-value = 0.08, non-ionic surfactant p-value = 0.64, complexing/sequestering agents p-value = 0.40, thickening agents/process aids p-value = 0.06, inorganic builders p-value = 0.37), which only means that we failed to reject H<sub>0</sub>. This means that we failed to prove that there is no association between the two variables (Vickers, 2009; Thisted, 2010). In other words, the influence of expertise profile on proxy type remains unproven.

Similarly, when testing the association between total experience years and proxy type (best/majority/best-majority/other), the authors found that for all functional chemical groups, the p-value was found to be greater than or equal to 0.05 (anionic surfactants p-value = 0.05, non-ionic surfactants p-value = 0.43, complexing/sequestering agents p-value = 0.12, thickening agents/process aids p-value = 0.64, and inorganic builders p-value = 0.29). This outcome is interpreted as the failure to reject that there is no association between the two variables. In other words, the influence of total experience years on proxy type remains unproven. The associated likelihood ratio and degrees of freedom for each of the p-values can be found in the Annex.

Given that the statistical association between expertise profile/experience years and proxy type (best/majority/best-majority/other) was not proven, it is not possible to establish the profile of experts who performed better than the others. The following bullets provide an insight into the selection behavior of experts:

- No experts selected either best proxy, best & majority proxy, merged best proxy and majority proxy for all five functional chemical groups; majority proxy as the sole proxy type was not included in the analysis as the goal was to obtain guidance from the best proxy selections, or best proxy and majority selections with a small difference (less than 5MJ) in CED.
- One expert made the aforementioned proxy type selections for four functional chemical groups; this expert had expertise in all the four areas (table 2), and total experience years that ranged from 31 to 40.
- Seven experts made the aforementioned proxy type selections for three functional chemical groups; four of these experts had expertise only in LCA with total experience years that ranged from 1 to 10, and the remaining experts had assorted proficiency in three of the four individual areas of expertise and a varied range of total experience years.

- Sixteen experts made the aforementioned proxy type selections for two functional chemical groups; the expertise profile and total years of experience of the experts varied.
- Five experts made the aforementioned proxy type selections for only one functional chemical group; the expertise profile and total years of experience of the experts varied. Proxy type selections of each expert along with their expertise profile and total experience years are available in the Annex.

### **Confidence and intuition in choices**

The two important aspects to making proxy choices are the level of confidence exerted and the level of intuition utilized. The amount of confidence and intuition serves as qualitative indicators of the criteria provided by experts for the best proxies. Statistical testing was performed to test the association between (1) expertise profile and confidence, (2) total experience years and confidence, (3) expertise profile and intuition, and (4) total experience years and intuition. In all the above four cases, the p-value was found to be greater than or equal to 0.05, thus failing to reject the null hypothesis that there is no association between the said four pairs of variables. In other words, the association between expertise profile and total experience years, and confidence and intuition remains unproven. The p-values, likelihood ratio, and the associated degrees of freedom for each of the five functional chemical groups for each of the four above-mentioned associations, can be found in the supplemental. On analyzing the expert responses on confidence and intuition, for the five functional groups, it was evident that roughly one-third of the experts maintained “just some” confidence and “just some” intuition in their proxy selections.

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## APPENDIX C

### CHAPTER 4: SUPPORTING INFORMATION FOR SENSITIVITY OF PRODUCT- EVOLUTION ON LCA RESULTS

## Additional Figures

Figure C1: Endpoint impact ranges associated with various detergents components exemplifying carbon-chain variability.

The two dash lines in each pane reflect the minimum and maximum endpoint impact values for each chemical component.

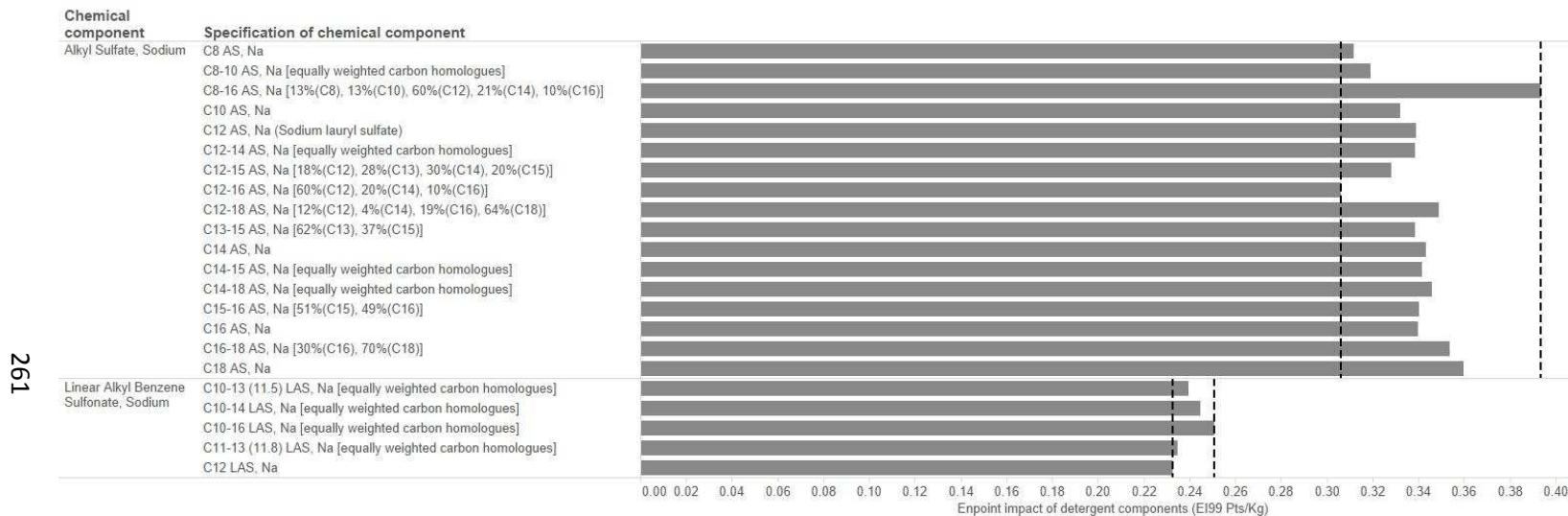
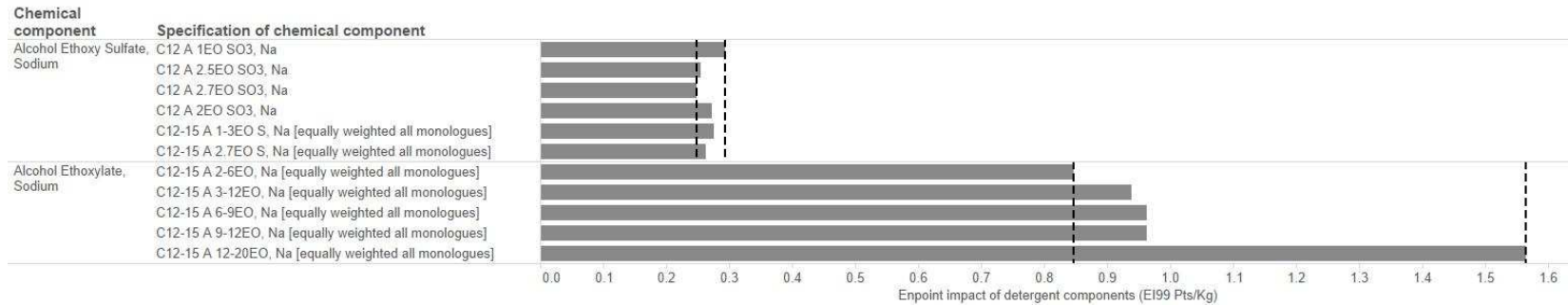


Figure C2: Endpoint impact ranges associated with various detergents components exemplifying ethoxylation variability.

The two dash lines in each pane reflect the minimum and maximum endpoint impact values for each chemical component.



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Figure C3: Endpoint impact ranges associated with various detergents components exemplifying homologue variability. The

two dash lines in each pane reflect the minimum and maximum endpoint impact values for each chemical component

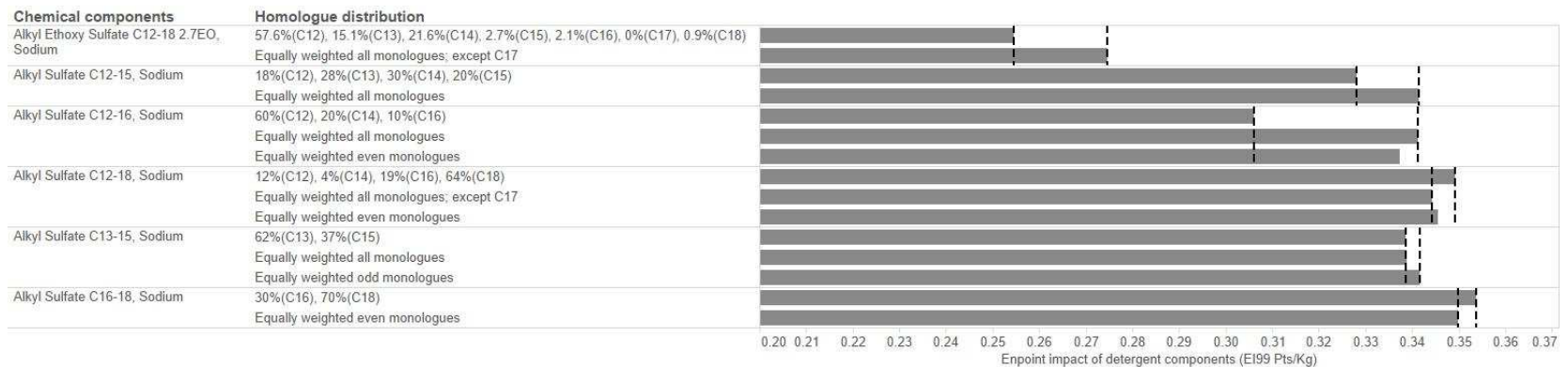
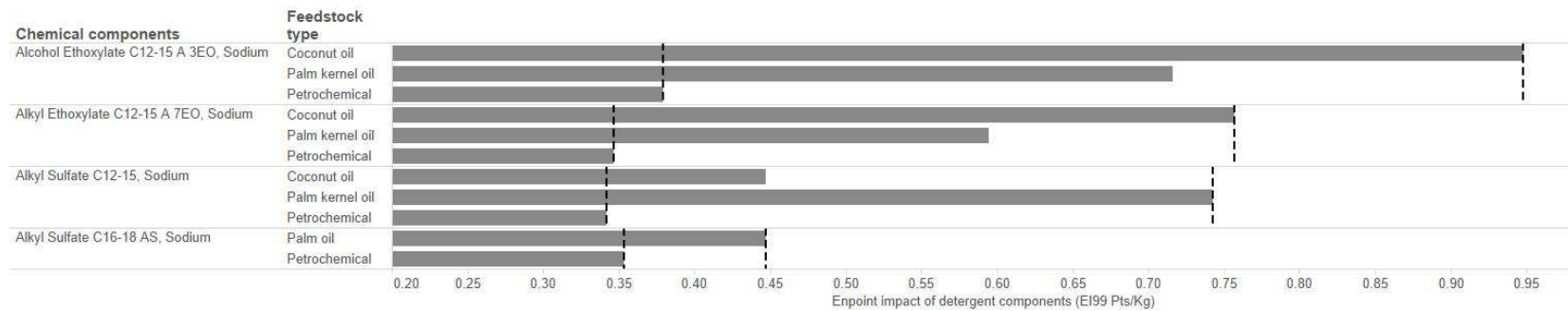


Figure C4: Endpoint impact ranges associated with various detergents components exemplifying feedstock variability. The two dash lines in each pane reflect the minimum and maximum endpoint impact values for each chemical component.



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Figure C5: Endpoint impact ranges associated with various detergents components exemplifying salt variability. The two dash lines in each pane reflect the minimum and maximum endpoint impact values for each chemical component.

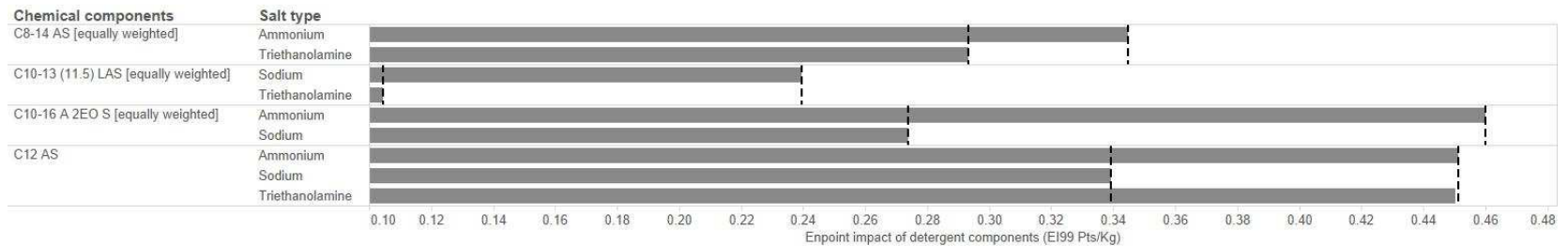
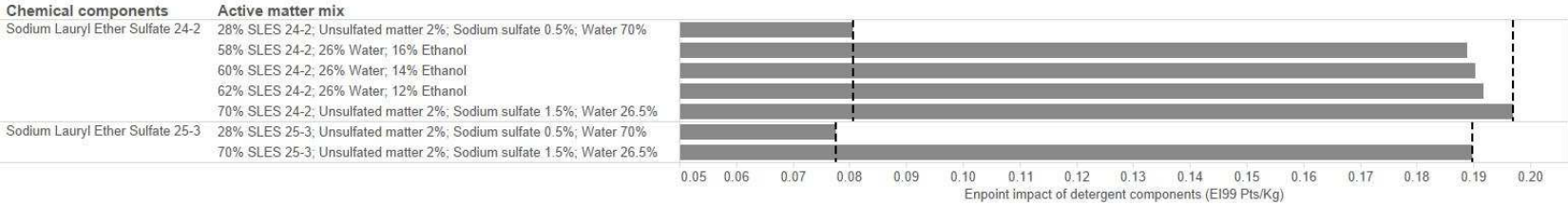


Figure C6: Endpoint impact ranges associated with various detergents components exemplifying active matter variability. The two dash lines in each pane reflect the minimum and maximum endpoint impact values for each chemical component.



## **Validity of the modeling**

Detergent formulations are highly sensitive to changes in chemical components, such that it can affect their physical and chemical stability. It is evident from formulators (Versteeg, 2012, Wolf, 2012) that a change in one chemical component in a detergent formulation, such as a surfactant, may require changes in several other detergent components to maintain stability – thereby changing the formulation from its original. For example, a change in carbon chain length (within acceptable limits) of Alcohol Ether Sulfate (AES) may increase the viscosity of the detergent, and therefore it necessitates that one or more ingredients be added to bring the viscosity back to an acceptable range, that which is determined by that brand/formulator. Therefore, a one-on-one substitution, to explore product variability may deem the formulation unstable in most cases. If a formulation is unstable, then there does not exist a possibility for it to be in the market. If it is not sold in the market, then the relevance of this research and its results is of questionable value.

In an ideal case, the exact formulation used by a brand based on the most detailed classification is tracked as it changes over time. This information provides the exact dynamics of the influence of product variability on the LCA of a detergent. There are two key reasons why the ideal case is not possible. Firstly, detergent formulations are trade secrets. Secondly, the knowledge of change in detergent ingredients has the potential to affect competition through insight into the economics of the cost and pricing, and through other factors. If the ideal case were possible, a detergent manufacturer would perform this analysis and would not publish a transparent report in order to protect trade secrets. In other words, the manufacturer will withhold key information such as formulations, ingredients, concentrations and other information. This prevents interested parties from

understanding the dynamics behind product variability. The following paragraphs shows how to chose to address this issue.

In place of exact formulations used by manufacturer, we use publicly available formulations found in publications (Flick, 1986; Flick, 1994; Ash and Ash, 1988; Davidsohn and Milwidsky, 1987; Showell, 2006). Publicly available formulations are most often not representative of formulations currently used in the market for several reasons: (1) they are formulations that were used two or three decades ago – ingredients and detergent classification have changed, and so have formulations (Bonvin, 2011), (2) they do not often provide specificity in the chemical names – Alcohol Ethoxylate is not a single chemical but a family of hundreds of chemicals with differing molecular structures and environmental impacts, (3) they often provide the function of the chemical as opposed to the chemical name – fabric whitening agents (FWA) for liquid HDL’s could cover several different chemicals, and (4) they, at times, provide ranges of the component concentration in the formulation, and so on. The implications of such non-representativeness decrease the reliability of results through LCA modeling, due to increased variability and uncertainty from assumptions. At the same time, the complexity associated with physical and chemical stability of publicly available formulations can be discounted because the formulations, as presented in the publications, may not in fact be stable based on points (2), (3) and (4). The only way to test their stability would be to actually create the formulation in a laboratory. Even if it were created, the stability requirements and ranges differ from brand to brand, based on the classifications listed in table 3. Therefore, there would be no way to know if right level of physical and chemical stability were achieved.

Based on the situation (lack of actual formulations that are currently used, lack of information on the actual frequency of change and the actual change in

ingredients, complexity with stability), we identified four ways to create a study that comprehensively captured the dynamics of product variability to produce results that could give insight . They are (1) perform one-on-one substitution and include other ingredient changes to address stability issues, (2) perform one-on-one substitution and do not address stability issues, (3) perform homologue based substitution for surfactants and do not address stability, and (4) perform substitution of one formulation with another, that fall within the same classification and price tier and assuming that they are stable. Homologue based substitution is when, C12-15 Alcohol Ethoxylate is split into C12 AE, C13 AE, C14 AE and C15 AE and substituted individually in place of the ingredient that is being substituted in the formulation.

The authors decided not pursue option 1, as stability was too complex an issue to systematically address, and that the use of publicly available formulations may not warrant addressing stability issues – reasons provided above. The authors decided to pursue option (2) to capture product variability, and option (3) to understand the dynamics of molecular structure change of an ingredient on the environmental impacts of the formulation.

In other words, based on the available resources, and the imminent need to explore and understand product variability, we chose to ignore the stability aspect of detergent until future opportunities provide more transparency into real formulations of products sold in the market and how price volatility influences its change over a period of time.

### **Methods: Data**

In preparation for this study, an extensive list of 245 chemical components used in detergents was collected from the Detergent Ingredient Database (Eskeland, 2007) and from publicly listed ingredients from detergent formulations (Henkel, 2012). The Finechem tool was used to calculate the impacts of 188 chemical



components. Assumptions used in the operation of the Finechem tool can be found in the supplemental. As previously mentioned, EI99(H/A) scores of 31 chemical components found in home-care and personal-hygiene products were sourced from Koehler and Wildbolz (2009). While Koehler and Wildbolz (2009) failed to provide the basis for Ecoindicator99 score of the chemical components, it seemed likely that they were for one-kilogram of the chemical, and so it was assumed. It must be noted that the impacts for some chemical components from Koehler and Wildbolz (2009), when compared with impacts obtained from Finechem, were off by a factor of three.

### **Methods: Datasets for the Base Case**

The base case rests on the choices made in the selection of the base formulation and the LCIA data for the chemical components, from different data sources, to calculate the environmental impact of the formulations. The base case serves as a reference point from which changes in the product formulations and its associated impacts are recorded and analyzed, using sensitivity analysis.

There are four data sources available for use in this study: Ecoinvent v2.2, Finechem Model, Koehler and Wildbolz (2009) and Novozymes (2010). The quality of data seems to follow the same order. To explain further, the data available in Ecoinvent is third-party vetted, and the Finechem model is based on Ecoinvent data and other high quality datasets (Wernet et al., 2009). On the other hand, data established by Koehler and Wildbolz (2009) and Novozymes (2010) have not been through a third party vetting process. Therefore, the priority in the choice of LCIA data for chemical components will follow the same order.

The names of some chemical components in the formulations lack sufficient specificity. For example, linear alkyl benzene sulfonate (LAS), which is given as chemical component in the premium-tier detergent, does not provide necessary

details such as its carbon chain length range. HERA (2010) identifies 10 CAS numbers for chemicals that fall under the name LAS with varying carbon chain length ranges. Similarly, Alcohol Ethoxylate (AE) is a chemical component present in the value-tier detergent, but which does not provide necessary information such as carbon chain length or the number of moles of ethoxylation. HERA (2010) indicates that potentially carbon chain length can vary between 8 and 18 and the number of moles of ethoxylation can vary from 0 to 40 for household detergent products. In such cases, a selection of carbon chain length range and/or ethoxylation degree will be based on production volume, use of such a chemical with carbon chain length range and/or ethoxylation degree in detergent manufacture, and availability of LCIA data.

All chemical components used in the base case utilized a petrochemical feedstock. This was done so because the Finechem model is limited to chemicals that are petrochemcially sourced, and that all data provided by Koehler and Wildboz (2009) are also petrochemcially sourced. Additionally, formulations with petrochemical feedstock provide a good basis for comparing with formulations that incorporate oleochemicals, as part of feedstock variability.

The CAS numbers of chemicals used in laundry detergents weren't provided. Therefore, assumptions were made based on conjectures, expert opinions, and the use of the precautionary principle.

- **Water:** The dataset "deionized water" was identified as the most appropriate dataset as opposed to "decarbonized water", "ultra-pure water", and "completely softened water", as Flick (1994) used it in the creation of several detergent formulations.
- **Fluorescent Whitening Agent (FWA):** The two types of FWA's presently used in laundry detergents are DAS-1 type and DSBP type (Stoll et al., 1997).

Given that many detergent formulations don't specify which FWA to use, we quantified the sensitivity of this detergent component on several formulations. The FWA with the highest impact was used in the base formulation,

- The typical content of DAS-1 type FWA is 0.05-0.4%
- The typical content of DSPB type FWA is 0.05-0.15%
- **Propanediol:** There are two types of propanediol: 1,2-propanediol and 1,3-propanediol. Based on the fact that the authors have not encountered 1,3-propanediol being used as a detergent ingredient, it is assumed that propanediol refers to 1,2-propanediol.
- **Enzymes:** Commonly used classes of enzymes in laundry detergents are: (1) protease, (2) cellulase, (3) lipase, (4) mannanase, and (5) amylase. The use of enzymes in detergents occurs as a mixture of two, three or four classes of enzymes. Protease, lipase, mannanase, and amylase act directly by hydrolizing and solubilizing the soils on the fabric. Cellulase acts indirectly by hydrolizing the glycosidic bonds, and is most desirable for its ability to bring more fiber smoothness by removing pills and color brightness to worn cotton fabrics. There are several products under each of these classes of enzymes produced by different manufacturers (Novozymes, 2012a, 2012b). The following are the datasets for enzymes was obtained from Novozymes in 2010.
  - Proteases:
    - Ovozyme
    - Liquinase Ultra 2.5 L
    - Liquinase Ultra 2.5 XL
  - Lipase:
    - Lipex 100T

- Amylase:
  - Termamyl 300L
- Cellulases:
  - Endo-A Glucanase
- Carezyme

### **Methods: Perfumes and Dyes**

Although perfumes and dyes don't contribute to the primary performance of the detergent, they have an important role in a detergent.

Detergents contain different levels of perfume as consumers perceive a fresh and clean smell as a key performance indicator, in general value detergent contain less perfume than mid-tier and particular premium detergents. However, laundry detergent fragrances contain easily 40+ ingredients and the composition changes frequently which makes it almost impossible to consider them in an LCA. Dyes are used for the esthetical differentiation of the different detergent brands and to mask to mostly off-white, yellow brownish base color of the detergent. The type of dyes and level used in all formulations are comparable so the impact can be calibrated for all detergents. For the reasons mentioned before perfumes and dyes were excluded from being part of the formulations

Additionally, detergents without perfumes and dyes are marketed by manufacturers as "free & clear" detergents to consumers who desire such a product and to others with allergies to perfumes and dyes. While it is not one of the goals of this study to compare the environmental impacts of the three detergent formulations, we feel it is important to explore the change in impacts of the three formulations through comparison. Therefore, it is important that the additional benefits (color and smell) offered by the detergent formulations be equivalent or

null. Lastly, LCI or LCIA data for dyes are not available, and that only one LCIA data point is available from Koehler and Wildbolz (2009) for perfumes. If perfumes and dyes were included in the formulations of all detergents, assumptions would have to be made regarding their concentration in mid-tier and premium-tier detergents. In assuming that equivalent concentrations of perfumes were used in all three formulations, their contribution to the environmental impacts of the formulation would be the same, and hence don't hold any value for potential comparisons.

### **Methods: Assumptions in the Use of Finechem Tool**

As mentioned in the article, the tool was used to estimate EI99(H/A) impacts for chemicals from DID, brochures of chemical suppliers, HERA reports, OECD reports et cetera.

Here are some assumptions that were employed when utilizing the tool:

- If the salt of any surfactant isn't mentioned, it was assumed that it was sodium salt. This assumption is based on the fact that sodium is the most common salt (HERA).

Firstly, it was difficult to interpret the chemicals provided in DID due to the following reasons:

- The full names of chemicals weren't provided. It took a while to decipher the chemical names
- Some described a family of chemicals, as opposed to a single chemical. Example: surfactants.

Other assumptions included the expansion of carbon chain length, moles of Ethoxylation, moles of propoxylation, in different chemicals so that we could better understand the impacts of those structural changes on the environmental impact. For

example, the chemical C 12/15 A, 3–12 EO refers to fatty alcohol with 3–12 moles of Ethoxylation. This was expanded to the following:

The case of multi-branched compounds further complicated our modeling efforts. The number of quaternary carbons in the chain was assumed to be the maximum number, to simplify the decision making process. In some cases, compounds were identified as predominantly linear, but lacked all other information necessary to make decisions on the molecular structure.

For the sake of consistency, the molecular weight of all chemicals were recalculated using the molecular weight calculator tool available at Lenntech (2012).

### **Methods: Uncertainty Considerations**

The Finechem tool, used to estimate LCA impacts of chemical components, did not provide an option to quantify the inherent uncertainty, but did include the uncertainty of the neural network prediction model. Given that it is a neural network based prediction model, there wasn't a straightforward process to identify options/methods to estimate parameter uncertainty, and therefore wasn't included. Chemical substances with EI99 (H/A) scores from Koehler and Wildbolz (2009) did not come with any uncertainty data. The impacts of chemical substances used in Koehler and Wildbolz (2009) came from establishing new LCI data, estimations from stoichiometric balances, using different data sources such as USEtox, HERA study, EPI suite et cetera. As with the previous case, the estimation of uncertainty for third party data that was estimated from different sources, seemed to require a new methodology, and therefore wasn't included.

SimaPro provides an option to calculate the inherent uncertainty of the Ecoinvent data using the embedded data quality indicators as factors for Monte Carlo simulation. As it was infeasible to develop a robust method to quantify inherent uncertainty for the data from Finechem and Koehler and Wildbolz (2009), it was

decided not incorporate inherent uncertainty data to theecoinvent data for the sake of preserving consistency in data quality. The use of data from different datasets was reason for some variability, and this was captured as data source uncertainty in the study. Peereboom et al. (1999) assessed the influence of LCI data from different databases, in a case study of PVC, and concluded that the LCA results changed from 10–100%. Miller et al. (2006) attempted to generate LCI data using three different database models and noted that there were significant differences due to disparities in assumptions. The quantified implications of data source uncertainty is compared with prior studies and discussed in Section 7.

Of the 339 detergent components gathered for this study, 66.67% didn't have any uncertainty data nor did they provide an option for users to calculate the uncertainty on their own.

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