

COMPARATIVE ASSESSMENT OF THE ENVIRONMENTAL FOOTPRINT OF INFANT
FORMULA PACKAGING CONTAINERS: A CRADLE-TO-GATE PLUS END-OF-LIFE
LCA USING FULL AND STREAMLINED SOFTWARE

By

Abigale Lewis

A THESIS

Submitted to
Michigan State University
in partial fulfillment of the requirements
for the degree of

Packaging – Master of Science

2023

ABSTRACT

Life cycle assessment (LCA) in the packaging industry is often centered around designing packages with the lowest environmental footprint (EF) by adjusting the design and prioritizing modeling end-of-life (EoL) scenarios. A LCA study was conducted comparing three packaging systems to deliver infant formula, including primary (plastic-package 1, composite-package 2, and steel container-package 3), secondary (corrugated box), and tertiary (pallet) packaging levels, all manufactured and distributed in North America. The goal was to inform a company of the footprint of the containers. The project involved quantifying the environmental impacts of each system, which could guide decision-making regarding which system would have the lowest EF. Additionally, it involved evaluating the effect of modeling choices and interpreting trade-offs among environmental impact for business decisions.

The functional unit was defined as the packaging needed to deliver 1,000g of infant formula from cradle-to-gate, plus the EoL. Complete modeling of the three packages and the recycling procedures was done using SimaPro 9.3.03 with TRACI 2.1 V1.06 Midpoint and ReCiPe 2016 Midpoint (H) V1.06 impact methods and compared with PackageSmart software. The LCA was conducted according to ISO 14040/14044 standards. EoL modeling included the cut-off method, 50/50 allocation, and circular footprint formula (CFF). The stochastic multi-attribute analysis (SMAA) method was implemented to evaluate trade-offs between indicators in all cases.

In both software tools, the primary container had the most significant contribution for the three systems for all categories evaluated. Adjusting the EoL models influences the results regarding the preferred packaging systems; however, contributions in each category vary slightly from the highest or lowest package footprints in all recycling models. With the cut-off EoL methodology, the highest impact was found in 4 of the 10 impact categories for Package 1, in 2 of the 10 categories for Package 2, and in the remaining 4 categories for Package 3. With 50/50 allocation and CFF EoL methodologies, different conclusions were reached about the preferred package; however, the ranking preference from SMAA across the recycling methods indicates that the plastic container is preferred, with the lowest EF with more than 50% probability.

Copyright by
ABIGALE LEWIS
2023

ACKNOWLEDGEMENTS

I would like to acknowledge and give a huge thanks to several people who made this work possible. First, thank you to Dr. Rafael Auras who provided valuable guidance, knowledge, and advice during this entire process, I cannot express enough gratitude for his help in each step of the way. I would also like to thank Dr. Anibal Bher, Dr. Matthew Daum, and Dr. Satish Joshi for participating in my guidance committee, providing further support, and providing comments to better this research. Finally, I would like to thank the team at Perrigo, for financial support of this research and allowing me to share findings and expand the initial project into my final thesis.

Additionally, I would like to share my appreciation for several of my friends and family who provided love and support throughout my entire graduate degree. To my parents and sister, Jason, Kathy, and Emily, and to my Fiancé, Patrick, I appreciate the patience, love, and guidance that allowed me to complete this work. To my various roommates and hometown friends, thank you for providing a stress-relieving outlet and for always motivating me to accomplish this work. And to the research team, particularly Anibal, Wan, Pooja, Dian, Jim, Carinna, and Dwi, thank you for all your help throughout this entire process.

Finally, a huge thank you to the entire School of Packaging community, a group I am so grateful to be a part of. This community has given me so much over the past 5 years as both an undergraduate and graduate student, and I cannot thank the faculty and fellow students I have interacted with enough for the patience, support, and encouragement I have received throughout my time here.

TABLE OF CONTENTS

LIST OF ABBREVIATIONS	vii
1.0 Introduction & Motivation	1
1.1 Research topic and problem statement	1
1.2 Research Objectives	3
REFERENCES	4
2.0 Literature Review	5
2.1 Introduction to LCA	5
2.1.1 Structure of LCA	5
2.1.2 Types of LCA	6
2.1.3 Full and Streamlined LCAs	7
2.2 Comparative LCA Studies in Packaging	7
2.2.1 Material-based comparisons	8
2.2.2 Processing and conversion-based comparisons	11
2.2.3 Design Thinking Comparisons	11
2.3 Use of LCA within the food and nutrition industry	14
2.4 Use of LCA to make informed business decisions	15
REFERENCES	18
3.0 Assessing environmental trade-offs in packaging systems for infant formula delivery. A cradle-to-gate plus end-of-life LCA	20
3.1 Abstract	20
3.2 Introduction	21
3.3 Materials and Methods	24
3.3.1 Goal definition	24
3.3.2 Scope definition	24
3.3.2.1 System boundaries	25
3.3.3 Functional unit and reference flows	27
3.3.4 End-of-life modeling	28
3.3.5 Life cycle inventory	29
3.3.6 Life cycle impact assessment	30
3.3.7 Assumptions and limitations	31
3.3.8 Data quality assessment	32
3.3.9 Life cycle interpretation	32
3.4 Results and Discussion	35
3.4.1 Contribution analysis	35
3.4.2 Comparative analysis	37
3.4.3 Scenario analysis	40
3.4.4 Biogenic carbon	42
3.4.5 Sensitivity analysis	42
3.4.6 Discernability analysis	47
3.4.7 Stochastic multi-attribute analysis	47
3.4.8 Keeping it in perspective	49
3.5 Conclusions, limitations, and recommendations	50
3.6 Supporting Information	55
3.6.1 Life Cycle Inventory	55

3.6.2 Life Cycle Impact Assessment	85
3.6.3 Life Cycle Interpretation	94
3.6.4 LCA Results	103
REFERENCES	108
4.0 Comparing LCA Software.....	112
4.1 Software Overview	113
4.2 Methods and Modeling.....	113
4.2.1 Streamline LCA modeling, assumptions, and end-of-life	114
4.2.2 Notable Differences between the two models	121
4.2.3 Comparison of Results	122
4.3 Results and Discussion	122
4.3.1 Contribution Analysis.....	122
4.3.2 Comparative Analysis	130
4.3.3 Scenario Analysis	133
4.4 Conclusions	137
REFERENCES	140
5.0 Conclusion and Recommendations for Future Work	141
5.1 Recommendations for Future Work	144

LIST OF ABBREVIATIONS

CFF	Circular Footprint Formula
EF	Environmental Footprint
EoL	End of Life
GWP	Global Warming Potential
HDPE	High Density Polyethylene
IPCC	Intergovernmental Panel on Climate Change
LCA	Life Cycle Assessment
LCI	Life Cycle Inventory
LCIA	Life Cycle Impact Assessment
LLDPE	Linear Low-Density Polyethylene
PP	Polypropylene
SMAA	Stochastic Multi-Attribute Analysis
TRACI	Tool for Reduction and Assessment of Chemicals and other Environmental Impacts

1.0 Introduction & Motivation

As environmental issues come forward in many of today's discussion topics, understanding the impact of various products, services, and ways of life has become extremely important. Many of the world's environmental problems come from the overconsumption of products, such as clothing or services such as media streaming. Our advanced society has developed a taste for constantly consuming products and services that all individually contribute to the environmental issues faced by the world population today. One sector frequently looked at when it comes to environmental impacts is the food industry. The United States is reported to have one of the highest per capita consumptions in the world, and the projected household spend on food is expected to reach \$1.1 Trillion in 2023 [1]. The large amount of food being purchased and consumed in the U.S. has an enormous environmental impact. One study from 2018 found that U.S. households generated 899 billion kg CO₂-eq from food spending in 2013, a number that has been thought to increase each year [2]. This environmental impact is equivalent to 174,922,532 U.S. homes' electricity use for an entire year [3].

With all the consumption of food in the U.S. and worldwide, much attention has been given to the packaging industry, as almost every food purchased today has some direct or indirect associated packaging. The packaging industry has been blamed for a lot of unnecessary environmental impact, which is now being quantified and sought to improve in many research areas. One way the environmental impact of food packaging is assessed is through Life Cycle Assessment (LCA). This methodology translates the inputs and outputs of making a product or using a process into a quantifiable measure of the environmental impact. LCA is also a methodology widely used by many business sectors and can be universally understood by various stakeholders, helping translate the environmental impact of products or processes into familiar terms for those interested.

1.1 Research topic and problem statement

The research presented in this thesis involves using LCA to compare the environmental footprint of three rigid package systems for delivery of infant formula. LCA is an internationally used methodology that can quantify the environmental effects of products, services, manufacturing techniques, or any other process. The ISO 14040 and 14044 standards outline proper ways in which to perform LCA studies, which allows the results from any study following the standards to be easily understood by the research community and add to the general

knowledge of the environmental impacts of various products and services [4, 5]. **Figure 1. 1** shows a schematic of the steps in performing an LCA study.

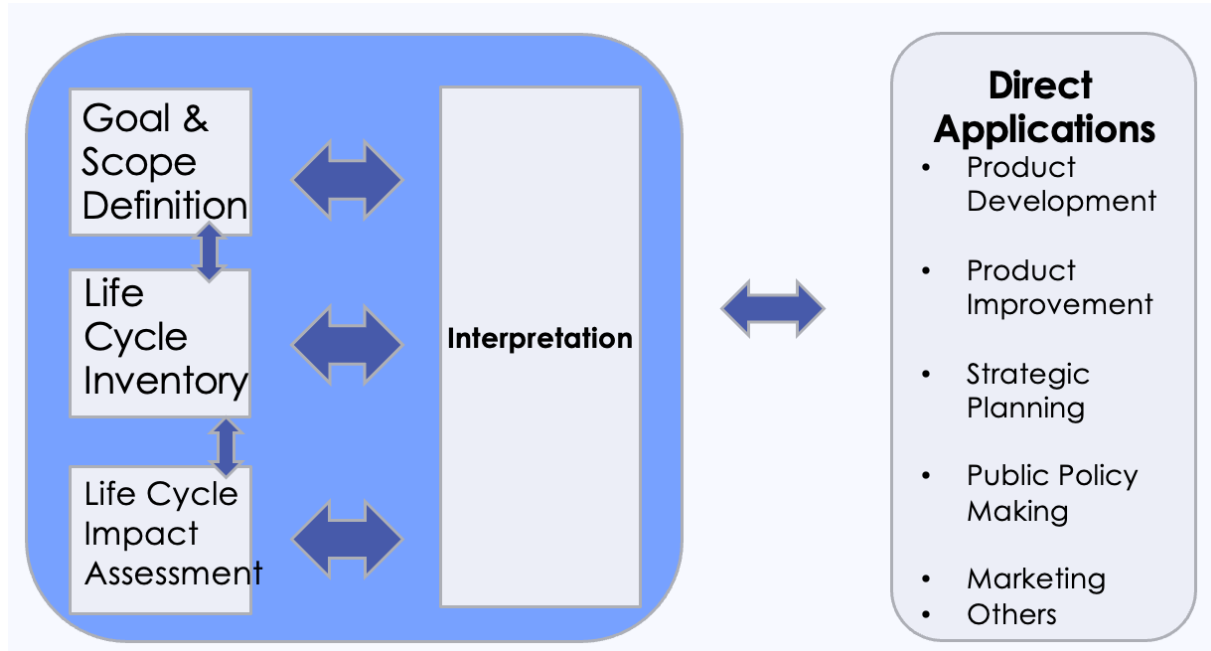


Figure 1. 1: Schematic describing the steps involved in LCA as well as possible applications for the results of the studies.

Although LCA is an iterative process, the first step is defining the goal and scope of the study, including the boundaries to be followed, the purpose of the study and the intended use of the results. From there, the Life Cycle Inventory (LCI) is done, which involves compiling information on the studied product or process, including all the inputs and outputs of the system. The Life Cycle Impact Assessment (LCIA) is then done using a particular methodology such as the Tool for Reduction and Assessment of Chemicals and other Environmental Impacts (TRACI) or ReCiPe. It takes all the inputs and outputs from the LCI and quantifies them in the methodology's impact categories. From there, the results can be interpreted and used for their previously specified purpose, such as informing decision-makers or implementing policies. In the packaging industry, LCA can quantify impacts associated with a specific package design, material, or overall packaging system for delivering a product.

The packaging industry often looks at lowering their packaging environmental footprint (EF), and LCA studies can inform businesses and packaging stakeholders of better packaging

options and to understand the EF ratio between product and packaging. As the use of LCA studies within the packaging industry increases, the availability of already published results can greatly benefit various interested parties in informing their decision-making without performing a study, which often involve large budgets and extended timelines.

Although many business sectors and stakeholders widely use and understand the LCA methodology, gaps in knowledge of how results may differ between studies still exist. Each LCA study differs in many aspects, including the system boundaries, modeling choices and assumptions, data sources, and many other factors that ultimately influence the final results. These choices made by LCA practitioners have unknown effects on results; therefore, each LCA can only be considered valid after considering all factors included in the study. One way these choices can be evaluated is by comparing these choices within the same LCA study and investigating how results change when changing specific inputs, boundaries, or modeling choices. For instance, how can LCA results differ when altering how a product's End-of-Life (EoL) is modeled?

1.2 Research Objectives

The main objective of the research presented in this thesis is to use LCA methodology to evaluate the EF of three infant formula package systems from cradle-to-gate plus EoL. Additionally, this research addresses how choices in modeling when performing LCA in the packaging industry can influence the comparative results of a study, particularly the EoL model and LCA software. Three different EoL models are compared using the same full LCA and results are evaluated using SMAA methodology, which assigns ranking preference to each package within all three methodologies, allowing for direct comparisons in results between the models. This research includes evaluating the abilities of a streamlined and full LCA software commercially available for business use. The results from each software can be compared to each other when using the same LCA parameters, such as assumptions and system boundaries. This LCA study follows ISO standards and can therefore add to the portfolio of already existing LCA results of consumer product goods and packaging materials.

The thesis contains a literature review of existing LCA studies and their relevance to the packaging industry. From there, a study covering a full LCA of infant formula containers and various EoL modeling methods is discussed. The comparison between the results of the full LCA and the streamlined LCA follows. Final conclusions and future recommendations are provided.

REFERENCES

- [1] Fitch Solutions, “United States Food & Drink Report,” 2023.
- [2] R. Boehm, P. E. Wilde, M. Ver Ploeg, C. Costello, and S. B. Cash, “A Comprehensive Life Cycle Assessment of Greenhouse Gas Emissions from U.S. Household Food Choices,” *Food Policy*, vol. 79, pp. 67–76, Aug. 2018, doi: 10.1016/j.foodpol.2018.05.004.
- [3] United States Environmental Protection Agency, “Greenhouse Gas Equivalencies Calculator.” Accessed: Aug. 21, 2023. [Online]. Available: <https://www.epa.gov/energy/greenhouse-gas-equivalencies-calculator>
- [4] “ISO14044 - 2006: Environmental management - Life cycle assessment - Requirements and guidelines”.
- [5] “ISO14040 - 2006: Environmental management - Life cycle assessment - Principles and framework”.

2.0 Literature Review

2.1 Introduction to LCA

With consumer and business focus shifting to environmental concerns, the packaging industry is specifically vulnerable for taking the blame due to the seemingly large impact on the environment. Therefore, tools and studies are needed to explore the actual impacts of packaging systems. Over the past several years, LCA has been used in various industries and further developed by international organizations as one tool to evaluate, analyze, and explain the environmental effects of different systems, goods, or services. LCA is outlined by ISO Standards 14040 and 14044, which gives general guidance on performing LCA studies and the interpretation to create a sense of uniformity in an area with many opportunities for variation [1, 2]. Utilizing LCA is becoming more common in many business sectors, especially as sustainability goals are being prioritized across the globe. The packaging industry has recently been under the microscope for the environmental impacts of common packaging designs, such as single-use plastics or multilayer materials that are difficult to recycle. LCA has been a handy tool for evaluating the environmental impacts of these types of designs and potentially justifying the continued use of these materials over other alternatives.

2.1.1 Structure of LCA

Figure 1. 1 shows an outline of the steps to conduct an LCA. The first step in LCA is to define the studies' goal and scope. The goal includes details such as the intended audience, the type of study (e.g., attributional or consequential, Types A, B, C), and the goal statement itself. The scope is much more in-depth and truly defines and illustrates the way in which the LCA study is intended to be performed. This includes a complete description of the system being studied and researched, the system boundaries, the definition and explanation of the functional unit, the allocation and cut-off procedures (pertaining to EoL modeling), the temporal and geographical boundaries, the specified technological coverage, the sophistication of the study, and the formatting of the finished work. The scope is essentially the detailed plan of how the LCA will be performed and should be written out prior to any work on the study being performed. As demonstrated **Figure 1. 1**, the goal and scope are subject to change if during the performance of the study the original scope is ill fitting or can no longer be followed. This change should be explained and made during the iteration process of the study.

The Life Cycle Inventory (LCI) portion of LCA studies is the portion involving all data collection for the system to be modeled. For packaging, this means collecting any data relevant to raw material acquisition, processing and conversion, transportation, and end-of-life data. The collection of the inputs and outputs of the system should pertain directly to the already defined system boundaries. The Life Cycle Inventory Assessment (LCIA) portion of the LCA studies is the portion that translates the inputs and outputs collected and modeled in the LCI portion into environmental categories. This is the portion that quantifies the data for the system into the selected environmental indicators and gives a numerical value that can be compared across other systems with the same unit. Finally, the Interpretation section of LCA studies involves drawing final conclusions about the system. These can be relating to which impact categories the studied system has the most influence in or how the studied system compares to other similar systems.

As demonstrated by the arrows between each section of the study, an LCA is designed to be an iterative process, which means that when conducting an LCA, a practitioner can go back and forth between each of the four steps. For instance, the goal and scope have been written and the LCI has begun, the practitioners are able to look at the data and what can start to be interpreted from the data and tweak the goal and scope if they see fit.

2.1.2 Types of LCA

As mentioned above, several different types of LCA studies are widely found today, varying in size and decision-making value. The two main categories of LCA include Attributional or Consequential. Attributional studies involve attributing the inputs and outputs to a functional unit, ignoring any outside factors of connections such as economics or social factors. These studies model any system as it is or was and usually utilize average data available. Consequential studies, on the other hand, involve studying a system's future impacts with any possible changes. Consequential-type LCA studies are typically used for decision support but are based on hypothetical models. LCA can also be broken down by size and usage of the study. These include “Situation A” studies, which are used for micro-level decision making, “Situation B” studies, which are used for meso or macro-level decision making, and “Situation C” studies that are not used for decision making but are rather more of an accounting study that may or may not involve other systems [3].

2.1.3 Full and Streamlined LCAs

Several different available software tools are available to perform LCA studies, which can then easily be translated to easy-to-digest results. These software tools are used for either streamlined or full LCA. A streamlined LCA is a relatively fast study with little detail, resulting in interpretations needing more support and detailed evidence. Benefits to utilizing streamlined LCA include that they are relatively simple to use with little information about the studied systems, still have the capability to compare EF results making it ideal when professionals outside the studied area need LCA results. Examples of various software tools available to perform streamlined LCA for the packaging industry specifically are PackageSmart from EarthShift Global, EcoIMPACT COMPASS from TRAYAK, and PIQUET from LIFECYCLES. Software tools are often derived from a full LCA software and are not considered to be fully ISO compliant. A full LCA study, on the other hand, is a much more involved process that requires more time, data, and detailed inputs to reach a reliable conclusion. Benefits of performing full LCA studies include that there is much more detail involved in the results and the main drivers of the results can be seen so the LCA practitioners can reach conclusions on why the environmental impacts are being quantified the way they are. In Full LCA studies, the inputs and outputs of the system are much more detailed and can be manipulated by the practitioner in almost every aspect, making the results much more robust, accurate, and able to answer specific questions that are wished to be answered. Streamlined LCA studies are often limited in these aspects, as input and output data is not easily manipulated and analysis capabilities are therefore restricted. Full LCA software includes SimaPro from Pré Sustainability, LifeCycle for Experts from Sphera®, and Umberto from iPoint, all software that are internationally recognized, fully ISO compliant, and used in most comparative studies.

Although both types of LCA software can provide decision making support and assist interested stakeholders in understanding a system's environmental impacts, many factors may influence which type of software to use. These factors include price, allotted time, availability of input and output data, and required amount of detail.

2.2 Comparative LCA Studies in Packaging

LCA studies can inform several business decisions or industry-wide trends, especially when the LCA is done in a comparative nature. Many studies done within the packaging industry, for instance, are to investigate the environmental impact of one package design

compared to another. These types of studies are typically done with packages that differ from each other slightly, such as with materials, processing techniques, amount of product in the package, and many other packaging-related decisions that packaging professionals make frequently in the design process. This section contains several examples of comparative life cycle assessments.

2.2.1 Material-based comparisons

Decisions on which materials will be used in packaging scenarios are usually based on the product to be packaged, such as fragile items or foods sensitive to oxygen. Other factors, especially those related to the sustainability of materials, are recently being considered more often; however, this is largely due to the influx of material based comparative LCA studies used to inform the general community of impacts associated with packaging materials. Studies like those mentioned below can be extremely helpful to companies looking to meet sustainability goals in a simple way such as shifting from one material to another. Because these studies directly compare the environmental impact of materials in the same application, other interested parties can use the LCA results to inform their own similar decisions, as long as study decisions and limitations are understood.

For example, Kliugaite and Staniskis performed and published an LCA study in 2013. The study compared three different multilayered flexible plastic materials and examined their impacts on the environment to provide evidence for packaging materials having lower impacts for most food products that they would be packaging. Type I was a multilayer of PET+AIOx, Paint, Adhesive, and LDPE. Type II was a PET, Paint, Adhesive, and PE-EVOH-PE. And Type III was a PET+PVOH, Paint Adhesive, and LDPE multilayer. All three types had equal thicknesses and a functional unit of 1 square meter. Although the study did not include food production, filling or consumption, one of the study's goals was to evaluate the overall impact of the packaging, which could then translate into another study to help prove the food product's higher effect on the environmental impacts. The study's findings included that the Type II package had the lowest impact due to the higher barrier properties. The study also found that the contribution of gas barrier materials to packaging is not significant enough in the production and raw material acquisition phases of the life cycle impacts to deter a packaging engineer from choosing other materials to lower environmental footprint [4].

A study published by Franklin Associates in April of 2018 is another example of comparing packaging materials; however, this study was completed on a much larger scale. Their study consisted of an LCA on plastic packaging in the U.S. and Canada. Substitution analysis was done during this study to answer the question: “If plastic packaging were replaced with alternative types of packaging, how would environmental impacts be affected?”. Essentially this LCA first was done on the major plastic resins used in the U.S. and Canadian packaging industries and then substitution or replacement was done using ratios and various functional units to compare the effect that an equivalent non-plastic package would have on the environment. The results from this LCA study provide evidence that plastic packaging is overall less impactful on the environment when compared to a direct equivalent package of a different material such as glass, metal, or paper. The reported average ratio of the weight of packaging comes out to about 4.4 million kg of other materials compared to 1 million kg of plastic packaging. The Global Warming Potential (GWP) indicated that when using plastic packaging instead of other packaging alternatives, 39.5 million metric tons of CO₂-eq was saved in a conservative scenario. Interpretation of the full study leads to the assertion that when looking across all plastic packaging categories, the use of any feasible substitute packaging formats results in much higher environmental impact across the studies impact categories. This study shows the capabilities of an LCA to analyze a specific material in a larger scale while also including some sort of scenario analysis [5].

Ferrara and De Feo published a comparative LCA that focused on five different packaging formats for Italian wines. This study aimed to question one of the recent packaging trends that is being driven by consumers, which is the push for using glass rather than plastic when possible. Consumers have a very negative perception of plastic as the concern regarding marine pollution and microplastics continue to make headlines, influencing many companies to start using other materials, including glass, in cases such as wine. The LCA evaluated the following packages for delivering wine to the consumer: an aseptic carton, a bag-in-box, a single-use glass bottle, a refillable glass bottle, and a multilayer PET bottle. Variations of three parameters were also included in the study, including the weight of the primary package containers, the distance of distribution, and the disposal scenario. The results of the study showed that the single-use glass bottle was the worst packaging format, closely followed by the multilayer PET bottle, which indicates that consumer perceptions may have been wrong about

the hunch that glass bottles had a lower environmental effect than plastic but also somewhat correct in the negative effect that plastic has in some situations. The bag-in-box had the lowest impact, presumably because of the low packaging weight and greater palletizing efficiency. The aseptic carton and refillable glass bottle had the second and third lowest impact in most of the impact categories. In terms of the variation scenarios, the change in weight of the primary container had little effect on the overall impacts of the system; however, the distribution distance did show opportunities for improvement, especially in the refillable glass bottle package. The disposal scenario variation had the largest effect on the environmental impacts, most prominent in the single-use glass bottle and PET bottle cases, as those packages are easily used again as post-consumer material. Consumer behavior was inherently studied in this variation as it demonstrated the consumer has an influence on the impact, as recycling rates can change the End-of-Life impact, changing the overall impact of the system [6].

Finally, a study published by Kang et al. in 2013 compares bacon packaging with different materials and, in turn, a weight reduction of the overall packaging. The first of the two packages is a traditional bacon package containing polyethylene and wax-coated paper board. The second is a new board consisting of reverse-printed oriented polypropylene (OPP) and expanded polystyrene (EPS) with an adhesive. The OPP/EPS board is lower in weight but maintains the same dimensions and is compatible with the functional unit chosen by the practitioners of the LCA. This LCA divided the systems into material production, intermediate processes, transportation, and disposal phases. The study found significant differences between the two packaging systems, such as the differing amounts of board material used (weight reduction) and the type of materials, which make the most significant difference in the global warming and eutrophication impact categories. Results from this LCA did not prove either package to be the most environmentally friendly, as the weight reduction of the new package lowered the footprint; however, the choice of materials of that new package had a higher environmental footprint. This emphasizes the importance of package design and how it can influence the impact a package or particular components of a package have. It is also essential to learn that LCA does not produce a specific answer as to which package is the “best” or least harmful to the environment. It is instead a tool that should be used to influence decisions and examine how a packaging system impacts its surroundings based on several different categories, such as emissions and water pollution [7].

2.2.2 Processing and conversion-based comparisons

Much like comparisons in packaging systems based on materials, comparisons about the effects of processing types on a package's overall impact can be made. Although LCA studies on manufacturing techniques are typically done in an accounting fashion, comparing processes directly within the guidelines of LCA may prove to be extremely useful in package design, as if one technique is known to have higher impacts than another feasible alternative, going with the latter alternative might be chosen if sustainability goals are to be met.

Packaging processes, specifically printing and plastic manufacturing, can be examined closely using LCA. He et. al. published a study comparing two different lamination processes to find opportunities to lessen the environmental impact caused by the process. The two processes in the LCA were solventless lamination, which involves a solventless adhesive and special composite equipment to bond the plastic substrates. Dry lamination is very similar to solventless lamination but includes using a drying tunnel after applying adhesive. Results found that solventless lamination was a more novel and cleaner process than traditional dry lamination for producing the same amount of flexible plastic packaging material [8].

As addressed earlier in this review, printing within the packaging industry and like processes, in general, are no exception to comparative LCA studies. Steve Barr, a Dupont employee, updated a 2008 study in 2021 that compared the impacts of flexographic printing and gravure printing. Updates continued to show that flexographic printing still has a lower environmental impact than gravure printing. Ink used in various ways is also something that LCA studies have been able to focus on [9].

A study published in 2000 and written by Tolle et. al. evaluated the impact of soy-based inks used for lithographic printing using a streamlined LCA. The study devised recommendations to lessen the impact of bio-based ink, such as shifting the ink formula by reducing the quantity of some ingredients that drive the amount of CO₂ released when the ink is in the landfill [10].

2.2.3 Design Thinking Comparisons

LCA is also used to evaluate various packaging inputs such as consumer perceptions, overarching trends, or the product and package size. Extensive studies can be performed to compare designed-based packaging decisions, which may also involve scenario analysis. Scenario analysis allows LCA practitioners to investigate possible changes in overall results

based on a hypothetical change in the system, in packaging cases, this could be lightweighting of any component, adjusting the serving size delivered to the consumer by the package, or streamlining the design in other ways. Examples of LCA studies that utilize comparisons based on packaging designs and/or scenario analysis are below.

Packaging companies and industry stakeholders have also been using LCA to evaluate the impacts of various trends such as e-commerce, reusability, and recyclability. For instance, Su et. al. studied the effects of increased demand for express delivery or e-commerce in China. This trend inherently increases the overall number of specific types of packaging being used across the world; this includes the amount of corrugated board, tape, mailing envelopes, cushioning materials, and various other types of plastic and paper packaging. Practitioners of the LCA used surveys to determine which packaging would be specifically studied and for developing scenarios to analyze, including the change in average per parcel weight or material reduction as well as a reduction in overall use of express delivery e-commerce purchases over the next 10 years. The study did find that the increase in e-commerce has led to an increase in environmental impact; however, it found that most of that increase comes from the raw material phase. Scenario analysis suggested the overall reduction of e-commerce and express delivery with possible government implementation and guidance, which is hypothesized to reduce impact by approximately 10%. This study highlights the possibilities of LCA to influence and analyze different types of packaging industry trends [11].

Gatt and Refalo performed and published an LCA study focusing on the reusability and recyclability of a plastic cosmetic product in 2022. The LCA had alternative scenarios involving varied recyclability rates of the plastic compact and varied levels of reusability of the plastic compact. The assessment results found that the aluminum pan had the largest impact within the cosmetic compact design, with the much larger and heavier plastic lid being the second largest in most impact categories. This study compared scenario-specific results directly to examine how the package's design and inherent recyclability and reusability changed the overall environmental impact. In the overall results of the study, it was reported that the reusability of the package has a positive effect on the impacts, meaning reusability can lower environmental impact. It was also found that adding any amount of recycled content to a package version that is already reusable has no added effect on the impacts generated by the system. The main takeaway is the positive outlook on reusability, when possible, in package design, with recyclable packaging also having

a positive impact when reusability is off the table. This was another study that incorporated packaging design and how design can alter the environmental effects of a package [12].

An LCA can also be performed to evaluate specific components often used in product packaging systems. A literature review was published by Deviatkin et. al. in 2019 that compiled all the LCI data and conclusions from 16 different studies involving pallets used in the distribution of various materials, types, and sizes. Cumulatively, the literature review analyzed 43 different pallet-based LCA's due to comparative studies that focused on the amount of reuse of a pallet, whether the pallet was wood or plastic, or the overall size and, therefore, the efficiency of the pallet in distributing large quantities of product. The literature review was able to make overarching conclusions and spark discussion on the ideal pallet and what impact categories have proven to be the most relevant in the impact of pallets on packaging systems. Conclusions of the literature review were also presented in a way that suggested ways that future LCA of pallets can be most efficient, such as a recommendation for the functional unit to be the number of trips through the supply chain rather than other functional units to make LCA studies more uniform. It also pointed out that the plastic pallets have much less variation in data, which is most likely because fewer LCAs have been performed specifically analyzing the environmental footprint of plastic pallets and they are less widely used [13].

A large-scale comparative LCA study was conducted by Thoma et. al and published in 2012. This study focused on the United States Dairy industry and specifically, the various packaging options available for milk. The different packaging types varied by in-home versus on-the-go consumption, chilled versus ambient temperature storage, amount of milk delivered to the consumer, and the packaging material, such as different plastic resins or paperboard. The functional unit of the study was the consumption of 8 oz of milk by the consumer, and the system boundaries varied as part of the study aimed to analyze the impacts of the systems from gate-to-grave (thus excluding the milk production), and another part analyzed from cradle-to-grave including all milk and packaging production. One unique characteristic of this study is that it includes the consumption phase of the product, something that is rather difficult to model, which is why it is often left out of most LCAs. Essentially, the consumption phase is modeled in terms of milk wasted by the consumer but includes car transportation, electricity for storage, dishwashing and water use, municipal wastewater treatment, and actual food waste of milk. The study utilized tables and figures in the LCIA and interpretation phases of the study while also

separating the results into four categories: the HDPE systems, the LDPE systems, the PET systems, and the Paperboard systems. Of the many results of this study, the two that the authors emphasize include that in the cradle-to-grave scenario, the milk product and, in particular, the production of the milk is by far the major contributor to the system's environmental impact in nearly each category. In the farm gate-to-grave scenario both the container stage and the processing plant stage can vary tremendously on their contributions, based on the size and material of the package itself. Both stages however definitely contribute the most to climate change, non-renewable fossil energy, toxicity, photochemical oxidant formation, and ecosystems impact categories. The primary recommendation that the study came up with was to reduce the material use and packaging weight of all milk containers in general. In addition, it would be beneficial for milk processors to reduce overall water consumption and improve practices for sewer discharge. Although this LCA was on a much larger scale than most of the other assessments discussed in this review, it shows many similarities in the way it was conducted and how conclusions and recommendations are brought up [14].

2.3 Use of LCA within the food and nutrition industry

Food packaging has been a focal point for many LCA studies, as it is seen as a necessity by many. The sheer amount of food and nutrition products that are made, packaged, and sold throughout the U.S. and other similar countries has been evaluated in a negative tone. LCA can be used to evaluate the environmental impact associated with this industry. For instance, Wikstrom et. al. used LCA to investigate the environmental effects on food waste, a huge issue being addressed by many company sustainability goals globally. This study was centered on a packaging specific LCA that was then altered to include waste of rice and yogurt products and how that wasted product factors into the overall impact of the entire system. Results found that including food waste in the analysis dramatically increased and altered the study's overall results in most impact categories [15].

Specifically, the infant formula and baby food market in the US reached a value of \$48.5 Billion in 2022, despite shortages of infant formula across the nation due to significant plant shutdowns after repeated foodborne illness outbreaks [16, 17] The market for infant formula alone is projected to grow from \$2.5 Billion in 2018 to roughly \$5 Billion by 2026, due to the population increase trends [18]. Major players in the infant formula market include Abbott Nutrition, Nestle, Danone, Mead Johnson, and Kraft, along with private label infant formula, that

primarily comes from Perrigo [19]. Like any product, infant formula manufacturing and distribution produced at such high-volume result in large environmental impacts, which was estimated using LCA in 2020 to be roughly 650,000 Tons of kg CO₂-eq for the United States alone [18].

The packaging involved in containing and selling food and nutrition products, including powdered infant formula, has the potential to greatly impact such a large market. Several packaging materials commonly found in this industry, such as plastic and paperboard, can easily be compared using LCA to quantify the environmental impacts of the package design, as discussed above. This methodology has the potential to reduce the environmental impacts of the packaging sector, considering the food and nutrition industry is so large and will in fact, be growing due to population increases. The plausible result of the growing need for food packages is an overall increase in the industry's environmental footprint, the opposite of the goals of many companies, so LCA may be the right tool to guide decision-making regarding package design.

2.4 Use of LCA to make informed business decisions.

As outlined in **Figure 1. 1**, the interpretation of LCA results can be used for several purposes, such as informing R&D in product development, public policy makers, or consumers concerned with environmental impacts. In the packaging industry, LCA is usually used to inform decision-makers of the impacts of package designs to assist in reaching sustainability goals. A simple example would be comparing the impact of a 50-gram PET bottle and a 50-gram steel can to package soda. The results of an LCA would compare the PET bottle and the steel can when looking at the global warming category. Suppose the company aimed to lower its impact on global warming. In that case, they may use the results of the LCA study to provide evidence to switch all soda packaging to use either PET bottles or steel cans in their packaging department. This, however, is a straightforward case, many companies are instead using LCA to evaluate the effects of several scenarios.

Bassani et al. advocated for the utilization of LCA in informing eco-design in packaging decision-making. The study incorporated LCA as a step in three different scenarios (referred to as strategies within the article) regarding the design of pharmaceutical packaging in terms of environmental footprint and how it was used to provide recommendations and justify future decisions when designing or redesigning the packaging of pharmaceuticals. Strategy 1 was the comparison of packaging formats before and after some weight or volume reduction. Strategy 2

was the comparison of pack formats, such as blister packs vs a bottle vs a sachet for storing the same pharmaceutical product. Finally, Strategy 3 was the comparison of transportation modes such as truck, train, airplane, ship, and commercial vehicles that are either diesel or electric-powered. An LCA was conducted in each strategy, and the impact assessment was used to inform recommendations on which of the compared packaging was more environmentally friendly. The first strategy found that reducing the weight or overall volume of the packaging could reduce the impacts for all categories by almost two times. Findings for strategy 2 were similar, finding that the blister package had the lowest impacts due to the higher volume utilization and less material production compared to the bottle packaging and the larger sachet packaging. Strategy 3 found that train transportation had lower impacts in most impact categories, and the airplane had the highest in all but one category. It was also found that electric vehicles had a lower impact in most categories if the transportation distance was less than 300 km. Recommendations based on these findings can be summed up by stating that packaging design with smaller dimensions and lower weight can improve the performance of the studied pharmaceutical packaging. It is also recommended by the study that the transportation mode selected should ideally be the most optimized cargo spacing and smallest transport based on where production and distribution centers are located. This study showcases the use of LCA in informing design decisions and how LCA can be incorporated into larger studies and not just a stand-alone piece in the analysis of packaging environmental footprint [20].

Finally, Kim and Park compared three different liquid laundry detergent packaging formats. The study used LCA to examine the footprints of the traditional HDPE pour bottle laundry detergent and two different packaging formats for liquid detergent that come in pod form: a rigid PET container and a multilayer flexible stand-up pouch. Excluded processes included the production, package filling, and use stages of the liquid detergent itself, again leaving only the packaging production, processing, distribution, and end-of-life phases. The study results showed that the traditional HDPE pour bottle had the lowest environmental impact in all categories except ecotoxicity. The remaining two systems with the detergent pods had higher impacts due to the PVA film needed to form the pods. Out of these two systems, the rigid PET container had the highest impact compared to the multi-layer flexible pouch in most impact categories because of its lighter weight, smaller volume, and less energy processing techniques. Results and conclusions from this LCA demonstrate that consumer perceptions of convenience

and environmental footprint sometimes differ from reality in terms of a package's environmental impacts. Consumers enjoy the convenience of the small pouches of liquid detergent as they are easy to use and provide the exact amount of detergent needed without worrying about spilling or wasting product while ensuring a proper clean. Unfortunately, the pods result in a higher environmental footprint than the bottle, requiring consumers to pour the correct amount of detergent [21]. This begs the question, if consumers understood that the more popular, convenient pod package design automatically resulted in higher environmental impacts, would they continue to purchase that product over the traditional package?

The studies mentioned above show that LCA can be a handy tool in evaluating the environmental impact of packaging materials, processes, and designs in the packaging industry. Like any methodology, however, improvements in accuracy and relevancy can always be made, which is something further research in the field can improve greatly. As mentioned in the Introduction, understanding how the results of LCA are impacted by various choices in modeling, such as EoL modeling or software being used to model, can enhance the use of LCA in all industries and increase the breadth of research relevant to packaging.

REFERENCES

- [1] “ISO14044 - 2006: Environmental management - Life cycle assessment - Requirements and guidelines”.
- [2] “ISO14040 - 2006: Environmental management - Life cycle assessment - Principles and framework”.
- [3] R. A. Auras and S. E. M. Selke, “Life Cycle Assessment,” in *Life Cycle of Sustainable Packaging: From Design to End-of-Life*, First., R. Auras and S. Selke, Eds., Hoboken, New Jersey: John Wiley & Sons, Inc., 2023 , 2022, pp. 179–215.
- [4] D. Kliagaitė and J. K. Staniškis, “Comparative Life Cycle Assessment of High Barrier Polymer for Selecting Resource Efficient and Environmentally Low-Impact Materials,” *International Journal of Environmental and Ecological Engineering*, vol. 7, no. 11, 2013, doi: doi.org/10.5281/zenodo.1088816.
- [5] Franklin Associates, “Life Cycle Impacts of Plastic Packaging Compared to Substitutes in the United States and Canada. Theoretical Substitution Analysis,” 2018.
- [6] C. Ferrara and G. De Feo, “Comparative life cycle assessment of alternative systems for wine packaging in Italy,” *J Clean Prod*, vol. 259, p. 120888, Jun. 2020, doi: 10.1016/j.jclepro.2020.120888.
- [7] D. Kang, N. Sgriccia, S. Selke, and R. Auras, “Comparison of bacon packaging on a life cycle basis: a case study,” *J Clean Prod*, vol. 54, pp. 142–149, Sep. 2013, doi: 10.1016/j.jclepro.2013.05.008.
- [8] H. He *et al.*, “Applied properties and life cycle assessment of flexible packaging lamination processes: a comparative study,” *Int J Life Cycle Assess*, vol. 26, no. 3, pp. 561–574, Mar. 2021, doi: 10.1007/s11367-021-01883-4.
- [9] S. Barr, “Life Cycle Assessment Flexographic Printing and Platemaking Update,” 2021.
- [10] D. A. Tolle, D. P. Evers, B. W. Vigon, and J. J. Sheehan, “Streamlined LCA of Soy-Based Ink Printing LCA Case Studies 374 LCA Case Studies Streamlined LCA of Soy-Based Ink Printing,” *Korea Int. J. LCA*, vol. 5, no. 6, pp. 374–384, 2000, doi: 10.1065/lca2000.11.040.
- [11] Y. Su, H. Duan, Z. Wang, G. Song, P. Kang, and D. Chen, “Characterizing the environmental impact of packaging materials for express delivery via life cycle assessment,” *J Clean Prod*, vol. 274, p. 122961, Nov. 2020, doi: 10.1016/j.jclepro.2020.122961.
- [12] I. J. Gatt and P. Refalo, “Reusability and recyclability of plastic cosmetic packaging: A life cycle assessment,” *Resources, Conservation & Recycling Advances*, vol. 15, p. 200098, Nov. 2022, doi: 10.1016/j.rcradv.2022.200098.

- [13] I. Deviatkin, M. Khan, E. Ernst, and M. Horttanainen, “Wooden and Plastic Pallets: A Review of Life Cycle Assessment (LCA) Studies,” *Sustainability*, vol. 11, no. 20, p. 5750, Oct. 2019, doi: 10.3390/su11205750.
- [14] G. Thoma *et al.*, “Comprehensive Life Cycle Assessment for Fluid Dairy Delivery Systems,” 2012.
- [15] F. Wikström, H. Williams, K. Verghese, and S. Clune, “The influence of packaging attributes on consumer behaviour in food-packaging life cycle assessment studies - a neglected topic,” *J Clean Prod*, vol. 73, pp. 100–108, Jun. 2014, doi: 10.1016/j.jclepro.2013.10.042.
- [16] Food & Beverage Close-Up, “Research and Markets Adds Report: Baby Food and Infant Formula Market,” Feb. 2020. [Online]. Available: www.researchandmarkets.com/r/p2aag7
- [17] J. Broadbent, “Abbott Laboratories to set up new factory amid infant-formula shortage plaguing US parents.” Accessed: Aug. 16, 2023. [Online]. Available: <https://search-ebscohost-com.proxy2.cl.msu.edu/login.aspx?direct=true&db=edsinc&AN=edsinc.A723601166&site=eds-live>.
- [18] K. Cadwell, A. Blair, C. Turner-Maffei, M. Gabel, and K. Brimdyr, “Powdered Baby Formula Sold in North America: Assessing the Environmental Impact,” *Breastfeeding Medicine*, vol. 15, no. 10, pp. 671–679, Oct. 2020, doi: 10.1089/bfm.2020.0090.
- [19] Perrigo, “Perrigo Pediatrics .” Accessed: May 10, 2023. [Online]. Available: <https://www.perrigopediatrics.com/>
- [20] F. Bassani, C. Rodrigues, P. Marques, and F. Freire, “Ecodesign approach for pharmaceutical packaging based on Life Cycle Assessment,” *Science of The Total Environment*, vol. 816, p. 151565, Apr. 2022, doi: 10.1016/j.scitotenv.2021.151565.
- [21] S. Kim and J. Park, “Comparative Life Cycle Assessment of Multiple Liquid Laundry Detergent Packaging Formats,” *Sustainability*, vol. 12, no. 11, p. 4669, Jun. 2020, doi: 10.3390/su12114669.

3.0 Assessing environmental trade-offs in packaging systems for infant formula delivery. A cradle-to-gate plus end-of-life LCA

A modified version of this chapter was submitted to the International Journal of Life Cycle Assessment as: Abigale LEWIS, Anibal BHER, Satish JOSHI, Matthew DAUM, Rafael AURAS (2023) **Assessing environmental trade-offs in packaging systems for infant formula delivery. A cradle-to-gate plus end-of-life LCA**

3.1 Abstract

Purpose A life cycle assessment (LCA) study was conducted comparing three packaging systems to deliver infant formula, including primary (plastic, composite, and steel containers), secondary (corrugated box), and tertiary (pallet) packaging levels, all manufactured and distributed in North America. The goal was to inform a company of the comparison of three manufactured containers. The project involved quantifying environmental impacts of each packaging system, which could guide decision-making regarding which system would have the lowest environmental footprint, evaluate the effect of end-of-life (EoL) modeling in LCA results, and interpret trade-offs among environmental impact for business decisions.

Methods The functional unit was defined as a packaging system delivering 1,000 g of infant formula from cradle to gate, plus the EoL. Complete modeling using full LCA of the three packages and the various recycling procedures was done using SimaPro 9.3.03 with TRACI 2.1 V1.06 Midpoint and ReCiPe 2016 Midpoint (H) V1.06 impact methods. The LCA was performed according to ISO 14040/14044 standards. The modeling of EoL included the cut-off method, the 50/50 allocation, and the circular footprint formula (CFF). The stochastic multi-attribute analysis (SMAA) method was implemented to evaluate the trade-offs among the midpoint indicators.

Results & Discussion The primary container had the largest contribution for the three systems for all midpoint categories evaluated. Adjusting the EoL models does influence the overall results regarding the packaging systems total impacts. Contributions in each category vary slightly, with minimal changeover from the highest or lowest package footprints in all recycling models. The ranking preference from SMAA for all recycling methods however indicates that the plastic container is preferred, as it has the lowest environmental footprint (EF) with more than 50% probability.

Conclusions The environmental impacts of the packages examined involved trade-offs and a discussion of priorities for consumers and the company's sustainability goals. With the initial EoL methodology used for modeling, *i.e.*, the cut-off method, the highest impact was found in 4 of the 10 impact categories for Package 1, in 2 of the 10 categories for Package 2, and in the remaining 4 categories for Package 3. With the 50/50 allocation and CFF EoL methodologies, different conclusions were reached about the impacts of each package; however, the SMAA methodology for assessing trade-offs found that ranking of the three packages within EoL methodologies did not change the final conclusions that the plastic container has the lowest EF.

Keywords: *Stochastic Multi-Attribute Analysis, SMAA, circular footprint formula, CFF, Recycling Allocation, LCA*

3.2 Introduction

In the packaging field, life cycle assessment (LCA) can be used to evaluate and compare the environmental impact of alternative packaging designs in terms of the package material, manufacturing, use, and end-of-life (EoL) contributions. LCAs conducted in the packaging industry have influenced the design of many of today's packaging systems available in the market, such as changing raw materials used for products to engage more sustainability-oriented customers, shifting from rigid to flexible packaging, implementing reuse systems, or lightweighting plastic containers for replacing glass or metal [1–4]. The United Nations (UN) published 17 “non-binding, broad, and flexible” Sustainable Development Goals (SDGs) that many corporations are choosing to incorporate in their sustainability reporting [5, 6]. These goals have been featured in several corporate sustainability reports, including companies such as Nike Inc., which reports on SDGs 3, 5, 8, 12, 13, and 17 on their website [7]. The Nike Impact Report for the fiscal year 2021 particularly outlines a goal of “10% waste reduction per unit in manufacturing, distribution, headquarters, and packaging through improved design and operational efficiency,” which can be evaluated through the use of LCA in packaging applications [8]. Hence, implementing LCA for packaging decision-making can help businesses understand which packaging alterations can be made to reduce the environmental footprint, and meet their corporate SDGs and reporting priorities. So, integration of LCA methodology to evaluate various packaging formats can assist businesses in making informed decisions on

package design, as long as the modeling of the packages accurately reflects the entire system, including transportation and EoL modeling. Comparing package performance side by side can put environmental performance in perspective for many companies looking to meet sustainability goals pertaining to packaging.

The United States (U.S.) infant formula and baby food market was valued at \$48.5 billion in 2022, despite shortages of infant formula nationwide due to significant plant shutdowns after repeated foodborne illness outbreaks [9, 10]. The U.S. market for infant formula alone was projected to grow from \$2.5 billion in 2018 to roughly \$5 billion by 2026 due to the increase in population [11]. Major players in the infant formula market include Abbott Nutrition®, Nestle®, Danone®, Mead Johnson®, and Kraft Heinz®, along with private-label infant formulas that primarily come from Perrigo® in the U.S. [12]. Infant formula manufacturing and distribution at such high-market volume result in large environmental impacts, which were estimated using LCA in 2020 to be roughly 650,000 tons of CO₂-eq for the U.S. alone [11]. This level is equivalent to the electricity use of 126,473 homes in one year in the U.S., according to the U.S. EPA Greenhouse Gas Equivalencies Calculator [13]. The packaging involved in containing and selling powdered infant formula may play a significant role in the impact of such a large market. The main package types in the powdered infant formula market include rigid containers that can hold a range of formulas to reduce the number of packaging stock-keeping units (SKUs). Although the impact of packaging materials is expected to be much lower than that of the infant formula product, LCA could help quantify the impacts and trade-offs of various current package types, help reduce their environmental impact, assist in decision-making, and deliver progress in packaging related Sustainable Development Goals.

Previous studies have evaluated the environmental impacts of products similar to powdered infant formula; however, many focus on the product itself without packaging, consider only certain impact categories such as global warming, or lack comparisons between other packaging alternatives to understand their relative environmental impacts [11], [14–16]. Ghenai et al conducted an LCA addressing the environmental impacts of packaging milk and dairy products; however, the study focused only on the energy and CO₂ footprint. There is a knowledge gap in how packaging system EoL modeling may or may not impact results, especially regarding recycling allocation. The circular footprint formula (CFF) is a relatively new way of modeling recycling and is being more frequently incorporated in LCA studies, particularly in the European

Union. The method for modeling EoL incorporates several parameters regarding the recycling processes, energy recovery processes, and final disposal of each individual component and material [17]. By comparing the CFF method of recycling allocation to those methods traditionally used, such as cut-off or 50/50 allocation, the LCA community can assess the use of CFF in various types of system modeling. The use of CFF in packaging-specific LCAs is rare in comparison to processing, infrastructure, or general recycling applications; however, CFF is becoming more prevalent in the packaging industry as the concerns about single-use packaging, reuse, and recycling increase [18, 19].

This study uses the stochastic multi-attribute analysis (SMAA) methodology to address the trade-offs that arise in comparative studies that need to show clear-cut results as to the system with the lowest environmental footprint [20]. The methodology was recently developed and in this research is used to compare results within various EoL modeling methodologies. The SMAA methodology is used when LCA results need to provide clear answers or ranking among options, providing a decision tool for companies when trade-offs are not clear [21- 23]. This method is a statistical approach that utilizes internal normalization and outranking along with weighting of impact categories to essentially rank each studied system as having a chance at having the highest or lowest EF. This ranking allows LCA practitioners to report highest or lowest EF in a way that is simple to understand while also emphasizing uncertainty in results.

Packaging systems generally involve more than the primary level or package that is directly in contact with the product and the consumer. Secondary and tertiary level packaging is necessary for handling, distribution, and transportation, which are often ignored in previous studies. This study compares the impact of three rigid containers used to package infant formula. The three containers differ in the material the package is primarily composed of; the three primary packages are plastic, composite (mostly paperboard), and steel. In addition, each system has a corrugated case as the secondary packaging, and a pallet with stretch wrap and slip sheets as the tertiary packaging. The containers are similar in that they are all only partially recyclable due to material differences, assumed consumer usage and disposal, and current recycling capabilities in the U.S. This LCA study was performed to assist a personal care company wishing to inform business decisions to reach SDGs related to packaging infant formula.

3.3 Materials and Methods

This LCA study followed the standards ISO 14040 and ISO 14044 during all its stages. SimaPro Analyst (version 9.3.03), developed by PRé Sustainability [24] was used to model, calculate, and analyze the trade-offs of the environmental footprint of the packages. Additionally, this study addressed the effect of EoL modeling, as several types of recycling modeling are used, and results are compared. The cut-off, the 50/50, and the CFF methodologies are used to model EoL [17]. These three EoL models are described in detail in **Section 3.3.4 End-of-life modeling**. SMAA methodology was used to evaluate the trade-offs present within each recycling model to compare and validate the LCA results; after weighing the midpoint category relevance, this method reports the preference for the specific package in percentage. Additionally, we compare the total environmental impact of the product itself (*i.e.*, milk powder) and its packaging.

3.3.1 Goal definition

The goal of this study was to evaluate the environmental footprint (EF) from cradle-to-gate plus selective EoL scenarios, as well as to identify the opportunities and potential EF trade-offs for three packaging systems for delivering powdered infant formula. Examining the trade-offs among the three rigid containers can bring up information about the impacts of recycling, as each container has a different dominant material. In addition, this LCA assessed the impact of recycling allocation methods on the comparative results. This study was initially performed to inform a global company specializing in packaging personal care products, including the infant formula products compared in the study. This study followed an attributional LCA situation A – micro-level decision support – case scenario [25]. The study did not aim at a comparative public assertion.

3.3.2 Scope definition

The scope of this study involved three packaging systems being evaluated in terms of the environmental footprint of their primary, secondary, and tertiary levels. The scope included all the relevant aspects of an LCA, such as the functional unit, system boundaries, cut-off criteria, allocation, assumptions, study limitations, and the impact assessment method. The packaging systems modeled are intended to distribute and protect powdered infant formula. The three packaging systems can deliver different amounts of formula in differently designed primary packages; however, the distribution systems are similar. The transportation and EoL scenarios

are included in the analysis; however, the shipping of the containers from the distribution center to the supermarket and the consumer use phase of the three packages are excluded from the study. **Table 3. 1** provides a detailed description of each package.

Table 3. 1 : Packaging system descriptions for the comparative LCA of the packages.

Infant Formula			
			
	Plastic container (Package 1)	Composite container (Package 2)	Steel can (Package 3)
Mass of formula contained per functional unit	1,000 g	1,000 g	1,000 g
Primary package composition	HDPE tub, PP lid and scoop, aluminum foil, multilayer labels	Paperboard, PP, aluminum composite material, steel bottom and peel-off lid, LLDPE overcap, PP scoop	Steel can, steel bottom and peel-off lid, LLDPE overcap, PP scoop
Weight of primary packaging unit	158.8 g	134.2 g	207.5 g
Secondary packaging composition	Corrugated case and dividers, hot melt glue	Corrugated case, packaging tape	Corrugated case, packaging tape
Weight of secondary packaging per unit of primary packaging	86.5 g	57.5 g	57.5 g
Tertiary packaging composition	Wood pallet, LLDPE stretch wrap, corrugated dividers	Wood pallet, LLDPE stretch wrap, corrugated dividers	Wood pallet, LLDPE stretch wrap, corrugated dividers
Weight of tertiary packaging per unit of primary packaging	23.8 g	17.8 g	17.8 g

3.3.2.1 System boundaries

The study includes cradle-to-gate plus the EoL scenarios, beginning with the raw material acquisition, packaging material production, package forming and conversion, shipping to filling plant, distribution, and disposal of the packaging materials, including recycling where applicable.

Capital equipment, land use, facilities (including administrative), infrastructure (public and private), and human resources support activities/requirements were omitted from the analysis. Furthermore, the manufacturing of the product (*i.e.*, infant formula) in all its stages was not considered but just presented for scenario analysis. Transportation of packaging raw materials was included for each component to the Allenton, MI (48002) assembly plant and from the assembly plant to the company distribution center located in Grand Rapids, MI (49512). Impacts associated with individual consumer purchases and use of the packages were not considered. Component disposal methods were determined according to U.S. EPA 2018 datasets [26].

In terms of temporal and geographical boundaries, this LCA study is intended to represent package production during the year when the study was conducted (2022) and for the U.S., with minor consideration for Canadian production. Data selected and assumptions made are intended to reflect current equipment, processes, technologies, and market conditions to fit the established best temporal and geographical boundaries. Although relevant geography data may only sometimes be available, the primary databases and reports used in this study were from 2000 or later; they are considered to represent the actual production conditions. Most of the data used for modeling was from North American databases, as indicated in **Section 3.6.1 Life Cycle Inventory**. In cases where data was unavailable for the North American region, supplemental data was adapted to the extent possible to represent the current North American inputs and practices and energy grid. Boundaries were chosen based on realistic and available primary data to focus the study on packaging impacts rather than the product. **Figure 3. 1** is a diagram representing the system boundaries.

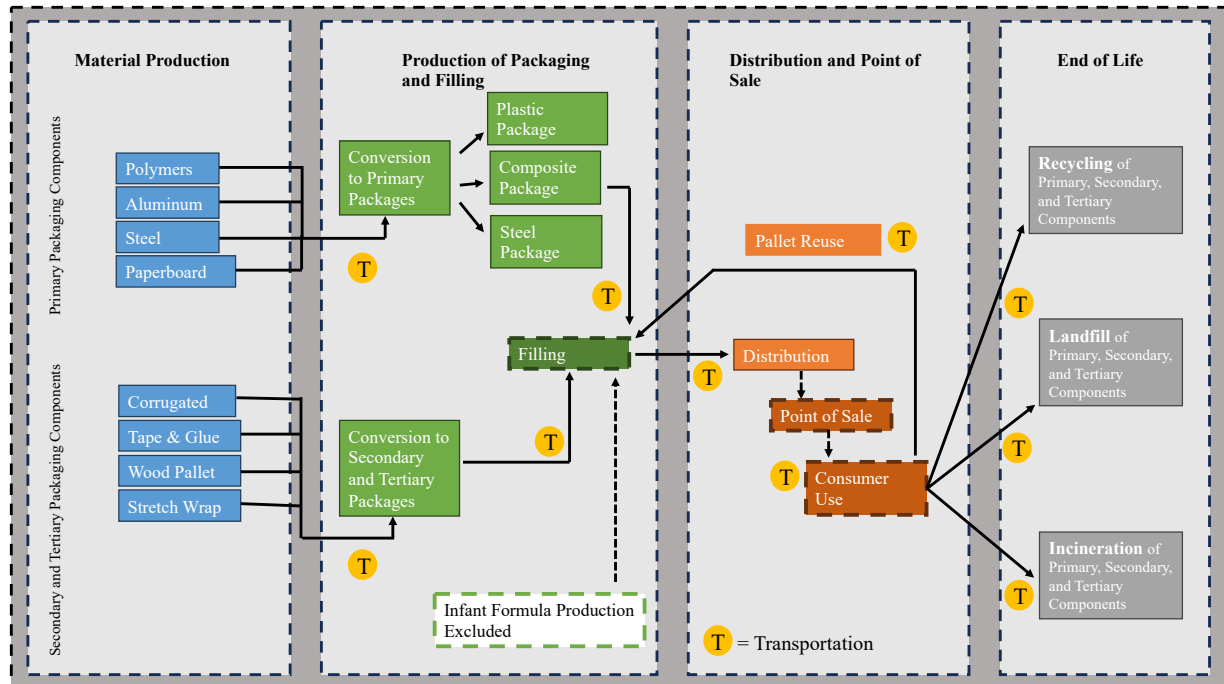


Figure 3. 1: System boundaries used for modeling the three packaging systems from cradle to gate plus EoL. Note: Dashed lines within the unit flow indicate processes not included in system boundaries.

3.3.3 Functional unit and reference flows

Package 1 is a 42-oz plastic container, Package 2 is a 36-oz composite container, and Package 3 is a 25.2-oz steel container. However, each primary package can contain a range of formula mass, with Package 1 being able to deliver anywhere between 824 and 1,023 g, and both Packages 2 and 3 being able to deliver 900 to 1,184 g of formula. Because of this range in the formula mass delivered to the consumer in all three packages, the functional unit was set to 1,000 grams. All three systems can deliver this amount of infant formula to the consumer, and in this way the systems can be evenly compared in a 1:1:1 ratio; therefore, the functional unit used in this study was *the delivery of 1,000 g of infant formula to the consumer*. To accurately reflect the system's secondary and tertiary packaging for each container, the number of primary packages for the plastic container is less than that for the other two packages. **Figure 3. 2** illustrates the functional unit and flows for the three systems.

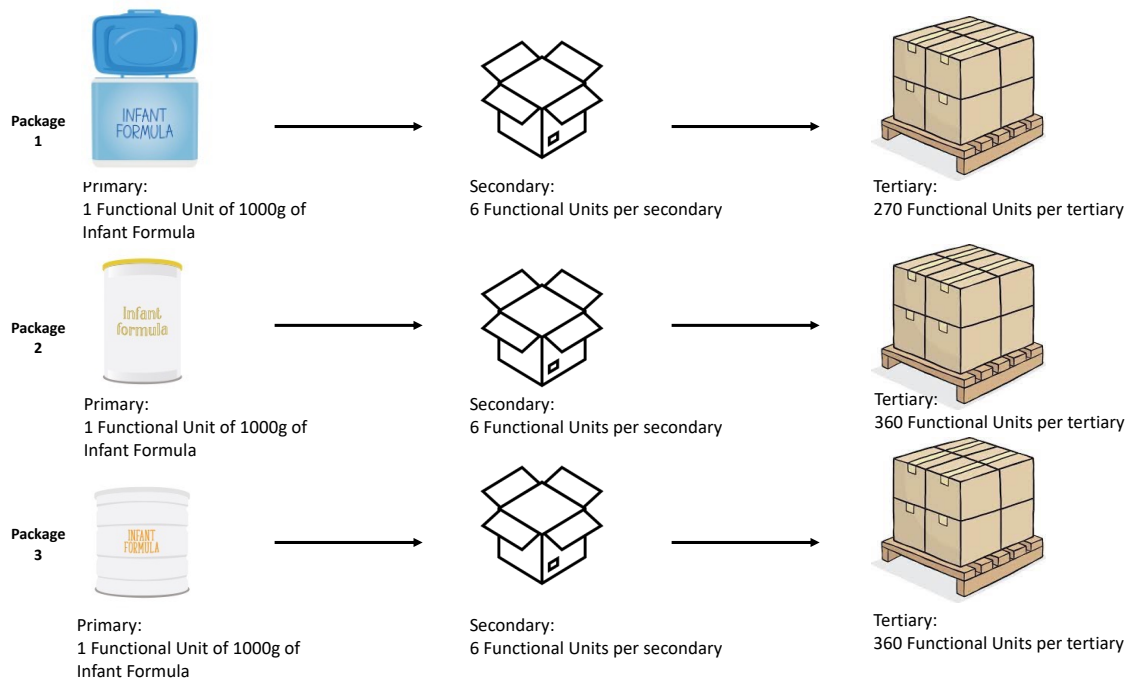


Figure 3. 2: Functional unit for all three packages and flows for all three packaging systems.

3.3.4 End-of-life modeling

In modeling the EoL of each component in each package, the best available foreground data from the company was used. For materials where specific information was unavailable, the U.S. EPA report reporting 2018 data was used to determine recycling percentages [26]. Each component's disposal method breakdown was found in relation to its primary material and the reported recycling percentage. The remaining percentage was broken down between landfill and incineration percentages, with incineration with energy recovery being 19.5% of the remaining values and landfill 80.5%.

Some components were not considered recyclable for several reasons, such as consumer perception and participation in the separation of components, and inclusion of other materials when recycling would take place. For example, the steel bottom attached to the composite container was considered not recyclable, as a U.S. consumer would likely not detach the steel from the composite material, which makes the combination of components not recyclable. For the steel can, however, the same steel bottom component was considered recyclable as it would be recycled as part of the steel can component. Detailed EoL for each component is provided in the Supplementary Information.

Three methods of EoL modeling were used in this study to evaluate the effect of EoL on the overall results. The cut-off method, 50/50 allocation method, and the CFF were used in SimaPro when modeling, and sensitivity analyses were carried out. In the cut-off method, the LCA does not include processes beyond the product life cycle, and there is no environmental burden associated with the products that are recycled. This means the system is not penalized for the environmental impact of the recycling process. On the other hand, in the 50/50 method, the system is penalized for 50% of the emissions generated due to the recycling process. The environmental burden of virgin material production and final disposal are split equally between the product using the virgin material and the product where the material is lost from the technosphere. For the recycling waste scenario, the environmental burden of each recycling process is split equally between the component of the system that supplies the recyclable material and the potential product where the recycled material is used. Finally, the CFF establishes environmental impact by accounting for recycling credits and energy usage. The CFF was developed to define the rules for allocating environmental burdens and benefits of recycling, reusing, or energy recovery [17]. This method of modeling a package EoL breaks down the package into individual components. It calculates a numerical value for each component, which is then added up to an overall value for a package. The CFF modeling was done with the SimaPro software. Modeling for the CFF EoL model can be found in **Section 3.6.3.1 Circular Footprint Formula Modeling**. Trade-offs among these options were evaluated using the SMAA method [20].

3.3.5 Life cycle inventory

Primary Package 1, a predominantly plastic package, consists of an HDPE injection-molded plastic container with a corresponding injection-molded plastic lid. The package is sealed with laminated aluminum foil, which is removed using a tear-off plastic area made of polypropylene. The package also consists of a tamper-evident sticker that touches both the lid and the tub, as well as three labels, one on the lid and two more on the base of the tub. A polypropylene (PP) scoop is also included in the package. Six primary packaging units are placed in a display-ready container (DRC) corrugated case with a set of corrugated dividers, identified as secondary packaging. The case is sealed with hot melt adhesive. Cases are placed on the tertiary packaging, which is a regular wood Grocery Manufacturers Association (GMA)

pallet (48"x40") unitized with stretch wrap film, with pallet slip sheets within the load itself. The tertiary package contains a total of 270 primary packages.

Primary Package 2, a composite package, consists of a composite container that is made up of Kraft paper (70%), polypropylene (20%), and aluminum (10%), per the company specification. The tube has a steel bottom and a peel-off aluminum closure to provide tamper evidence. In addition, the package has a LLDPE overcap, a full label that wraps around the entire tube, and a PP scoop. Six primary packages are placed in a regular slotted container (RSC) corrugated case that is sealed with packaging tape and placed on the same tertiary packaging as described for package 1; however, there are 360 primary packages in the tertiary package for Package 2.

Primary Package 3, a predominantly steel package, consists of a steel tube with a steel bottom. The package also has a peel-off aluminum closure to provide tamper evidence and a PP scoop. This system has a LLDPE overcap, but the graphics are printed directly on the can, not on a separate label. Printing of the can in this study was not included. Six primary packages are placed in an RSC corrugated case that is sealed with packaging tape and placed on the tertiary packaging as also described for Package 2.

3.3.6 Life cycle impact assessment

The life cycle impact assessment (LCIA) methodology relies on modeling Packages 1, 2, and 3 as a process sequence that transforms inputs into outputs while consuming energy and resources and releasing environmental emissions. Thus, the total life cycle and its associated impacts are estimated for each product system from cradle to gate plus EoL. The ISO standards do not dictate which impact assessment method to use for a full LCA study (International Organization for Standardization 2006). However, the methodology should rely on an internationally recognized and accepted method, and the main category should correspond to the main impact associated with the LCIA. For this study, TRACI 2.1 V1.06 was chosen as the primary midpoint impact indicator method, including the categories ozone depletion, global warming, smog, acidification, eutrophication, carcinogens, non-carcinogens, respiratory effects, ecotoxicity, and fossil fuel depletion. ReCiPe 2016 Midpoint (H) V1.06 was selected to check for the robustness of the results and presented in **Section 3.6.4.2 Comparative Results in ReCiPe**. Midpoint impact indicator methods were used in this study rather than endpoint impact indicator methods to focus on more specific effects, as endpoint assessment methods further

quantify or summarize impacts rather than pinpoint impacts associated with common midpoints. Five main impact categories were selected to focus the analysis for the purpose of the discussion: Global Warming, Eutrophication, Carcinogens, Ecotoxicity, and Fossil Fuel Depletion. These categories are chosen to narrow down discussions pertaining to impacts on the atmosphere, water, human health, ecosystems, and resources. A complete table of indicators is shown in **Section 3.6.3.1 Circular Footprint Formula Modeling.**

The main comparative results were obtained using 1,000 g as the functional unit. The full LCA study also included various scenarios to answer questions about possible packaging changes the company could make to reduce its packaging environmental footprint.

3.3.7 Assumptions and limitations

Assumptions were made during testing to fill in gaps in the primary data. These assumptions could be for individual packages in terms of ratios of materials or types of processing or could be used for the entire comparative study, such as transportation values.

Key assumptions related to the overall modeling of all three package systems include that the values for recycling for each component and material, which were taken from the U.S. EPA report with data from 2018 [26]. The transportation values for all components were obtained based on data provided by the company; an average assumed value was used for components or groups of components with no reported transportation value. The assumed value for the transportation of raw materials needed for the primary, secondary, and tertiary packages was adopted as 100 miles (160 km) for modeling, and the transportation value for the EoL modeling was 50 miles (80 km). These values consider the availability of resources and facilities within this distance range, which seems a fair assumption for the North American market and when considering the company's distribution locations. In modeling EoL, the default incineration with energy recovery values was 19.5%, and the landfill value was 80.5%, as reported by the U.S. EPA [26]. The system boundaries for each system do not include any secondary and tertiary packaging involved in delivering the actual packaging components to the manufacturing facilities. Additionally, secondary, and tertiary packaging printing was not included in the system boundaries due to lack of available and provided data as well as inconsistencies across represented SKUs. Depreciation and environmental impact of infrastructure processes were excluded when analyzing the systems. When analyzing scenarios, it was assumed that any weight reduction did not compromise the integrity of the component. The analysis did not

consider material waste during processing and leaks during the transportation stages as the main focus was the packaging system not the product. The energy and electricity grid were considered for the medium grid of the United States. The primary recycling allocation method assumed in the modeling was the cut-off approach.

Further assumptions and limitations used to model each individual package can be found in **Section**

3.6.2.1 Assumptions and Limitations.

3.3.8 Data quality assessment

Data quality indicators have been assigned to each component using the quality matrix approach. The Pedigree matrix evaluated five data quality indicators to assign uncertainty to the data model using scores from 1 to 5 [27]. The results from the data quality assessment for this study can be found in the Supplementary Information.

In addition, a completeness check was conducted to ensure that the required information and data from all phases have been used and are available for interpretation. Data gaps are identified, and the need to complete the data acquisition was evaluated. **Table 3. 6** in **Section 3.6.2.2 Data quality assessment** summarizes the completeness check. According to this check, all the requirements have been met for each assembly level, transportation of the assembly, and end-of-life scenarios. The cut-off criteria have been met and no additional action items are to be completed. This indicates that the LCA study has complete data, and where data was not fully provided, an assumption was made and documented to fill in any gaps.

3.3.9 Life cycle interpretation

Scenario, sensitivity, and uncertainty analyses were performed to assess trade-offs among the package systems.

3.3.9.1 Contribution analysis

The contribution to the overall environmental footprint from the assembly and EoL of the primary, secondary, and tertiary packaging levels was determined for the three packages. The assembly portion involves all impacts associated with the materials and processing and conversion of the components. The EoL portion involves all impacts associated with recycling, incineration, and landfill of the components. Transportation within these categories was not included. For this analysis, modeling did not change, however, the data was grouped into six

categories: Assembly of the Primary, EoL of the Primary, Assembly of the Secondary, EoL of the Secondary, Assembly of the Tertiary, and EoL of the Tertiary.

3.3.9.2 Comparative analysis

A comparison analysis was conducted to determine each package's overall EF. The comparison was based on the functional unit of delivering 1,000 g of infant formula to the consumer, which compares one of each package to the other.

3.3.9.3 Scenario analysis

Several scenarios were run to evaluate various ways in which the environmental footprint of the three infant formula packages could be reduced. Scenarios highlighted in this paper include lightweighting the plastic and steel containers and swapping the steel bottom in the composite container with the same composite material.

In the lightweighting scenarios, the main component(s) were lightweighted by 30%, a percentage chosen to observe the overall trend for the effect of lightweighting. It was understood that a 30% lightweighting of all components is not feasible. For the plastic package, the plastic lid and plastic tub were both lightweighted. For the steel package, only the steel can component was lightweighted. In the remaining scenario, the steel bottom component is taken out of the assembly and is replaced with a bottom component made of the same composite material as the main body of the package.

3.3.9.4 Biogenic carbon

Increasing importance is given to materials of biobased origin; therefore, the carbon sequestered from the atmosphere during biomass growth that may later be released due to combustion or decomposition accounts for the biogenic carbon. Two main approaches can account for carbon storage in biobased materials. The approach used for this LCA study considers biogenic carbon to be CO₂ neutral and excluded from the inventory analysis at the end-of-life phase (cradle-to-grave LCA). The central rationality for this scenario is to understand whether biomass as a material source or material production significantly impacts the Global Warming Potential (GWP). The method used in the LCIA in SimaPro and reported was the Intergovernmental Panel on Climate Change (IPCC) 2021 GWP100 (including CO₂ uptake) V1.00 method (100 years). The midpoint indicator for this method is the Global Warming Potential in kg CO₂-eq.

3.3.9.5 Sensitivity analysis

To assess how modeling choices affect the results of an LCA, sensitivity analysis was considered to determine if the recycling allocation or method of modeling impacts the results following the ISO 14044 standard. The modeling for EoL for each package varied based on different allocation methods. The cut-off (0/100), 50/50, and CFF methods were all considered in this analysis. Details pertaining to the three recycling allocation methods are found in **Section 3.3.4 End-of-life modeling**.

3.3.9.6 Uncertainty and discernability analysis

Monte Carlo analysis allows for only a direct comparison of two items; therefore, an uncertainty analysis was run to compare Package 1 with Package 2, Package 1 with Package 3, and Package 2 with Package 3, with $n=10,000$ runs. Since there were three packages involved, the analysis is typically deemed a discernability analysis rather than uncertainty; hence, it is referred to as a discernability analysis for the remainder of the paper.

3.3.9.7 Stochastic multi-attribute analysis

To examine the trade-offs observed in the results of this comparative LCA, the SMAA normalization method was used. This method provides a methodology for directly examining trade-offs utilizing internal normalization with outranking as well as exploration of weighting that does not favor one impact category over any others [20]. The SMAA method relies on uncertainty, or in this case the discernability analysis to assign weighting coefficients as well as a ranking of important impact categories by the practitioners of the LCA. From there, an overall score is given to each package. The parameters used in running the SMAA analysis include that all Monte Carlo analyses done in SimaPro involved 10,000 runs. Then, within the SMAA software (Stochastic Multi Attribute Analysis for Life Cycle Assessment [SMAA-LCA], software version 1.0.8-alpha, affiliated with Arizona State University) all impact categories were weighted equally, with 2,000 runs.

3.3.9.8 Keeping it in perspective

The product is generally not included in LCA studies concerning packaging systems; however, the product typically has a much higher impact [25]. In the case of this LCA study, the infant formula product was not easily replicated in modeling; however, a milk powder product was chosen to mimic the infant formula product, albeit with lower EF, and it was included to

understand the overall impact of product plus package. In this scenario, 1,000 g of milk powder was added to the assembly of the packages and the life cycle of each is reported.

3.4 Results and Discussion

The following section addresses the LCA results, followed by the discussions and the impact of infant formula packaging in three types of rigid containers. In addition, the section evaluates the recycling methodology on the overall results of comparative LCA for packaging containers. Results from incorporating SMAA methodology to address trade-offs in final decision-making is also reported, as the results of the LCA were unable to provide clear answers about the packaging systems with the lowest EF.

The main results of the comparative LCA study include individual and comparative results demonstrating trade-offs. TRACI 2.1 V1.06 midpoint impact methodology was used as the primary impact assessment method for reporting the results.

3.4.1 Contribution analysis

Contribution analysis allows for identifying the phases that are the main EF contributors to the life cycle of each system. A contribution analysis provides an overall picture of where the opportunities for improvement exist. For this work, the specific categories analyzed are the primary, secondary, and tertiary levels as well as the assembly and EoL portions within those categories. shows that for the Package 1 system, the assembly of the primary package has the highest contribution for the carcinogens and fossil fuel depletion categories. Significant contributions can be observed for the EoL of the primary level in the categories of global warming, eutrophication, and ecotoxicity. The transportation level contribution to the overall impact is negligible in all three systems; therefore, they are not shown in this contribution analysis. For Package system 2 (*Figure 3. 11*) the highest contribution is the assembly of the primary level for all impact categories analyzed, and the EoL for the primary level is the next highest contributor in all categories. Package system 3 (*Figure 3. 12*) has similar trends to those of Package system 2; however, the second highest contributor in the eutrophication category is the disposal scenario for tertiary packaging. These figures are found in **Section 3.6.4.1 Contribution Analysis.**

Figure 3. 3 indicates that for the plastic package specifically, the primary components contribute the most to the environmental footprint of the system. This breakdown of contributions from package levels, however, can also demonstrate the idea of trade-offs, as seen

with a direct comparison of the results of the ecotoxicity and fossil fuel depletion categories. For the ecotoxicity indicator, the EoL of the primary package has the highest contribution at 79%. For the fossil fuel depletion indicator, the assembly of the primary package has the highest contribution at 91%. This comparison can be seen as a trade-off because, depending on the indicators prioritized by LCA practitioners or businesses, the optimization of the package can be focused on different aspects. If a business is mainly concerned with fossil fuel usage in its packaging, they may focus on optimizing the package assembly; however, if they are more concerned with impacts on the ecosystem, then they would want to focus more on the EoL of the package.

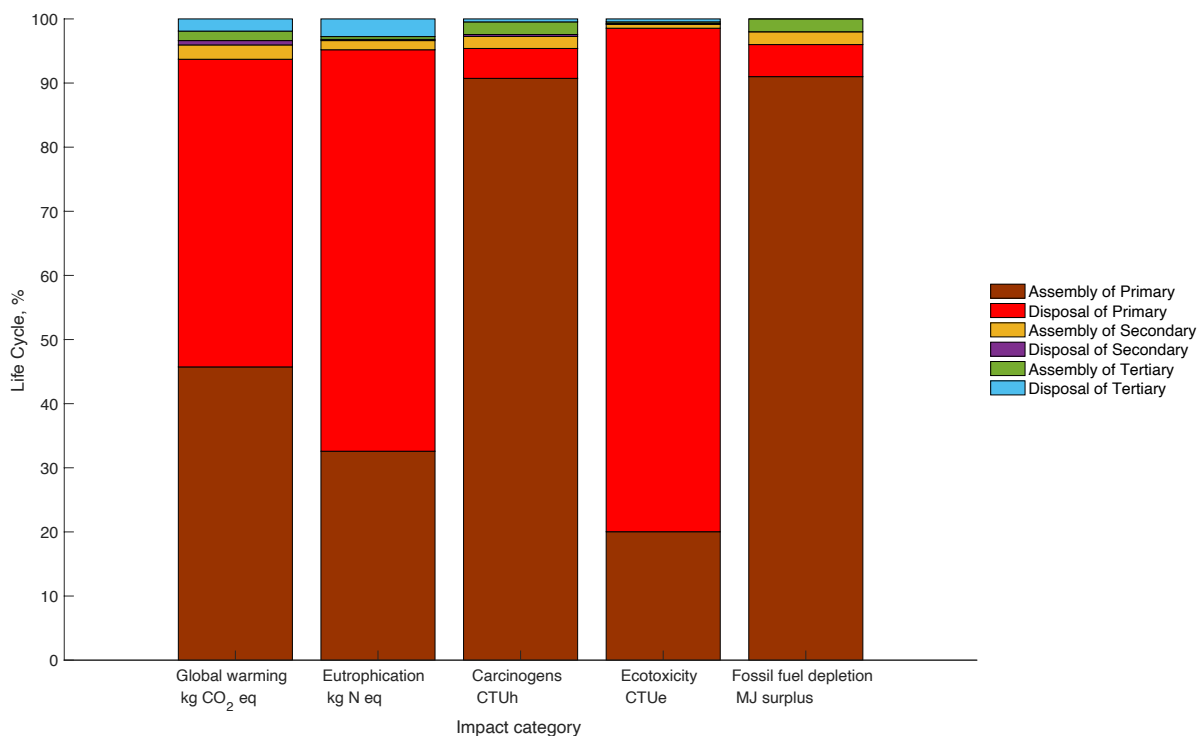


Figure 3. 3: Main contributions to midpoint indicators global warming, eutrophication, carcinogens, ecotoxicity, and fossil fuel depletion of assemblies and disposal scenarios for the (plastic) Package system 1, according to TRACI 2.1 V1.06.

3.4.2 Comparative analysis

Figure 3.4 presents the comparative analysis results for the packages with a functional unit of 1,000 g of formula. When the three packages were compared with TRACI 2.1 V1.06, a more extreme case of trade-offs can be seen as no package has the highest contribution in the most impact categories. The plastic package, Package 1, has the highest contribution in 4 of the 10 impact categories, including ozone depletion, global warming, eutrophication, and fossil fuel depletion. The composite container, Package 2, has the highest contribution in 2 of the 10 impact categories, including smog and acidification. The steel can, Package 3, has the highest contribution in the remaining 4 of 10 impact categories, including carcinogens, non-carcinogens, respiratory effects, and ecotoxicity. **Table 3. 2** provides the mean values for the impact categories for each packaging system. This table is the discernability analysis results, which indicate that in all TRACI 2.1 V1.06 impact categories, the impact values among the three packages are significantly different. The graphical representation and the tabulated data of the results for ReCiPe are shown in **Section 3.6.4.2 Comparative Results in ReCiPe (Figure 3. 13)** and demonstrate a similar case of trade-offs. Therefore, further exploration is needed to fully understand if any package should be recommended over another.

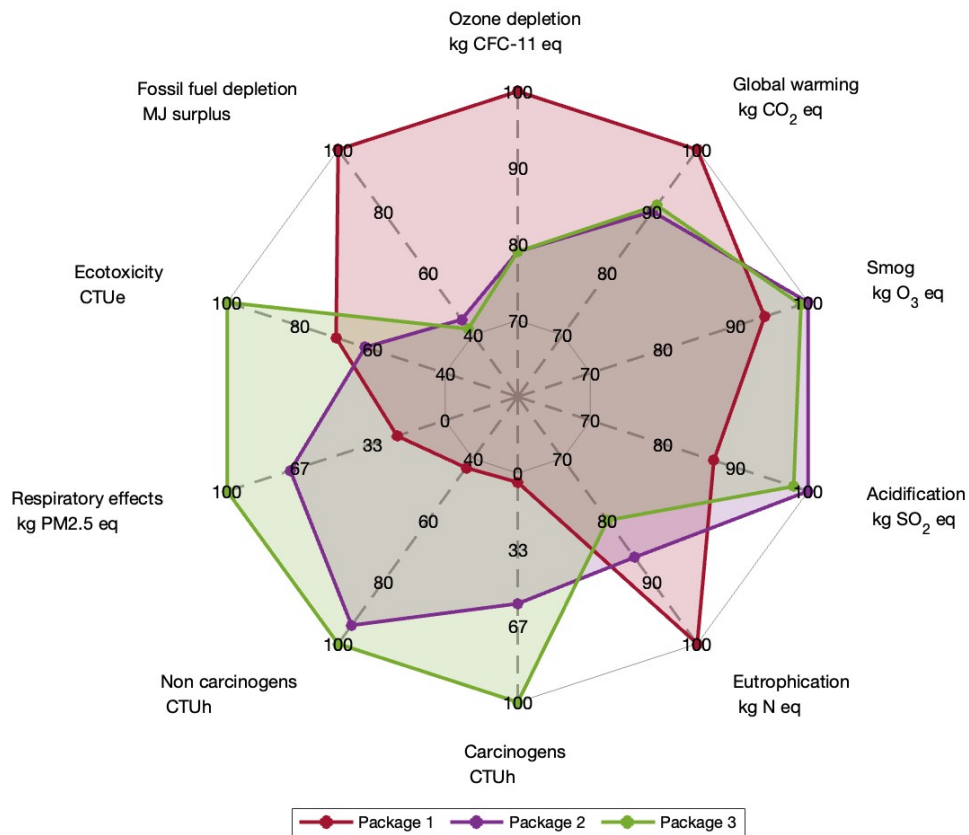


Figure 3. 4 : Spider chart comparative results of all three package systems using TRACI 2.1 V1.06. Note: Middle ticks for each indicator differ between 0 and 100% midpoint environmental impact, but they are not the same to facilitate visualization.

Table 3. 2: Discernability analysis results for the three packaging systems for the cut-off EoL model, according to TRACI 2.1 V1.06. Monte Carlo runs $n=10,000$.

Impact category	Unit	Package 1		Package 2		Package 3	
		Mean	SD	Mean	SD	Mean	SD
Ozone depletion	kg CFC-11 eq	5.33E-08 ^a	9.10E-09	4.19E-08 ^b	8.45E-09	4.39E-08 ^c	8.44E-09
Global warming	kg CO ₂ eq	0.8070939 ^a	0.0773455	0.7277925 ^b	0.0485788	0.7475012 ^c	0.056484
Smog	kg O ₃ eq	0.0427722 ^a	0.0034498	0.0446433 ^b	0.0027438	0.0451122 ^c	0.003289
Acidification	kg SO ₂ eq	0.0026352 ^a	0.0003014	0.0029379 ^b	0.0002380	0.0029553 ^c	0.000254
Eutrophication	kg N eq	0.0025193 ^a	0.0014276	0.0022748 ^b	0.0009017	0.0021683 ^c	0.001462
Carcinogens	CTUh	2.11E-08 ^a	6.09E-08	2.32E-07 ^b	8.13E-08	4.05E-07 ^c	1.35E-07
Non-carcinogens	CTUh	1.57E-07 ^a	6.22E-08	3.49E-07 ^b	2.94E-07	3.76E-07 ^c	1.87E-07
Respiratory effects	kg PM2.5 eq	0.0001535 ^a	0.0000192	0.0004824 ^b	0.0000529	0.0006854 ^c	0.000081
Ecotoxicity	CTUe	13.376281 ^a	7.4163912	12.682551 ^b	3.3715603	20.558919 ^c	6.201392
Fossil fuel depletion	MJ surplus	2.4086545 ^a	0.1089644	1.0834917 ^b	0.0709547	1.0248102 ^c	0.087573

Note: Within each row, column values (means) followed by a different letter are significantly different at $p \leq 0.05$ (Tukey's test).

Although there is no clear-cut “winner” in the final comparison, there are several opportunities to make sustainable decisions to reduce the EF of the packages. The impact categories all correlate to environmental issues, which are often prioritized as issues in businesses. For example, most businesses have goals pertaining to reducing GHG emissions; however, they may not specifically call out goals for reducing water pollution. In cases like this, businesses can still make informed decisions with package trade-offs in mind. Trade-offs are instances in which a package or material may have very low impact in certain categories but simultaneously have very high impact in others. In this comparative LCA, the steel can package has the highest impact in human-health related categories like carcinogens and respiratory effects; however, it has lower impact in atmospheric related indicators like climate change and fossil fuel depletion due to the largest recycling content and type of energy used. The results of this study can also be an example of LCA giving results that are not typically expected. In comparing the materials of plastic and steel, it was expected that steel would have a

much higher impact in most categories than plastic due to the greater weight. Particularly interesting is the observation that the plastic container has a higher impact than the steel in the global warming impact category, mainly due the large amount of recycling content in steel.

3.4.3 Scenario analysis

3.4.3.1 Lightweighting

Figure 3. 5 presents the scenario analysis results for the plastic container in which the plastic lid and tub components are lightweighted by 30%. The value of 30% was chosen as a proxy to use in this scenario; it is understood that lightweighting these components by this amount may not be feasible. It was assumed that the lightweighting of these components does not compromise the ability of the package to deliver the same amount of infant formula product. This scenario analysis shows that lightweighting both the plastic lid and tub components of the plastic package can lower the environmental impact. The lightweighting of the steel can component in the steel package system also shows the same trend, as seen in **Figure 3. 14** in **Section 3.6.4.3 Scenario Analysis**

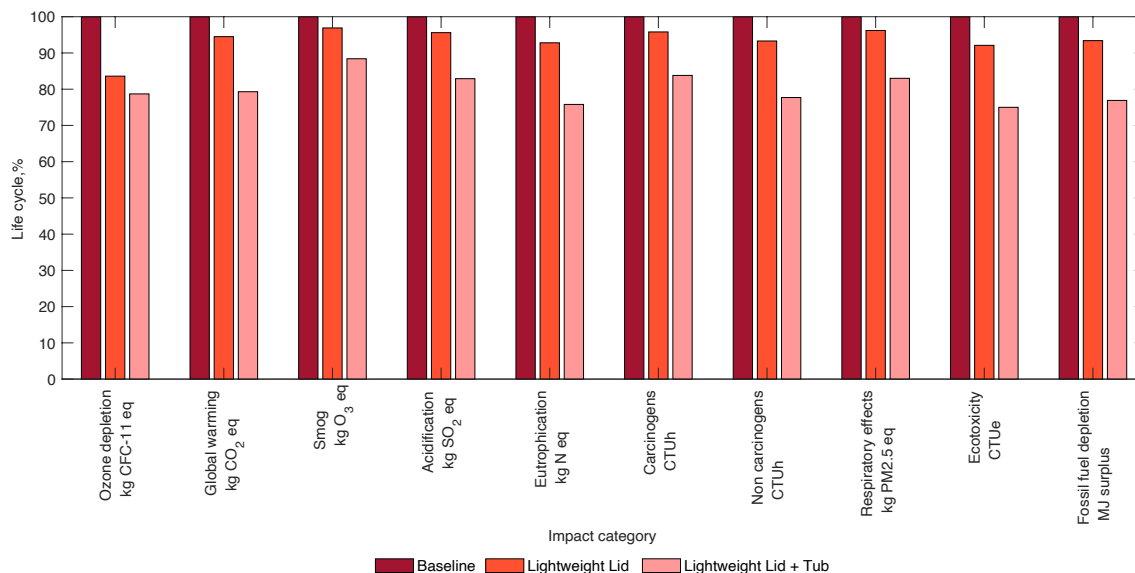


Figure 3. 5: Lightweighting scenario (30%) for Package 1, the plastic package, according to TRACI 2.1 V1.06.

3.4.3.2 Component replacement

Figure 3. 6 presents the scenario analysis results for the composite container in which the steel bottom component of the primary package is removed, and a new component comprised of the same composite material as the base of the can is incorporated as a replacement. The amount of composite material needed to cover the bottom and the weight of the replacement bottom were calculated, and a new component was modeled. In this scenario, it was assumed that replacing the steel bottom with composite material does not compromise the ability of the package to deliver the same amount of infant formula product; however, it is understood that this assumption may not be feasible. From this scenario analysis, it can be concluded that replacing the steel bottom component with a composite bottom decreases the environmental impact in all categories.

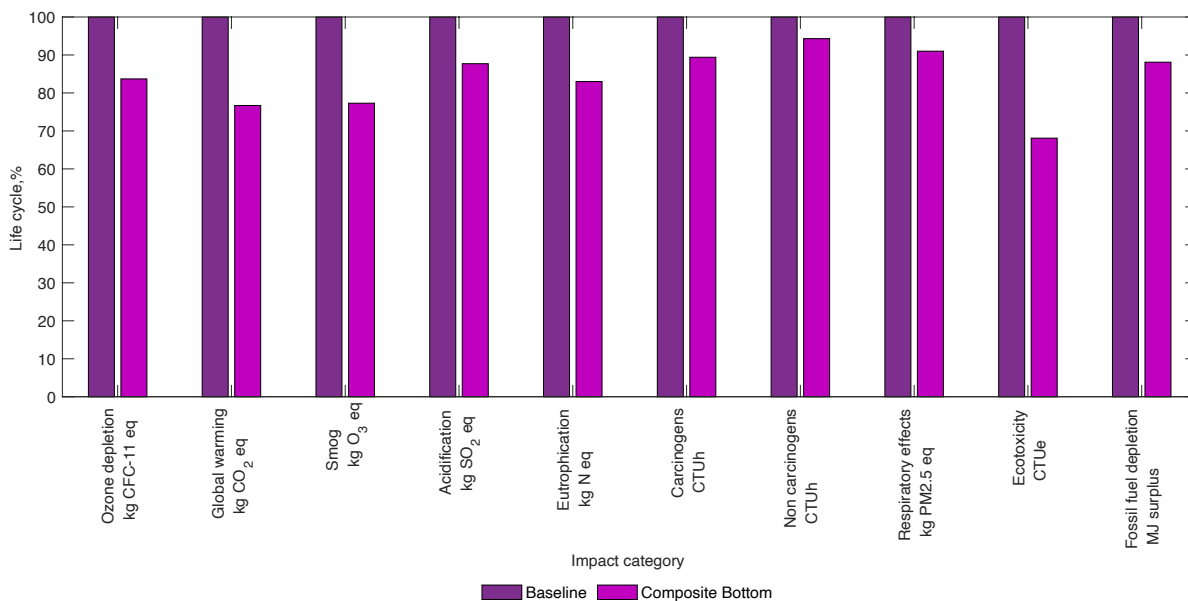


Figure 3. 6: Composite bottom scenario for Package 2, the composite container, according to TRACI 2.1 V1.06.

From the above scenarios involving lightweighting and component replacement, it can be assumed that by reducing the weight of primary packaging components, the overall environmental impact of the packaging systems for all three packages is reduced in all impact categories. As observed, the lightweighting of both the plastic lid and tub components of Package 1 lowers the environmental impact. For Package 2, changing the bottom of the package

from steel to the same composite material and inherently reducing the weight of the bottom component reduces the environmental impact. For Package 3, lightweighting the steel can component will also reduce environmental impact. Although the reduction is not linear across all categories, it is still concluded that within each individual category, impact is reduced.

3.4.4 Biogenic carbon

The approach used for this LCA study considers biogenic carbon to be CO₂ neutral and excluded from the inventory analysis at the EoL phase (cradle-to-grave LCA). **Figure 3. 7** shows the effect of biogenic carbon accounting on the global warming potential indicator for all three package systems. When adding the biogenic carbon credit to all three packages, the environmental impact in terms of the global warming impact category is lowered. The largest decrease in impact is seen for the composite container (Package 2), as it contains the most biobased material in the primary and secondary packaging systems (*i.e.*, paperboard).

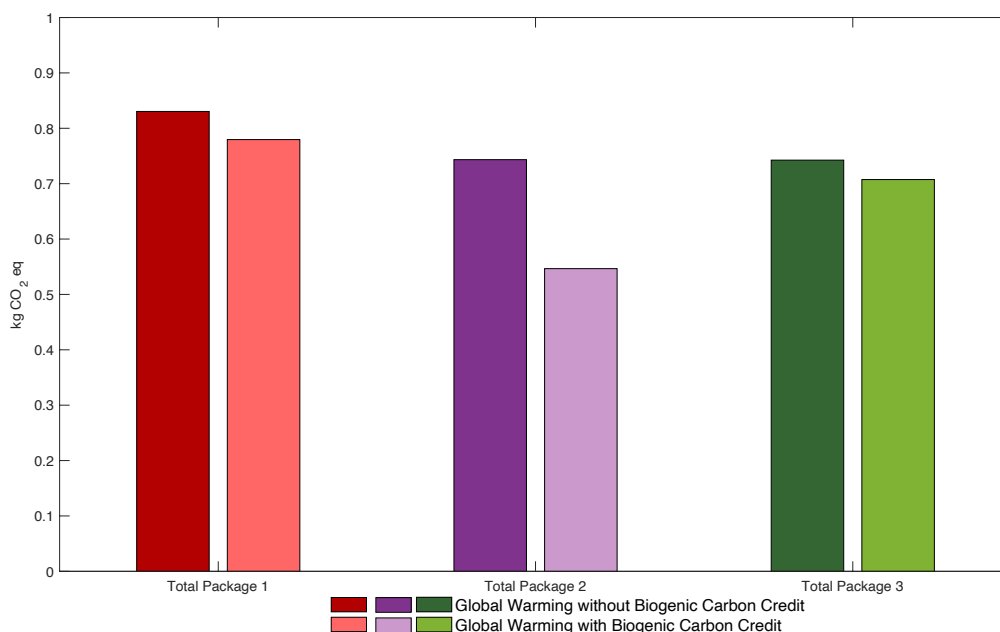


Figure 3. 7: Biogenic carbon accounting for the three package systems using the IPCC GWP with CO₂ uptake methodology.

3.4.5 Sensitivity analysis

Since the secondary and tertiary packaging levels are similar, a sensitivity analysis was conducted focused on the primary level of all packaging system options considering the cut-off, 50/50, and CFF allocation models. This analysis can be used to check if the recycling allocation

method used in modeling affects the results and trade-offs among the environmental footprints of the three package systems. **Figure 3. 8** presents the comparative results among the three packaging system EFs using TRACI 2.1 v1.06 methodology with the cut-off, 50/50, and CFF allocation models; and **Table 3. 3** presents the corresponding numerical values. The CFF modeling results do not match those obtained with the cut-off or 50/50 recycling allocation methods. The steel package, Package 3, has the highest impact in all categories except fossil fuel depletion; the plastic package, Package 1, had the highest impact for fossil fuel depletion. These findings indicate that the decision on how to model the EoL for this case of infant formula packages significantly influences the results. When looking at **Table 3. 3**, however, the values obtained for the final results of Package 1 with the three methods of EoL modeling vary between being significantly different or not significantly different from one another when statistically analyzed, depending on the impact category. This same trend can also be seen with the composite and steel can packages. For the steel package, Package 3, the values obtained with the three EoL models in most impact categories are significantly different. The cut-off and 50/50 methods are determined to be not significantly different in all impact categories, however, the CFF methodology obtains values that are different.

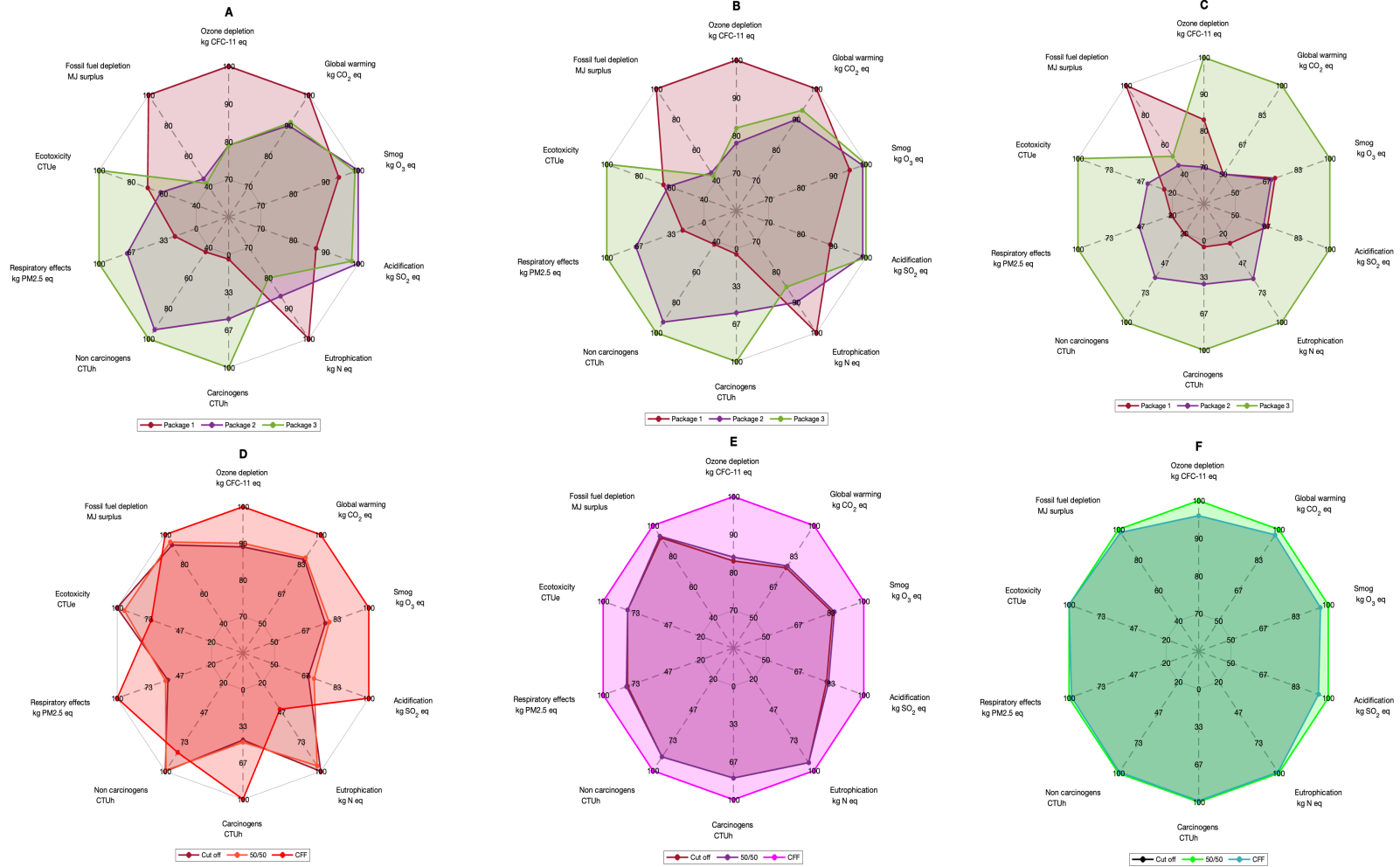


Figure 3. 8: Spider chart comparative results of the three package systems using TRACI 2.1 V1.06.

Top row (Left to Right): Environmental footprint according to TRACI v1.06 discussing **A)** Package 1, 2, and 3, cut-off; **B)** Package 1, 2, and 3, 50/50; and **C)** Package 1, 2, and 3, CFF. Bottom row (Left to Right): **D)** Package 1 cut-off, 50/50, and CFF;

Figure 3.8 (cont'd):

E) Package 2 cut-off, 50/50, and CFF; and ***F)*** Package 3 cut-off, 50/50, and CFF. Note: Middle ticks for each indicator differ between 0 and 100% midpoint environmental impact, but they are not the same to facilitate visualization.

Table 3. 3: Comparison of EoL values for the three packages according to the cut-off, 50/50, and CFF methods, according to TRACI 2.1 V1.06. Monte Carlo runs $n=10,000$.

Package 1 - Plastic		Cut-off Method		50/50 Method		CFF Method	
Impact Category	Unit	Mean	Standard Deviation	Mean	Standard Deviation	Mean	Standard Deviation
Ozone depletion	kg CFC-11 eq	5.07E-08 ^a	8.94E-09	5.17E-08 ^a	9.00E-09	5.94E-08 ^a	9.31E-09
Global warming	kg CO ₂ eq	0.800 ^a	0.068	0.821 ^a	0.068	0.932 ^b	0.068
Smog	kg O ₃ eq	0.044 ^a	0.003	0.045 ^a	0.003	0.054 ^b	0.003
Acidification	kg SO ₂ eq	0.00273 ^a	0.00027	0.00285 ^a	0.00027	0.00369 ^b	0.00027
Eutrophication	kg N eq	0.0024 ^b	0.0014	0.0024 ^b	0.00143	0.00116 ^a	0.000839
Carcinogens	CTUh	2.34E-08 ^a	3.97E-08	2.37E-08 ^a	2.71E-08	4.25E-08 ^a	3.28E-08
Non carcinogens	CTUh	1.35E-07 ^a	1.09E-07	1.39E-07 ^a	6.73E-08	1.33E-07 ^a	1.81E-07
Respiratory effects	kg PM _{2.5} eq	0.00017 ^a	1.79E-05	0.00019 ^a	1.81E-05	0.00026 ^b	1.85E-05
Ecotoxicity	CTUe	12.9 ^a	7.4	13.2 ^a	7.2	10.1 ^a	5.6
Fossil fuel depletion	MJ surplus	2.32 ^a	0.09	2.35 ^a	0.10	2.54 ^b	0.09
Package 2 - Composite		Cut-off Method		50/50 Method		CFF Method	
Impact Category	Unit	Mean	Standard Deviation	Mean	Standard Deviation	Mean	Standard Deviation
Ozone depletion	kg CFC-11 eq	4.14E-08 ^a	8.45E-09	4.53E-08 ^a	8.28E-09	4.96E-08 ^a	8.67E-09
Global warming	kg CO ₂ eq	0.72 ^a	0.05	0.75 ^a	0.05	0.93 ^b	0.05
Smog	kg O ₃ eq	0.044 ^a	0.003	0.047 ^b	0.003	0.053 ^c	0.003
Acidification	kg SO ₂ eq	0.00289 ^a	0.00022	0.00312 ^a	0.00022	0.00356 ^b	0.00023
Eutrophication	kg N eq	0.00227 ^a	0.00088	0.00229 ^a	0.00090	0.00244 ^a	0.00096
Carcinogens	CTUh	2.32E-07 ^a	1.23E-07	2.38E-07 ^a	8.05E-08	2.85E-07 ^b	8.97E-08
Non carcinogens	CTUh	3.57E-07 ^a	5.54E-07	3.53E-07 ^a	2.48E-07	3.92E-07 ^a	2.14E-07
Respiratory effects	kg PM _{2.5} eq	0.00048 ^a	5.30E-05	0.00050 ^a	5.21E-05	0.00060 ^b	5.59E-05
Ecotoxicity	CTUe	12.7 ^a	3.7	13 ^a	3.6	15.7 ^a	5.1
Fossil fuel depletion	MJ surplus	1.07 ^a	0.07	1.11 ^{ab}	0.07	1.17 ^b	0.07
Package 3 - Steel		Cut-off Method		50/50 Method		CFF Method	
Impact Category	Unit	Mean	Standard Deviation	Mean	Standard Deviation	Mean	Standard Deviation
Ozone depletion	kg CFC-11 eq	4.11E-08 ^a	8.20E-09	4.17E-08 ^a	8.22E-09	7.14E-08 ^b	1.12E-08
Global warming	kg CO ₂ eq	0.714 ^a	0.055	0.725 ^a	0.056	1.860 ^b	0.073
Smog	kg O ₃ eq	0.0421 ^a	0.0032	0.0429 ^a	0.0032	0.0768 ^b	0.0044
Acidification	kg SO ₂ eq	0.00276 ^a	0.00025	0.00283 ^a	0.00025	0.00550 ^b	0.00032
Eutrophication	kg N eq	0.00209 ^a	0.00106	0.00211 ^a	0.00110	0.00396 ^b	0.00146
Carcinogens	CTUh	4.04E-07 ^a	1.33E-07	4.03E-07 ^a	1.29E-07	7.12E-07 ^b	2.27E-07
Non carcinogens	CTUh	3.79E-07 ^a	8.29E-07	3.75E-07 ^a	2.61E-07	6.71E-07 ^b	7.56E-07
Respiratory effects	kg PM _{2.5} eq	0.00066 ^a	8.16E-05	0.00067 ^a	8.28E-05	0.00126 ^b	0.00012
Ecotoxicity	CTUe	20.5 ^a	6.1	20.4 ^a	6.0	38.3 ^b	24.3
Fossil fuel depletion	MJ surplus	0.97 ^a	0.08	0.98 ^a	0.09	1.33 ^b	0.11

Note: Within each row, column values (means) followed by a different letter are significantly different at $p \leq 0.05$ (Tukey's test).

3.4.6 Discernability analysis

A discernability analysis is an extension of a statistical analysis that leads to the pair-wise comparisons of the mean values of environmental impact among 10,000 Monte Carlo runs.

Table 3. 2 denotes the mean values for the impact categories among the packages that are deemed significantly significant from one another for the cut-off method. The results demonstrate that the three packages have statistically significant differences in their environmental impact in all 10 impact categories, which indicates that the assumptions and boundaries followed in this study do not significantly impact the results. This is concluded due to the fact that in 10,000 runs of the study, a statistically significant difference among all three packages is found for each impact category.

3.4.7 Stochastic multi-attribute analysis

SMAA was used to compare results and trade-offs for all three EoL modeling methodologies. Results obtained through SMAA rank the three packages in terms of the chance that each package has the lowest, second lowest (middle), and highest EF. For instance, as shown in **Figure 3. 9**, the plastic container, Package 1, has a 40% chance (Rank 1) of being the option with the lowest EF and a 28% chance (Rank 3) of having the highest EF when considering the cut-off method of recycling allocation.

Figure 3. 9 also shows that in the ranking among the three EoL models, the SMAA methodology still indicates that Package 1 has the highest chance of having the lowest EF, with the cut-off probability being 40% (Rank 1 cut-off), the 50/50 probability being about 48% (Rank 1 50/50), and the CFF probability being about 60% (Rank 1 CFF). The middle-ranked package system also remains the same across EoL models, with the composite container, Package 2, having the highest probability in Rank 2 for all three methodologies (Rank 2 cut-off, 50/50, and CFF). The lowest-ranked package, meaning the largest EF, was the steel can, Package 3, for the cut-off probability at 42% and the CFF probability at 99.6% (Rank 3 cut-off and CFF). However, the 50/50 method indicates that the highest probability for the highest EF is the plastic package, Package 1. Within the 50/50 ranking results, the plastic package, Package 1 has the highest probability of being Rank 1 meaning the lowest EF with the probability of 48% (Rank 1 cut-off) compared to the probability of being Rank 3 at 35% (Rank 3 50/50). This would lead one to reach the conclusion that within the 50/50 methodology the plastic package has the lowest EF

and the steel package the highest EF, which matches the results for the other two EoL methodologies.

The discrepancy among Rank 3 probabilities would indicate that results obtained through SMAA do change depending on the EoL method used to model the packaging system. Despite the small discrepancy in Rank 3, the same conclusions can still be reached in this case, which include that Package 1 has the highest probability of having the lowest EF, Package 3 has the highest probability of having the highest EF, and Package 2 has the highest probability of being ranked second lowest EF.

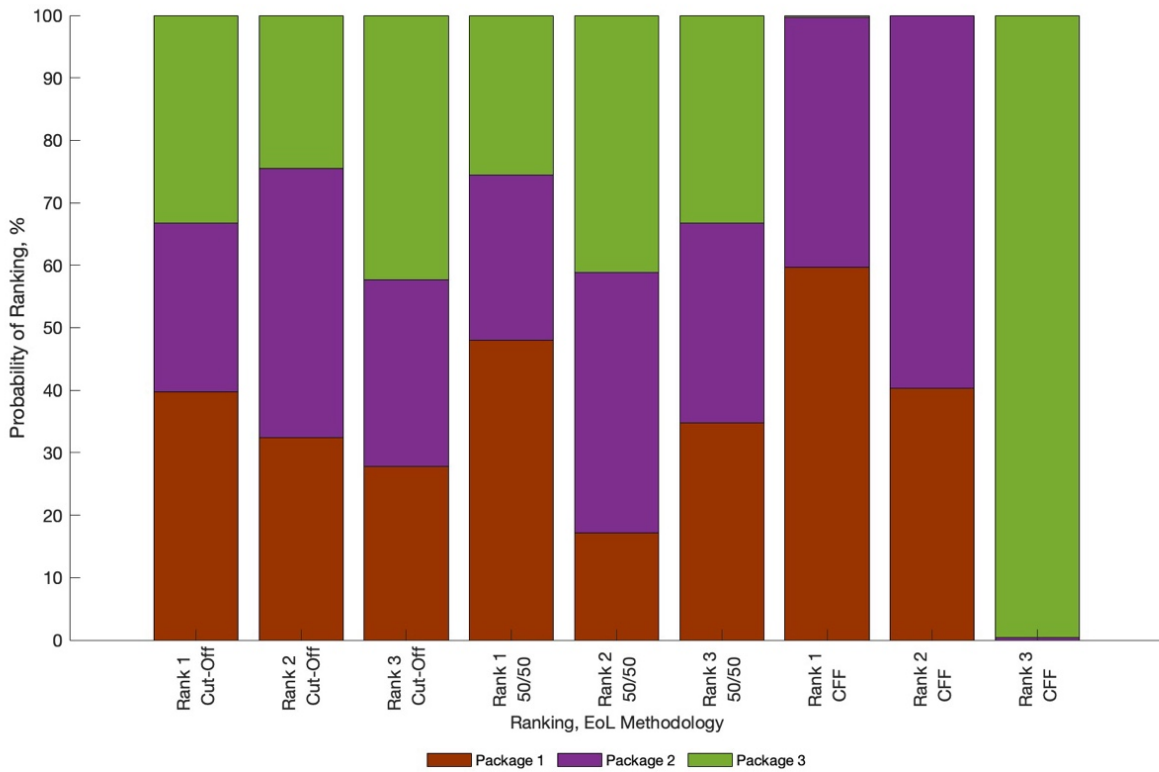


Figure 3. 9: Results of SMAA ranking among EoL models: cut-off, 50/50, and CFF. Rankings were obtained using TRACI 2.1 V1.06, and an initial 10,000 Monte Carlo runs, and then 2,000 runs using SMAA methodology.

3.4.8 Keeping it in perspective

In addition to package-specific analysis, the product in this case was rather complex to model to allow for package-product comparison, so milk powder was used as a proxy.

Figure 3. 10 shows the breakdown among all the components of the steel can (Package 3) packaging system as well as the 1,000 g of a milk powder product. This analysis demonstrates the concept that the product being packaged often has a much higher impact than the packaging alone. The lime green color dominating 8 of the 10 impact categories represents the 1,000 g of milk powder, which presumably has less of an impact than most infant formula products. This result suggests that in all three package systems, since the metal packaging has the largest impact according to SMAA results, the infant formula product has a much higher impact than all the packaging involved in delivering the product to consumers. The breakdowns for the plastic package (Package 1) and composite package (Package 2) with the milk powder product can be found in **Figure 3. 15** and **Figure 3. 16** respectively, in **Section 3.6.4.4 Keeping it in perspective scenario**.

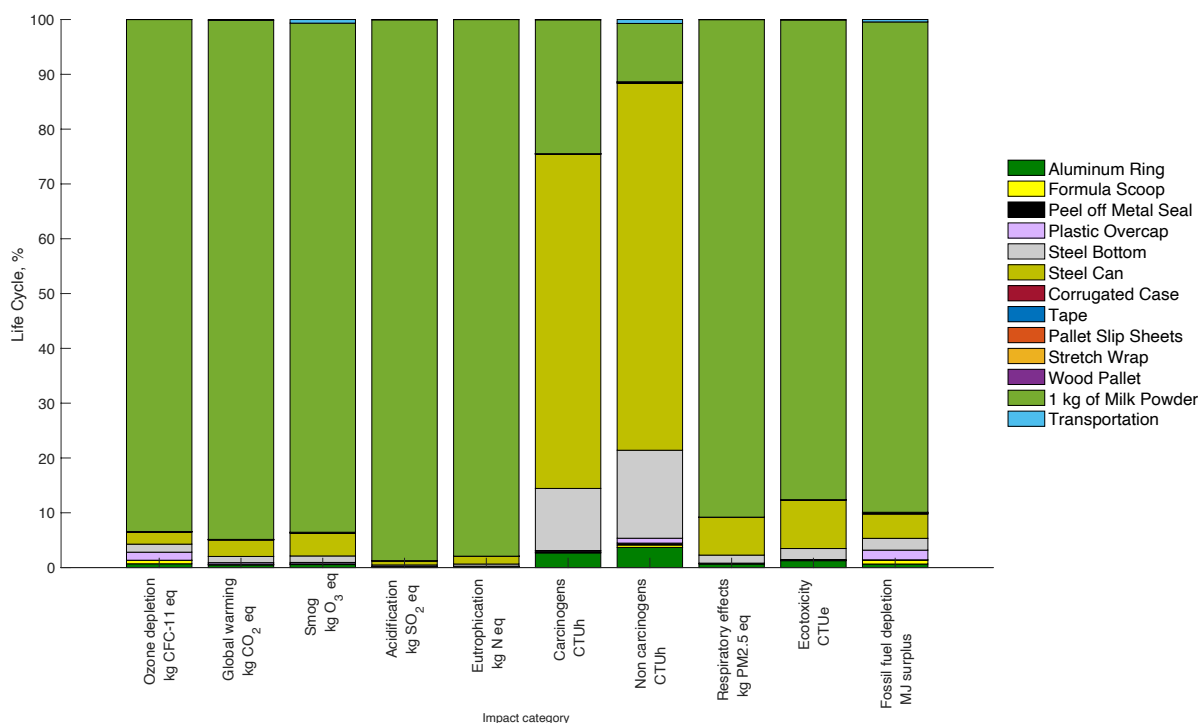


Figure 3. 10: Contribution breakdown of the assembly portion of the steel can packaging system, Package 3, with addition of 1 kg of milk powder, according to TRACI 2.1 V1.06.

Previous LCA studies performed for infant formula and similar products, such as powdered milk, have typically been done to evaluate the impact of those products compared to breastfeeding rather than in terms of packaging. Those studies, however, can provide insight into the impact of the product itself. Infant formula has several major ingredients, including milk powder, whey powder, and various proteins and sugars, including lactose and glucose, which all impact the environment. Milk powder, for example, has several reported values for CO₂-eq for every kg, including 12.64 per kg [11] and an average of 1.54 per kg in milk powder processing [15]. In comparison to breastfeeding, the use of infant formula is found to have a higher impact on the environment, as the calculated weight of formula used in a 6-month period is 21 kg. This formula weight was calculated to have an impact of roughly 226–288 kg CO₂-eq, whereas breastfeeding only generates about half the impact at 123–162 kg CO₂-eq. However, this study reports that infant formula packaging contributes little to this difference; instead, it is the product's manufacturing [28]. Infant formula packaging is often not included in studies on infant formula and nutrition products. Overall, we can conclude that although assessing the EF of the packaging systems is relevant and essential, we cannot disregard the importance of lowering the EF of the product/packaging systems.

3.5 Conclusions, limitations, and recommendations

The environmental impacts of three infant formula packages were estimated. The results did not provide clear-cut answers as to which package had the highest or lowest EF and instead involved trade-offs, which would require prioritizing sustainability goals. For the TRACI 2.1 V1.06 midpoint method, the plastic package, Package 1, has the highest impact in the ozone depletion, global warming, eutrophication, and fossil fuel depletion categories. The composite package, Package 2, has the highest impact in the smog and acidification categories. The remaining categories of carcinogens, non-carcinogens, respiratory effects, and ecotoxicity show the highest impact from the steel package, Package 3.

From the scenario analysis, it can be concluded that lightweighting the plastic lid and tub components of Package 1 can lower the environmental impact. For Package 2, changing the bottom of the package from steel to the same composite material used in the can component reduces the environmental impact. For Package 3, lightweighting the steel can component could lower the environmental impact.

Results vary only slightly when using the 50/50 recycling allocation method. For the TRACI 2.1 V1.06 midpoint method, the plastic package, Package 1, has the highest impact in the ozone depletion, global warming, eutrophication, and fossil fuel depletion categories. The composite package, Package 2, has a low impact in all categories. The remaining categories of smog, acidification, carcinogens, non-carcinogens, respiratory effects, and ecotoxicity show the highest impact from the steel package, Package 3. A different conclusion was reached with the CFF method for modeling EoL as well. The difference in results among these methods occurs due to the various assumptions used; for instance, the CFF incorporates primary and secondary materials as well as energy recovery while the cut-off method assumes that none of the environmental impacts from recycling are included in the EF. For the TRACI 2.1 V1.06 midpoint method, Package 1 has the highest impact in the fossil fuel depletion category; Package 2 does not have the highest impact in any category; and the remaining categories of ozone depletion, global warming, smog, acidification, eutrophication, carcinogens, non-carcinogens, respiratory effects, and ecotoxicity show the highest impact from Package 3.

Using the SMAA methodology for addressing trade-offs within each set of comparative results, it was found that the final ranking of each package from lowest to highest overall environmental footprint remains the same. In all three cases, Package 1 (plastic) ranks as having the lowest environmental footprint compared to the others, and Package 2 (composite) ranks as the second lowest environmental footprint compared to the other packages. Package 3 (steel can) has the highest probability of having the largest environmental footprint for the cut-off and CFF EoL methodologies. In the 50/50 methodology, Package 1 (plastic) has the highest probability of being ranked with the highest environmental footprint. Still, the probability is lower than that, ranking the plastic package as having the lowest environmental footprint. This finding indicates that all three EoL methodologies result in the same conclusions when addressing trade-offs using SMAA. The results of this comparative LCA for infant formula packages show that Package 1 is the option with the lowest environmental footprint and Package 3 is the option with the highest environmental footprint, with Package 2 being between the two.

Finally, adding the milk powder product to all three systems demonstrates that the packaging components of similar products have much lower environmental impacts than the products themselves. By keeping this in perspective, along with the demonstration of few differences among EoL modeling, LCA practitioners in the packaging industry can worry less

about the choice of EoL modeling, at least in terms of the environmental impacts. Interested parties can also recognize that when looking to lower the environmental footprint of a SKU, adjusting the packaging may not make a large difference and instead they should reduce overall product/package EF impacts.

LCIA results present relative and potential, not measured, environmental impacts. They are relative expressions (to the functional unit) that cannot be used to predict specific instances of adverse impacts or risk or whether standards or safety margins are exceeded. So, the direct comparison with other studies may not be representative. The use of a similar functional unit and goal and scope could provide insights; however, it is uncertain that solid conclusions can be derived since assumptions and background and foreground data may differ. LCIA models generally attempt to represent the most probable case rather than considering a worst case, safety margin, or similar conservative approaches often taken in a regulatory context.

Additionally, the categories evaluated here do not cover all the environmental impacts associated with human activities. For example, impacts such as noise, odors, electromagnetic fields, microplastics, and others are not included in the present assessment. The methodological developments regarding such impacts are insufficient to allow for their consideration. LCIA methodologies cannot characterize the full array of emissions released to soil, air, and water from processes. However, they do characterize the most well-known pollutants and, in doing so, provide the best estimate to evaluate environmental impact.

For the results of this study, the environmental impact of the product delivered (infant formula) is not analyzed at any stage. The transportation of the different EoL disposal scenarios was modeled based on the assumption of standard distances in urban cities for landfill, incineration, and recycling. For raw materials and/or conversion, the main database for modeling the packaging systems uses U.S. data and/or technologies described in European operations adapted to the U.S. and updated with U.S. electricity data. For these reasons, the results may not be directly applicable to geographies outside this boundary. Additionally, social and economic impacts were beyond the scope of this work, and therefore they were excluded. The above conclusions presented must be considered only within the context of the study and by keeping in mind the main assumptions listed in the previous section and study limitations presented here.

Overall recommendations can be made based on the above conclusions, results, and limitations of this LCA study. The results of this study can inform recommendations based on

the sustainability approach of a particular company. If the company prioritizes reducing their impact in the fossil fuel depletion and global warming categories, it may be beneficial to produce and sell more steel and composite containers, as the plastic container has the highest impact in those two categories. On the other hand, if it is more ideal to reduce impact in the respiratory effects and ecotoxicity categories, producing and selling more plastic and composite containers would be beneficial, as the steel container has a much higher impact in those categories. According to the SMAA methodology, Package 1 (plastic) will be the best option if a company would like to reduce its overall package environmental footprint. As another recommendation, the results suggest an advantage in lightweighting of primary package components to reduce the overall impact in all three systems. In each lightweighting scenario, each TRACI 2.1 V1.06 category experienced a reduction, which can result in overall impact reduction.

Acknowledgments

The authors thank Perrigo® for providing primary data for this work and collaborating on assessing the environmental footprint of packaging designs, and providing partial financial support for A.L. and A.B. The authors thank Lise Laurin and Bryton Moeller for introducing them to the SMAA methodology and Valentina Prado Lopez for providing access to the beta version of LCA-SMAA software. The authors also thank Wanwarang Limsukon for assistance in creating figures.

Supporting Information

Further information about the modeling and results of the full LCA can be found in the Supporting Information (SI), **3.6 Supporting Information**.

Conflict of interest

The authors declare no conflict of interest.

Authors responsible

Abigale Lewis: Data Curation, Formal Analysis, Writing – Original Draft. **Anibal Bher:** Methodology, Visualization, Writing – Review and Editing. **Satish Joshi:** Review and Editing. **Matthew Daum:** Review and Editing, Funding acquisition. **Rafael Auras:** Conceptualization, Project Administration, Supervision, Writing – Review and Editing, Funding acquisition. All the authors approved the final version of the manuscript.

3.6 Supporting Information

3.6.1 Life Cycle Inventory

3.6.1.1 Data Used in Modeling

All packaging systems' components have been modeled independently of the other components. This allows a more objective analysis and review of individual components besides their contribution to the overall life cycle for each packaging system.

Package 1, Plastic Package

Components Package 1, primary level

- Back Label: This component was modeled with four different materials, the first being “Polypropylene resin, at plant NREL/RNA U”, which was taken from modified US LCI data modified by Long Trail Sustainability for DATASMART in 2008. The processes included in this dataset were unspecified; however, the geography was for North America. The manufacturing process was considered with the raw materials, energy, infrastructure, land use, and the generation of solid wastes and emissions into air and water. Transportation of raw materials and solid wastes was also included. The geography of this data was from European manufacturers, with no further information from said companies being provided. Finally, the process “Printing Colour, Offset, 47.5% solvent, at plant/US- US-EL U” was used to model the printing of the label. This data was part of an Ecoinvent 2.2 dataset modified by Long Trail Sustainability for DATASMART in 2003. It includes the material inputs (solvents, binders, pigments, fillers) and estimation of energy consumption; however, no emissions to air and water were included. The geography of the data was based on a survey from Switzerland. The processing and conversion process chosen for the Back Label was “Extrusion, plastic film/US- US-EL U”. This data was modified by Long Trail Sustainability from Ecoinvent v2.2 dataset for DATASMART in 2005. The processes included in this dataset were the auxiliaries and energy demand for the mentioned conversion process of plastics. The geography of this data was from different European and Swiss converting companies. In addition, there was the component “Laminating, foil, with acrylic binder/US- US-EL U”. The data was chosen from an Ecoinvent v2.2 dataset that was modified by Long Trail Sustainability for DATASMART in 2007. The data included estimating electricity use for the laminating and cutting of foils. Only glue from laminating processes was included,

and estimation for waste processing of glue overspray was included. The data had no specific geographic origin, and the energy values were undefined but modified to represent the US. Another process added was transportation (see Transportation).

- Metal Film: This component was modeled as two materials, the first being “Aluminum, primary, at plant/US- US-EL U”. This data was modified by Long Trail Sustainability from an Ecoinvent v2.2 dataset for DATASMART in 2003. The data includes cast aluminum ingot production, transport of the material to the plant, and disposal of the wastes. The geography was from Swiss plants as well as European data. The second material chosen was “Acrylic Binder, 34% in H₂O, at plant/US- US EL U”. This data was part of an Ecoinvent 2.2 dataset modified by Long Trail Sustainability for DATASMART in 2003. The manufacturing process was considered with the raw materials, energy, infrastructure, land use, and generation of solid wastes and emissions into air and water. Transportation of raw materials and solid wastes was also included. The geography of this data from European manufacturers, with no further information from said companies being provided. The component also involved two converting processes, the first being “Laminating, foil, with acrylic binder/US- US-EL U”. The data was chosen from an Ecoinvent v2.2 dataset that was modified by Long Trail Sustainability for DATASMART in 2007. The data included estimating electricity use for the laminating and cutting of foils. Only glue from laminating processes was included, and estimation for waste processing of glue overspray was included. The data had no specific geographic origin, and the energy values were undefined but modified to represent the US. The other converting process used in modeling was “Sheet Rolling, Aluminum/US- US-EL U”. This data was modified by Long Trail Sustainability from an Ecoinvent v2.2 dataset for DATASMART in 2003. The processes included were all the process steps, which can be attributed to semi-fabrication (sawing, scalping, hot rolling, cold rolling, solution heat treatment, finishing, and packaging). Another process added was transportation (see Transportation).
- Formula Scooper: This component was modeled as “Polypropylene resin, at plant NREL/RNA U”, taken from a US LCI dataset modified by Long Trail Sustainability for DATASMART in 2008. The processes included in this dataset were unspecified; however, the geography was for North America. The component also included a

converting process of “Injection Moulding/US US-El U” taken from an Ecoinvent v2.2 dataset modified by Long Trail Sustainability for DATASMART in 2003. The data included the auxiliaries and energy demand for the mentioned conversion process of plastics. The geography data was from different European and Swiss conversion companies. The energy values were undefined but modified to represent the US. Another process added was transportation (see Transportation).

- Lid Label: This component was modeled with four different materials, the first being “Polypropylene resin, at plant NREL/RNA U”, which was taken from a modified US LCI dataset that was modified by Long Trail Sustainability for DATASMART in 2008. The processes included in this dataset were unspecified; however, the geography was for North America. The manufacturing process was considered the raw materials, energy, infrastructure, land use, and the generation of solid wastes and emissions into air and water. Transportation of raw materials and solid wastes was also included. The geography of this data from European manufacturers, with no further information from said companies being provided. Finally, the process “Printing Colour, Offset, 47.5% solvent, at plant/US- US-EL U” was used to model the printing of the label. This data was part of an Ecoinvent 2.2 dataset modified by Long Trail Sustainability for DATASMART in 2003. It includes the material inputs (solvents, binders, pigments, fillers) and energy consumption estimation; however, no emissions to air and water were included. The geography of the data was based on a survey from Switzerland. The processing and conversion process chosen for the Back Label was “Extrusion, plastic film/US- US-El U”. This data was modified by Long Trail Sustainability from an Ecoinvent 2.2 dataset for DATASMART in 2005. The processes included in this dataset were the auxiliaries and energy demand for the mentioned conversion process of plastics. The geography of this data was from different European and Swiss converting companies. In addition, the process of “Laminating, foil, with acrylic binder/US- US-EL U” was included in modeling. The data was chosen from an Ecoinvent v2.2 dataset modified by Long Trail Sustainability for DATASMART in 2007. The data included estimating electricity use for the laminating and cutting of foils. Only glue from laminating processes was included, and an estimation for the waste process of glue overspray was included. The data had no specific geographic origin, and the energy

values were undefined but modified to represent the US. Another process added was transportation (see Transportation).

- Plastic Lid: This component was modeled as “Polypropylene resin, at plant NREL/RNA U”, taken from a modified US LCI data modified by Long Trail Sustainability for DATASMART in 2008. The processes included in this dataset were unspecified; however, the geography was for North America. The component also included a converting process of “Injection Moulding/US US-El U” taken from an Ecoinvent v2.2 dataset modified by Long Trail Sustainability for DATASMART in 2003. The data included the auxiliaries and energy demand for the mentioned conversion process of plastics. The geography data was from different European and Swiss conversion companies. The energy values were undefined but modified to represent the US. Another process added was transportation (see Transportation).
- Plastic Tub: The plastic tub was modeled with two different materials, the first being “High Density Polyethylene resin, at plant NREL/RNA U”. This data was a US LCI dataset modified by Long Trail Sustainability for DATASMART in 2008. The processes included for this data were unspecified, and the geography was from North America (US and Canada). The second material used to model was “Ethylene Vinyl Acetate copolymer, at plant/US- US-EL U”. The data was chosen from an Ecoinvent v2.2 dataset that was modified by Long Trail Sustainability for DATASMART in 2007. The included processes were the raw materials and chemicals used for production, transport of materials to the manufacturing plant, estimated emissions to air and water from production, estimation of energy demand, and plant infrastructure; however, solid wastes were omitted. The dataset has no specific geographical origin. This component was also modeled with two main processing and conversion techniques, the first being “Blow moulding/US- US-EL U”. This process contains the auxiliaries and energy demand for the mentioned conversion process of plastics. The geography of the data was from various Swiss and European converting companies. The second conversion process used was “Extrusion, plastic film/US- US-El U”. This data was modified by Long Trail Sustainability from an Ecoinvent v2.2 dataset for DATASMART in 2005. The included processes in this dataset were the auxiliaries and energy demand for the mentioned conversion process of plastics. The geography of this data was from different European

and Swiss converting companies. The energy values were undefined but modified to represent the US. Another process added was transportation (see Transportation).

- Silver Tamper-Evident Sticker: This component was modeled as “Kraft paper, unbleached, at plant/US- US-El U”, which was taken from a modified Ecoinvent v2.2 dataset that was modified by Long Trail Sustainability for DATASMART in 2003. The included processes were the European production of unbleached kraft paper in an integrated mill – including transportation, wood handling, chemical pulping, paper production, energy production on-site, and internal wastewater treatment. The geography was data from one European producer and a Finnish database used as European average data. Another material used to model this component was “Aluminum, primary, at plant/US- US-El U”. This material was chosen from a US LCI dataset modified by Long Trail Sustainability for DATASMART in 2003. The set includes the primary aluminum ingot production, including the plant itself. It also includes transporting materials to the plant and disposing of waste. The geography was North America, and the processes were updated for US data; however, some Swiss datasets were used to model European data. The binder between the Kraft Paper and Aluminum was “Acrylic Binder, 34% in H₂O, at plant/US- US EL U”. This data was part of an Ecoinvent 2.2 dataset that was modified by Long Trail Sustainability for DATASMART in 2003. The manufacturing process was considered the raw materials, energy, infrastructure, land use, and generation of solid wastes and emissions into air and water. Transportation of raw materials and solid wastes was also included. The geography of this data was from European manufacturers, with no further information from said companies being provided. In addition, the process “Laminating, foil, with acrylic binder/US- US-EL U” was used in modeling. The data was chosen from an Ecoinvent v2.2 dataset modified by Long Trail Sustainability for DATASMART in 2007. The data included estimating electricity use for the laminating and cutting of foils. Only glue from laminating processes was included, and estimation for waste processing of glue overspray was included. The data had no specific geographic origin, and the energy values were undefined but modified to represent the US. Another process added was transportation (see Transportation).
- Tear-Off Plastic Area: This component was modeled as “Polypropylene resin, at plant NREL/RNA U”, taken from a modified US LCI data modified by Long Trail

Sustainability for DATASMART in 2008. The included processes in this dataset were unspecified; however, the geography was for North America. The component also included a converting process of “Injection Moulding/US US-El U” taken from a modified Ecoinvent v2.2 dataset modified by Long Trail Sustainability for DATASMART in 2003. The data included the auxiliaries and energy demand for the mentioned conversion process of plastics. The geography data was from different European and Swiss conversion companies. Another process added was transportation (see Transportation).

- **Wrap Around Label:** This component was modeled with four different materials, the first being “Polypropylene resin, at plant NREL/RNA U”, which was taken from a modified US LCI data that was modified by Long Trail Sustainability for DATASMART in 2008. The included processes in this dataset were unspecified; however, the geography was for North America. The manufacturing process was considered with the raw materials, energy, infrastructure, land use, and generation of solid wastes and emissions into air and water. Transportation of raw materials and solid wastes was also included. The geography of this data from European manufacturers, with no further information from said companies being provided. Finally, the process “Printing Colour, Offset, 47.5% solvent, at plant/US- US-EL U” was used to model the printing of the label. This data was part of an Ecoinvent 2.2 dataset modified by Long Trail Sustainability for DATASMART in 2003. It includes the material inputs (solvents, binders, pigments, fillers) and estimation of energy consumption; however, no emissions to air and water were included. The geography of the data was based on a survey from Switzerland. The processing and conversion process chosen for the Back Label was “Extrusion, plastic film/US- US-El U”. This data was modified by Long Trail Sustainability from an Ecoinvent v2.2 dataset for DATASMART in 2005. The included processes in this dataset were the auxiliaries and energy demand for the mentioned conversion process of plastics. The geography of this data was from different European and Swiss converting companies. In addition, the process “Laminating, foil, with acrylic binder/US- US-EL U” was used in modeling. The data was chosen from an Ecoinvent v2.2 dataset that was modified by Long Trail Sustainability for DATASMART in 2007. The data included estimation of electricity use for the laminating and cutting of foils. Only glue from

laminating processes was included and an estimation for waste processing of glue overspray was included. The data had no specific geographic origin, and the energy values were undefined but modified to represent the US. Another process added was transportation (see Transportation).

Components Package 1, secondary level

- Corrugated Case: This component was modeled as “Corrugated board, mixed fibre, single wall, at plant/US- US-EI U”. This data was modified by Long Trail Sustainability from an Ecoinvent v2.2 dataset for DATASMART in 2007. The processes included were producing corrugated board out of corrugated base papers. Energy production, corrugated board production, and wastewater treatment were also included. The geography of this data was estimated based on average European data. Another process added was transportation (see Transportation).
- Dividers: This component was modeled as “Corrugated board, mixed fibre, single wall, at plant/US- US-EI U”. This data was modified by Long Trail Sustainability from an Ecoinvent 2.2 dataset for DATASMART in 2007. The processes included were producing corrugated boards out of corrugated base papers. Energy production, corrugated board production, and wastewater treatment were also included. The geography of this data was estimated based on average European data. Another process added was transportation (see Transportation).
- Glue: This component was modeled as “Polyurethane adhesive {GLO}|market for polyur”. This dataset was included in the Ecoinvent v3 and was created in 2021. Included processes start with polyurethane adhesives leaving the production facility and end with receiving the glue at the place it was to be applied. The geography of this data was global. Another process added was transportation (see Transportation).

Components Package 1, tertiary level

- Pallet Slip Sheets: This component was modeled as “Corrugated board, mixed fibre, single wall, at plant/US- US-EI U”. This data was modified by Long Trail Sustainability from an Ecoinvent v2.2 dataset for DATASMART in 2007. The processes included were producing corrugated boards out of corrugated base papers. Energy production, corrugated board production, and wastewater treatment were also included. The

geography of this data was estimated based on average European data. Another process added was transportation (see Transportation).

- **Stretch Wrap:** This component was modeled as two components, the first being the stretch wrap itself as “Stretch Wrap, LLDPE film, at plant/US U”. This data was modified by Long Trail Sustainability from an Ecoinvent 2.2 dataset for DATASMART in 2003. It includes the plastic amount and transport from the production site and the dataset “Extrusion, plastic film”. The geography was based on average European converting companies. The second component was the core board in which the stretch wrap was stored, which was modeled as “Core Board, at plant/US- US-EI U”. This dataset was also modified by Long Trail Sustainability from an Ecoinvent 2.2 dataset for DATASMART in 2003. Included processes were the material input, water (cooling and process) consumption, energy consumption, and emissions to air and water. The geography includes one Finnish plant and average European data. The energy values were undefined but modified to represent the US. Another process added was transportation (see Transportation).
- **Wood Pallet:** This component was modeled as “Pallet (22kg)/US- US-EI U”. This data was modified by Long Trail Sustainability from an Ecoinvent 2.2 dataset for DATASMART in 2003. The process included only the materials and not the actual construction of the pallet itself. The pallet system examined was gate to gate, and because the lifespan of a pallet was so long, the waste treatment was not included either. The energy values were undefined but modified to represent the US. Another process added was transportation (see Transportation).

Package 2, Composite Package

Components Package 2, primary level

- **Aluminum Ring:** This component was modeled as “Aluminum, primary, at plant/US- US-EI U”. This material was chosen in modeling from a US LCI dataset modified by Long Trail Sustainability for DATASMART in 2003. The set includes the primary aluminum ingot production, including the plant itself. It also includes transporting materials to the plant and disposing of waste. The geography was North America, and the processes were updated for US data; however, some Swiss datasets were used to model European data. This component also includes a processing and conversion portion of the

modeling, named “Metal working, average for aluminum production manufacturing {GLO}| market for | Cut-Off U”. This data was a global average that includes all the processes needed to make semi-manufactured aluminum, starting with service generation, and ending with the service being delivered to the consumers. This data also includes transportation in the manufacturing process, machinery, infrastructure, metal operations, and any additional aluminum input. The modeled dataset was built in 2011 within the Ecoinvent v3.3 database. Another process added was transportation (see Transportation).

- Composite Can: This component was modeled with three different materials as it was a composite material with plastic, paperboard, and metal portions. The most abundant portion was the paperboard portion, modeled as “Kraft paper, unbleached, at plant/US-US-El U”. This data was a version of an Ecoinvent v2.2 dataset that was modified by Long Trail Sustainability for DATASMART in 2003. The data includes the European production of unbleached kraft paper in an integrated mill, which includes transportation to and from the mill, wood handling, chemical pulping, paper production, energy production on-site and internal wastewater treatment. The geography of the data was from one European producer and a Finnish database used as the European average. The second largest material portion was modeled as “Polypropylene resin, at plant NREL/RNA U”, taken from a modified US LCI dataset modified by Long Trail Sustainability for DATASMART in 2008. The included processes in this dataset were unspecified; however, the geography was for North America. The third material portion was modeled as “Aluminum, primary, at plant/US-US-El U”. This material was chosen in modeling from a US LCI dataset modified by Long Trail Sustainability for DATASMART in 2003. The set includes the primary aluminum ingot production, including the plant itself. It also includes transporting materials to the plant and disposing waste. The geography was North America, and the processes were updated for US data; however, some Swiss datasets were used to model European data. This component also included a processing and conversion technique, which was modeled as “Laminating, foil, with acrylic binder/US-US-EL U”. The data was chosen from a Ecoinvent v2.2 dataset that was modified by Long Trail Sustainability for DATASMART in 2007. The data included estimating electricity use for the laminating and cutting foils. Only glue from laminating processes was included, and an estimation for the waste process of glue

overspray was included. The data had no specific geographic origin, and the energy values were undefined but modified to represent the US. Additionally, the process “Industrial machine, heavy, unspecified, at plant/US-/I US-El U” was used to represent the tubing process in manufacturing. This dataset includes the essential materials and the transportation of new parts to the assembly parts. The geography includes specific elementary flows from Swiss companies. Another process added was transportation (see Transportation).

- Formula Scooper: This component was modeled as “Polypropylene resin, at plant NREL/RNA U”, taken from a modified US LCI dataset modified by Long Trail Sustainability for DATASMART in 2008. The included processes in this dataset were unspecified; however, the geography was for North America. The component also included a converting process of “Injection Moulding/US US-El U” taken from an Ecoinvent v2.2 dataset modified by Long Trail Sustainability for DATASMART in 2003. The data included the auxiliaries and energy demand for the mentioned conversion process of plastics. The geography data was from different European and Swiss conversion companies. Another process added was transportation (see Transportation).
- Full Label: This component was modeled as two materials, the first being “Kraft paper, bleached, at plant/US- US-El U”. This data was a modified version of an Ecoinvent v2.2 dataset that was modified by Long Trail Sustainability for DATASMART in 2003. The data includes the European production of unbleached kraft paper in an integrated mill, which includes transportation to and from the mill, pulp handling, paper production, energy production on-site, and internal wastewater treatment. The geography of the data was from one Swiss producer used as the European average. The second material was “Acrylic Binder, 34% in H₂O, at plant/US- US EL U”. This data was part of an Ecoinvent 2.2 dataset modified by Long Trail Sustainability for DATASMART in 2003. The manufacturing process was considered with the raw materials, energy, infrastructure, land use, and the generation of solid wastes and emissions into air and water. Transportation of raw materials and solid wastes was also included. The geography of this data from European manufacturers, with no further information from said companies being provided. Additionally, the process “Use, printer, laser jet, colour, per kg printed paper/US- US-El U” was used to model printing of the label. This data was modified by

Long Trail Sustainability from an Ecoinvent v2.2 dataset for DATASMART in 2007. The data describes using a color laser jet printer in an office per 1 kg of printed paper. This dataset operates on a specified lifespan and energy consumption. The geography of this data was international. Another process added was transportation (see Transportation).

- Peel Off Metal Seal: This component was modeled as “Steel, low-alloyed, at plant/ US- US-El U”. This data was a version of an Ecoinvent v2.2 dataset that was modified by Long Trail Sustainability for DATASMART in 2007. Included processes were a mix of differently produced steels and hot rolling. The geography of the data was from various plants in the EU. The processing portion of this component was “Steel product manufacturing, average metalworking/US- US-El U”. This data was a version of Ecoinvent v2.2 data modified by Long Trail Sustainability for DATASMART in 2007. It includes manufacturing processes to make a semi-manufactured product into a final product, using average values for machine processes, factory infrastructure, and operations. The main geography used was from Germany and Europe; however, the energy was for the US. Another process added was transportation (see Transportation).
- Plastic Over cap: This component was modeled as “Linear low density polyethylene resin, at plant NREL/RNA U”. This dataset was US LCI data with dummy data filled by Long Trail Sustainability for DATASMART in 2008. The included processes were unspecified, and the geography was from North America. The processing portion of this component was modeled as “Injection Moulding/US US-El U” which was taken from an Ecoinvent v2.2 dataset modified by Long Trail Sustainability for DATASMART in 2003. The data included the auxiliaries and energy demand for the mentioned conversion process of plastics. The geography data was from different European and Swiss conversion companies. Another process added was transportation (see Transportation).
- Steel Bottom: This component was modeled as “Steel, low-alloyed, at plant/ US- US-El U”. This data was a version of Ecoinvent v2.2 data modified by Long Trail Sustainability for DATASMART in 2007. Included processes were a mix of differently produced steels and hot rolling. The geography of the data was from various plants in the EU. The processing portion of this component was “Metal working machine operation, average process heat/US- US-El U”. This data was a version of an Ecoinvent v2.2 dataset modified by Long Trail Sustainability for DATASMART in 2007. It includes the

materials, energies, and emissions related to the machines used for machining metal products. It was mainly electricity, compressed air, and solvents. The geography was mainly focused on Germany and Europe. A second processing and converting technique used to model this component was “Sheet Rolling, Steel/US- US-EL U”. This data was modified by Long Trail Sustainability from an Ecoinvent v2.2 dataset for DATASMART in 2003. The data includes the process steps of continuous picking line, cold rolling, annealing, tempering, inspecting, and finishing, packing coils and sheets, and roll maintenance. The geography of the dataset was representative of the European Union. Another process added was transportation (see Transportation).

Components Package 2, secondary level

- Corrugated Case: This component was modeled as “Corrugated board, mixed fibre, single wall, at plant/US- US-El U”. This data was modified by Long Trail Sustainability from an Ecoinvent v2.2 dataset for DATASMART in 2007. The processes included were producing corrugated boards out of corrugated base papers. Energy production, corrugated board production, and wastewater treatment were also included. The geography of this data was estimated based on average European data. The energy values were undefined but modified to represent the US. Another process added was transportation (see Transportation).
- Tape: This component was modeled as “Polypropylene resin, at plant NREL/RNA U”, which was taken from modified US LCI data that was modified by Long Trail Sustainability for DATASMART in 2008. The included processes in this dataset were unspecified; however, the geography was for North America. In addition, the material, “Ethyl vinyl acetate copolymer, at plant/US- US-El U” was used to model the adhesive of the tape. This data was modified by Long Trail Sustainability from an Ecoinvent v2.2 dataset for DATASMART in 2007. It includes the raw materials and chemicals used for production, transport of materials to manufacturing plant, estimated emissions to air and water from production, estimations of energy demand and infrastructure of the plant. Geography of this data has no specific origin. The conversion and processing modeling chosen was “Extrusion, plastic film/US- US-El U”. This data was modified by Long Trail Sustainability from an Ecoinvent v2.2 dataset for DATASMART in 2005. The included processes in this dataset were the auxiliaries and energy demand for the

mentioned conversion process of plastics. The geography of this data was from different European and Swiss converting companies. Another process added was transportation (see Transportation).

Components Package 2, tertiary level

- Pallet Slip Sheets: This component was modeled as “Corrugated board, mixed fibre, single wall, at plant/US- US-EI U”. This data was modified by Long Trail Sustainability from an Ecoinvent v2.2 dataset for DATASMART in 2007. The processes included in this date were the production of corrugated board out of corrugated base papers. Energy production, corrugated board production, and wastewater treatment were also included. The geography of this data was estimated based on average European data. Another process added was transportation (see Transportation).
- Stretch Wrap: This component was modeled as two components, the first being the stretch wrap itself being “Stretch Wrap, LLDPE film, at plant/US U”. This data was modified by Long Trail Sustainability from an Ecoinvent v2.2 dataset for DATASMART in 2003. It includes the plastic amount and transport from the production site and the dataset “Extrusion, plastic film”. The geography was based on average European converting companies. The second component of this was the core board in which the stretch wrap was stored, which was modeled as “Core Board, at plant/US- US-EI U”. This dataset was also modified by Long Trail Sustainability from an Ecoinvent v2.2 dataset for DATASMART in 2003. Included processes were the material input, water (cooling & process) consumption, energy consumption, and emissions to air and water. The geography includes one Finnish plant and average European data. Another process added was transportation (see Transportation).
- Wood Pallet: This component was modeled as “Pallet (22kg)/US- US-EI U”. This data was modified by Long Trail Sustainability from an Ecoinvent v2.2 dataset for DATASMART in 2003. The included process in this data was only the materials and not the actual construction of the pallet itself. The pallet system examined was gate to gate and because the lifespan of a pallet was so long the waste treatment was not included either. Another process added was transportation (see Transportation).

Package 3, Steel Package

Components Package 3, primary level

- Aluminum Ring: This component was modeled as “Aluminum, primary, at plant/US-US-EI U”. This material was chosen in modeling from a US LCI dataset modified by Long Trail Sustainability for DATASMART in 2003. The set includes the primary aluminum ingot production, including the plant itself. It also includes transporting materials to the plant and disposing waste. The geography was North America, and the processes were updated for US data; however, some Swiss datasets were used to model European data. This component also includes a processing and conversion portion of the modeling, named “Metal working, average for aluminum production manufacturing {GLO}| market for | Cut-Off U”. This data was a global average that includes all the processes needed to make semi-manufactured aluminum, starting with service generation, and ending with the service being delivered to the consumers. This data also includes transportation in the manufacturing process, the machinery, infrastructure, metal operations, and any additional aluminum input. The modeled dataset was built in 2011 within the Ecoinvent v3.3 database. Another process added was transportation (see Transportation).
- Formula Scooper: This component was modeled as “Polypropylene resin, at plant NREL/RNA U”, taken from a modified US LCI data modified by Long Trail Sustainability for DATASMART in 2008. The included processes in this dataset were unspecified, however the geography was for North America. The component also included a converting process of “Injection Moulding/US US-EI U” taken from an Ecoinvent v2.2 dataset modified by Long Trail Sustainability for DATASMART in 2003. The data included the auxiliaries and energy demand for the mentioned conversion process of plastics. The geography data was from European and Swiss conversion companies. Another process added was transportation (see Transportation).
- Peel Off Metal Seal: This component was modeled as “Steel, low-alloyed, at plant/ US-US-EI U”. This data was a version of an Ecoinvent v2.2 dataset that was modified by Long Trail Sustainability for DATASMART in 2007. Included processes were a mix of differently produced steels and hot rolling. The geography of the data was from various plants in the EU. The processing portion of this component was “Steel product

manufacturing, average metalworking/US- US-El U”. This data was a version of Ecoinvent v2.2 data modified by Long Trail Sustainability for DATASMART in 2007. It includes manufacturing processes to make a semi-manufactured product into a final product, using average values for machine processes, factory infrastructure, and operations. The main geography used was from Germany and Europe; however, was energy for the US. Another process added was transportation (see Transportation).

- Plastic Over cap: This component was modeled as “Linear low density polyethylene resin, at plant NREL/RNA U”. This dataset was US LCI data with dummy data filled by Long Trail Sustainability for DATASMART in 2008. The included processes were unspecified, and the geography was from North America. The processing portion of this component was modeled as “Injection Moulding/US US-El U” which was taken from an Ecoinvent v2.2 dataset modified by Long Trail Sustainability for DATASMART in 2003. The data included the auxiliaries and energy demand for the mentioned conversion process of plastics. The geography data was from European and Swiss conversion companies. Another process added was transportation (see Transportation).
- Steel Bottom: This component was modeled as “Steel, low-alloyed, at plant/ US- US-El U”. This data was a modified version of an Ecoinvent 2.2 dataset modified by Long Trail Sustainability for DATASMART in 2007. Included processes were a mix of differently produced steels and hot rolling. The geography of the data was from various plants in the EU. The processing portion of this component was “Metal working machine operation, average process heat/US- US-El U”. This data was a version of an Ecoinvent 2.2 dataset modified by Long Trail Sustainability for DATASMART in 2007. It includes the materials, energies, and emissions related to the machines used for machining metal products. It was mainly electricity, compressed air, and solvents. The geography was mainly focused on Germany and Europe. A second processing and converting technique used to model this component was “Sheet Rolling, Steel/US- US-EL U”. This data was modified by Long Trail Sustainability from an Ecoinvent 2.2 dataset for DATASMART in 2003. The data includes the process steps of continuous picking line, cold rolling, annealing, tempering, inspecting, and finishing, packing coils and sheets, and roll maintenance. The geography of the dataset was representative of the European Union. Another process added was transportation (see Transportation).

- Steel Can: This component was modeled as “Steel, low-alloyed, at plant/ US- US-El U”. This data was a version of an Ecoinvent v2.2 dataset that was modified by Long Trail Sustainability for DATASMART in 2007. Included processes were a mix of differently produced steels and hot rolling. The geography of the data was from various plants in the EU. Processing and converting techniques were used to model this component, which was “Sheet Rolling, Steel/US- US-EL U”. This data was modified by Long Trail Sustainability from an Ecoinvent 2.2 dataset for DATASMART in 2003. The data includes the process steps of continuous picking line, cold rolling, annealing, tempering, inspecting, and finishing, packing coils and sheets, and roll maintenance. The geography of the dataset was representative of the EU. Another processing and converting technique used to model this component was “Welding, arc, steel/US- US-El U”. This data was modified by Long Trail Sustainability from an Ecoinvent 2.2 dataset for DATASMART in 2003. The data includes the MAG-welding of non-alloyed steel and the transport of the filler rod and the protective gas to the place of use. The geography of the dataset was representative of the EU. The energy values were undefined but modified to represent the US. Another process added was transportation (see Transportation).

Components Package 3, secondary level

- Corrugated Case: This component was modeled as “Corrugated board, mixed fibre, single wall, at plant/US- US-El U”. This data was modified by Long Trail Sustainability from an Ecoinvent v2.2 dataset for DATASMART in 2007. The processes included in this date were producing corrugated boards out of corrugated base papers. Energy production, corrugated board production, and wastewater treatment were also included. The geography of this data was estimated based on average European data. The energy values were undefined but modified to represent the US. Another process added was transportation (see Transportation).
- Tape: This component was modeled as “Polypropylene resin, at plant NREL/RNA U”, taken from a modified US LCI dataset that was modified by Long Trail Sustainability for DATASMART in 2008. The included processes in this dataset were unspecified; however, the geography was for North America. In addition, the material, “Ethyl vinyl acetate copolymer, at plant/US- US-El U” was used to model the tape adhesive. This data was modified by Long Trail Sustainability from an Ecoinvent v2.2 dataset for

DATASMART in 2007. It includes the raw materials and chemicals used for production, transport of materials to the manufacturing plant, estimated emissions to air and water from production, estimations of energy demand, and plant infrastructure. The geography of this data has no specific origin. The conversion and processing modeling chosen was “Extrusion, plastic film/US- US-El U”. This data was modified by Long Trail Sustainability from an Ecoinvent v2.2 dataset for DATASMART in 2005. The included processes in this dataset were the auxiliaries and energy demand for the mentioned conversion process of plastics. The geography of this data was from different European and Swiss converting companies. Another process added was transportation (see Transportation).

Components Package 3, tertiary level

- Pallet Slip Sheets: This component was modeled as “Corrugated board, mixed fibre, single wall, at plant/US- US-El U”. This data was modified by Long Trail Sustainability from an Ecoinvent v2.2 dataset for DATASMART in 2007. The processes included in this date were producing corrugated boards out of corrugated base papers. Energy production, corrugated board production, and wastewater treatment were also included. The geography of this data was estimated based on average European data. The energy values were undefined but modified to represent the US. Another process added was transportation (see Transportation).
- Stretch Wrap: This component was modeled as two components, the first being the stretch wrap itself “Stretch Wrap, LLDPE film, at plant/US U”. This data was modified by Long Trail Sustainability from an Ecoinvent v2.2 dataset for DATASMART in 2003. It includes the plastic amount and transport from the production site and the dataset “Extrusion, plastic film”. The geography was based on average European converting companies. The second component of this was the core board in which the stretch wrap was stored, which was modeled as “Core Board, at plant/US- US-El U”. This dataset was also modified by Long Trail Sustainability from an Ecoinvent v2.2 dataset for DATASMART in 2003. Included processes were the material input, water (cooling & process) consumption, energy consumption, and emissions to air and water. The geography includes one Finnish plant and average European data. Another process added was transportation (see Transportation).

- Wood Pallet: This component was modeled as “Pallet (22kg)/US- US-EI U”. This data was modified by Long Trail Sustainability from an Ecoinvent v2.2 dataset for DATASMART in 2003. The included process in this data was only the materials and not the actual construction of the pallet itself. The pallet system examined was gate to gate, and because the lifespan of a pallet was so long, the waste treatment was not included either. Another process added was transportation (see Transportation).

Transportation

- Transportation for each component of every level (primary, secondary, and tertiary) was modeled as “Transport, combination truck, average fuel mix NREL/US U”. This was US LCI data with dummy data filled by LTS for DATASMART. Technology: Mixing process for combination truck, assuming 100% diesel and 0% gasoline.
- Transportation for waste management/disposal scenarios was modeled as “Transport, municipal waste collection, lorry 21t/US* US-EI U”. This process was modified from the Ecoinvent 2.2 database by LTS for DATASMART. Processes updated with US energy. Included processes: Diesel fuel consumption, air emissions from fuel combustion for Stop & Go driving, tire abrasion, brake lining abrasion, road abrasion, and re-suspended road dust. Remark: Based on a vehicle lifetime of 540,000 vehicle kilometers. Geography: Fuel consumption and uncertainty derived from literature values for settlement structure in Swiss and German municipalities. Technology: Waste collection and hydraulic compression vehicle. Gross load capacity 8.2 tons. Load factor 50%. Average load 4.1 tons. Emissions extrapolated from data for lorry 16t class (Ecoinvent 2000 report No. 14). Adaptations for air emissions to Stop & Go driving from average driving emission factors.

Electricity

- Electricity modeling was general grid for US electricity, “Electricity, medium voltage, production UCTE*, at grid/UCTE US-EI U” and “Electricity, at grid, US NREL/US U”.

Ink

- Environmental burdens of ink were selectively included with some processes and described when included. Otherwise, inks were not included in the inventory since they represent a small amount of the weight and environmental footprint.

Filling of product

- The product and the burdens of filling the containers with a product were not considered.

End-of-Life Modeling

Table 3. 4: *End of Life Breakdown for each component.*

Component Name	Recycling, %	Landfill, %	Incineration with energy recovery, %
Package 1, Plastic Package			
Back Label	0.00	80.50	19.50
Formula Scooper	3.00	78.09	18.92
Lid Label	0.00	80.50	19.50
Metal Film	34.90	52.41	12.69
Plastic Lid	3.00	78.00	18.92
Plastic Tub	18.10	65.93	15.97
Tear Off Plastic	0.00	80.50	19.50
Wrap Around Label	0.00	80.50	19.50
Corrugated Case	96.50	2.82	0.68
Corrugated Dividers	96.50	2.82	0.68
Hot Melt Glue	0.00	80.50	19.50
Pallet Slip Sheets	96.50	2.82	0.68
Stretch Wrap	13.30	69.79	16.91
Wood Pallet	26.90	58.85	14.25
Package 2, Composite Can			
Aluminum Ring	0.00	80.50	19.50
Composite Can	0.00	80.50	19.50
Formula Scoop	3.00	78.09	18.92
Full Label	0.00	80.50	19.50
Peel off Seal	81.00	15.30	3.71
Plastic Overcap	0.00	80.50	19.50
Steel Bottom	70.90	23.43	5.67
Corrugate Case	96.50	2.82	0.68
Packaging Tape	0.00	80.50	19.50
Pallet Slip Sheets	96.50	2.82	0.68
Stretch Wrap	13.30	69.79	16.91
Wood Pallet	26.90	58.85	14.25
Package 3, Steel Can			
Aluminum Ring	34.90	52.41	12.69
Formula Scoop	3.00	78.09	18.92
Peel off Seal	81.00	15.30	3.71
Plastic Overcap	0.00	80.50	19.50
Steel Bottom	70.90	23.43	5.67
Steel Can	70.90	23.43	5.67
Corrugate Case	96.50	2.82	0.68
Packaging Tape	0.00	80.50	19.50
Pallet Slip Sheets	96.50	2.82	0.68
Stretch Wrap	13.30	69.79	16.91
Wood Pallet	26.90	58.85	14.25

Package 1, Plastic Package

Components Package 1, primary level

- **Back Label:** The waste scenarios for the Back Label included modeling for the Undefined, PET, and PP (identified in SimaPro) waste types for “Incineration/US US-EI U”, “Landfill/US US-EI U”, and recycling cut-off. The rate for incineration, landfill, and recycling for the Back Label, as a function of its material composition, were modeled as 19.5%, 80.5%, and 0%, respectively [26]. Another process associated was transport (see Transportation). Additional scenario analysis was conducted as explained in Scenario modeling.
- **Formula Scooper:** The waste scenarios for the Formula Scooper included modeling for the PP (identified in SimaPro) waste type for “Incineration/US US-EI U”, “Landfill/US US-EI U”, and recycling cut-off. As a function of its material composition, the incineration, landfill, and recycling rate for the Formula Scooper were modeled as 18.9%, 78.1, and 3%, respectively [26]. Another process associated: transport (see Transportation). The recycling scenario was modeled as a process without emissions as outlined by the cut-off methodology (i.e., no emission allocated to the disposal of the material sent for recycling). Additional scenario analysis was conducted as explained in Scenario modeling.
- **Lid Label:** The waste scenarios for the Lid Label included modeling for the Undefined, PET, and PP (identified in SimaPro) waste types for “Incineration/US US-EI U”, “Landfill/US US-EI U”, and recycling cut-off. The incineration, landfill, and recycling rate for the Lid Label, as a function of its material composition, were modeled as 19.5%, 80.5%, and 0%, respectively [26]. Another process associated: transport (see Transportation). Additional scenario analysis was conducted as explained in Scenario modeling.
- **Metal Film:** The waste scenarios for the Metal Film included modeling for the Undefined and Aluminum (identified in SimaPro) waste types for “Incineration/US US-EI U”, “Landfill/US US-EI U”, and recycling cut-off. The rates for incineration, landfill, and recycling for the Metal Film, as a function of its material composition, were modeled as 12.7%, 52.4%, and 34.9%, respectively [26]. Another process associated: transport (see Transportation). The recycling scenario was modeled as a process without emissions as

outlined by the cut-off methodology (i.e., no emission allocated to the disposal of the material sent for recycling).

- Plastic Lid: The waste scenarios for the Plastic Lid included modeling for the PP (identified in SimaPro) waste type for “Incineration/US US-EI U”, “Landfill/US US-EI U”, and recycling cut-off. The incineration, landfill, and recycling rates for the Plastic Lid, as a function of its material composition, were modeled as 18.9%, 78.1%, and 3%, respectively [26]. Another process associated: transport (see Transportation). The recycling scenario was modeled as a process without emissions as outlined by the cut-off methodology (i.e., no emission allocated to the disposal of the material sent for recycling). Additional scenario analysis was conducted as explained in Scenario modeling.
- Plastic Tub: The waste scenarios for the Plastic Tub included modeling for the Plastics/Thermoplasts identified in SimaPro) waste type for “Incineration/US US-EI U”, “Landfill/US US-EI U”, and recycling cut-off. The incineration, landfill, and recycling rates for the Plastic Tub, as a function of its material composition, were modeled as 16.8145%, 65.2855%, and 18.9%, respectively respectively [26]. Another process associated: transport (see Transportation). The recycling scenario was modeled as a process without emissions as outlined by the cut-off methodology (i.e., no emission allocated to the disposal of the material sent for recycling). Additional scenario analysis was conducted as explained in Scenario modeling.
- Silver Tamper-Evident Sticker: The waste scenarios for the Silver Tamper-Evident Sticker included modeling for the Undefined, Paper/Packaging Paper, and Aluminum (identified in SimaPro) waste types for “Incineration/US US-EI U”, “Landfill/US US-EI U”, and recycling cut-off. The incineration, landfill, and recycling rates for the Silver Tamper-Evident Sticker, as a function of its material composition, were modeled as 19.5%, 80.5%, and 0% respectively [26]. Another process associated: transport (see Transportation). Scenario analysis was conducted as explained in Scenario modeling.
- Tear-Off Plastic Area: The waste scenarios for the Tear-Off Plastic Area included modeling for the PP (identified in SimaPro) waste type for “Incineration/US US-EI U”, “Landfill/US US-EI U”, and recycling cut-off. As a function of its material composition, the incineration, landfill, and recycling rates for the Tear-Off Plastic Area were modeled

as 19.5%, 80.5% and 0%, respectively [26]. Another process associated: (see Transportation).

- **Wrap Around Label:** The waste scenarios for the Lid Label included modeling for the undefined, PET, and PP (identified in SimaPro) waste types for “Incineration/US US-EI U”, “Landfill/US US-EI U”, and recycling cut-off. As a function of its material composition, the incineration, landfill, and recycling rates for the Lid Label were modeled as 19.5%, 80.5%, and 0%, respectively [26]. Another process associated: transport (see Transportation). Additional scenario analysis was conducted as explained in Scenario modeling.

Components Package 1, secondary level

- **Corrugated Case:** The waste scenarios for the disposal of the Corrugated Case included modeling for the Cardboard (identified in SimaPro) waste type for “Incineration/US US-EI U”, “Landfill/US US-EI U”, and recycling. The incineration, landfill, and recycling rates for the Corrugated Case, as a function of its material composition, were modeled as 0.7%, 2.8%, and 96.5%, respectively [26]. Another process associated: transport (see Transportation). The recycling scenario was modeled as a process without emissions.
- **Dividers:** The waste scenarios for the disposal of the Dividers included modeling for the Cardboard (identified in SimaPro) waste type for “Incineration/US US-EI U”, “Landfill/US US-EI U”, and recycling. The rates for incineration, landfill, and recycling for the Dividers, as a function of its material composition, were modeled as 0.7%, 2.8%, and 96.5%, respectively [26]. Other process associated: transport (see Transportation). The recycling scenario was modeled as a process without emissions.
- **Glue:** The waste scenarios for the disposal of the Corrugated Case included modeling for the Undefined (identified in SimaPro) waste type for “Incineration/US US-EI U”, “Landfill/US US-EI U”, and recycling. The incineration, landfill, and recycling rates for the corrugated box, as a function of its material composition, were modeled as 19.5%, 80.5%, and 0%, respectively [26]. Other process associated: transport (see Transportation).

Components Package 1, tertiary level

- **Pallet Slip Sheets:** The waste scenarios for the disposal of the Pallet Slip Sheets included modeling for the Cardboard (identified in SimaPro) waste type for “Incineration/US US-

EI U”, “Landfill/US US-EI U”, and recycling. The incineration, landfill, and recycling rates for the Pallet Slip Sheets, as a function of its material composition, were modeled as 0.7%, 2.8%, and 96.5% respectively [26]. Other process associated: transport (see Transportation). The recycling scenario was modeled as a process without emissions.

- Stretch Wrap: The waste scenarios for the disposal of the Stretch Wrap included modeling for the PE and Cardboard (identified in SimaPro) waste types for “Incineration/US US-EI U”, “Landfill/US US-EI U”, and recycling. The incineration, landfill, and recycling rates for the Stretch Wrap, as a function of its material composition, were modeled as 16.9%, 69.8%, and 13.3% respectively [26]. Other process associated: transport (see Transportation). The recycling scenario was modeled as a process without emissions.
- Wood Pallet: The waste scenarios for the disposal of the Wood Pallet included modeling for the Wood (identified in SimaPro) waste type for “Incineration/US US-EI U”, “Landfill/US US-EI U”, and recycling. The incineration, landfill, and recycling rates for the Wood Pallet, as a function of its material composition, were modeled as 14.3%, 58.8%, and 26.9% respectively [26]. Other process associated: transport (see Transportation). The recycling scenario was modeled as a process without emissions.

Package 2, Composite Package

Components Package 2, primary level

- Aluminum Ring: The waste scenarios for the Aluminum Ring included modeling for the Aluminum (identified in SimaPro) waste type for “Incineration/US US-EI U”, “Landfill/US US-EI U”, and recycling cut-off. As a function of its material composition, the incineration, landfill, and recycling rates for the Aluminum Ring were modeled as 19.5%, 80.5%, and 0%, respectively [26]. Another process associated: transport (see Transportation).
- Composite Can: The waste scenarios for the Silver Tamper-Evident Sticker included modeling for the PP, Paper/Packaging Paper, and Aluminum (identified in SimaPro) waste types for “Incineration/US US-EI U”, “Landfill/US US-EI U”, and recycling cut-off. The incineration, landfill, and recycling rates for the Composite Can, as a function of its material composition, were modeled as 19.5%, 80.5%, and 0%, respectively [26]. Another process associated: transport (see Transportation).

- **Formula Scoop:** The waste scenarios for the Formula Scoop included modeling for the PP (identified in SimaPro) waste type for “Incineration/US US-EI U”, “Landfill/US US-EI U”, and recycling cut-off. The rates for incineration, landfill, and recycling for the Formula Scoop, as a function of its material composition, were modeled as 18.9%, 78.1%, and 3%, respectively [26]. Another process associated: transport (see Transportation). The recycling scenario was modeled as a process without emissions as outlined by the cut-off methodology (i.e., no emission allocated to the disposal of the material sent for recycling).
- **Full Label:** The waste scenarios for the Full Label included modeling for the Undefined and Paper/Packaging Paper (identified in SimaPro) waste types for “Incineration/US US-EI U”, “Landfill/US US-EI U”, and recycling cut-off. The incineration, landfill, and recycling rates for the Full Label, as a function of its material composition, were modeled as 19.5%, 80.5%, and 0%, respectively [26]. Another process associated: transport (see Transportation). Scenario analysis was conducted as explained in SCENARIO MODELING.
- **Peel Off Metal Seal:** The waste scenarios for the Peel Off Metal Seal included modeling for the Steel (identified in SimaPro) waste type for “Incineration/US US-EI U”, “Landfill/US US-EI U”, and recycling cut-off. The incineration, landfill, and recycling rates for the Peel Off Metal Seal, as a function of its material composition, were modeled as 3.7%, 15.3%, 81%, respectively [26]. Another process associated: transport(see Transportation). The recycling scenario was modeled as a process without emissions as outlined by the cut-off methodology (i.e., no emission allocated to the disposal of the material sent for recycling).
- **Plastic Over cap:** The waste scenarios for the Plastic Over cap included modeling for the PE (identified in SimaPro) waste type for “Incineration/US US-EI U”, “Landfill/US US-EI U”, and recycling cut-off. The incineration, landfill, and recycling rates for the Plastic Over cap, as a function of its material composition, were modeled as 19.5%, 80.5%, and 0%, respectively [26]. Another process associated: transport (see Transportation). The recycling scenario was modeled as a process without emissions as outlined by the cut-off methodology (i.e., no emission allocated to the disposal of the material sent for recycling).

- **Steel Bottom:** The waste scenarios for the Steel Bottom included modeling for the Steel (identified in SimaPro) waste type for “Incineration/US US-EI U”, “Landfill/US US-EI U”, and recycling cut-off. As a function of its material composition, the incineration, landfill, and recycling rates for the Steel Bottom were modeled as 5.7%, 23.4%, and 70.9%, respectively [26]. Another process associated: transport (see Transportation). The recycling scenario was modeled as a process without emissions as outlined by the cut-off methodology (i.e., no emission allocated to the disposal of the material sent for recycling). Additional scenario analysis was conducted as explained in Scenario modeling.

Components Package 2, secondary level

- **Corrugated Case:** The waste scenarios for the disposal of the Corrugated Case included modeling for the Cardboard (identified in SimaPro) waste type for “Incineration/US US-EI U”, “Landfill/US US-EI U”, and recycling. The incineration, landfill, and recycling rates for the corrugated box, as a function of its material composition, were modeled as 0.7%, 2.8%, and 96.5 respectively [26]. Another process associated: transport (see Transportation). The recycling scenario was modeled as a process without emissions.
- **Tape:** The waste scenarios for the disposal of the Tape included modeling for the PP and Plastics (identified in SimaPro) waste types for “Incineration/US US-EI U”, “Landfill/US US-EI U”, and recycling. As a function of its material composition, the incineration, landfill, and recycling rates for the Tape was modeled as 19.5%, 80.5%, and 0%, respectively [26]. Another process associated: transport (see Transportation). The recycling scenario was modeled as a process without emissions.

Components Package 2, tertiary level

- **Pallet Slip Sheets:** The waste scenarios for the disposal of the Pallet Slip Sheets included modeling for the Cardboard (identified in SimaPro) waste type for “Incineration/US US-EI U”, “Landfill/US US-EI U”, and recycling. The incineration, landfill, and recycling rates for the Pallet Slip Sheets, as a function of their material composition, were modeled as 0.7%, 2.8%, and 96.5%, respectively [26]. Another process associated: transport (see Transportation). The recycling scenario was modeled as a process without emissions.
- **Stretch Wrap:** The waste scenarios for the disposal of the Stretch Wrap included modeling for the PE and Cardboard (identified in SimaPro) waste types for

“Incineration/US US-EI U”, “Landfill/US US-EI U”, and recycling. The incineration, landfill, and recycling rates for the Stretch Wrap, as a function of its material composition, were modeled as 16.9%, 69.8%, and 13.3 %, respectively [26]. Another process associated: transport (see Transportation). The recycling scenario was modeled as a process without emissions.

- Wood Pallet: The waste scenarios for the disposal of the Wood Pallet included modeling for the Wood (identified in SimaPro) waste type for “Incineration/US US-EI U”, “Landfill/US US-EI U”, and recycling. The incineration, landfill, and recycling rates for the Wood Pallet, as a function of its material composition, were modeled as 14.3%, 58.8%, and 26.9%, respectively [26]. Another process associated: transport (see Transportation). The recycling scenario was modeled as a process without emissions.

Package 3, Steel Package

Components Package 3, primary level

- Aluminum Ring: The waste scenarios for the Aluminum Ring included modeling for the Aluminum (identified in SimaPro) waste type for “Incineration/US US-EI U”, “Landfill/US US-EI U”, and recycling cut-off. As a function of its material composition, the incineration, landfill, and recycling rates for the Aluminum Ring were modeled as 19.5%, 80.5%, and 0%, respectively [26]. Another process associated: transport (see Transportation).
- Formula Scoop: The waste scenarios for the Formula Scoop included modeling for the PP (identified in SimaPro) waste type for “Incineration/US US-EI U”, “Landfill/US US-EI U”, and recycling cut-off. The rates for incineration, landfill, and recycling for the Formula Scoop, as a function of its material composition, were modeled as 18.9%, 78.1%, and 3%, respectively [26]. Another process associated: transport (see Transportation). The recycling scenario was modeled as a process without emissions as outlined by the cut-off methodology (i.e., no emission allocated to the disposal of the material sent for recycling).
- Peel Off Metal Seal: The waste scenarios for the Peel Off Metal Seal included modeling for the Steel (identified in SimaPro) waste type for “Incineration/US US-EI U”, “Landfill/US US-EI U”, and recycling cut-off. The incineration, landfill, and recycling rates for the Peel Off Metal Seal as a function of its material composition, were modeled

as 3.7%, 15.3%, 81%, respectively [26]. Other process associated: transport (see Transportation). The recycling scenario was modeled as a process without emissions as outlined by the cut-off methodology (i.e., no emission allocated to the disposal of the material sent for recycling).

- Plastic Overcap: The waste scenarios for the Plastic Over cap included modeling for the PE (identified in SimaPro) waste type for “Incineration/US US-EI U”, “Landfill/US US-EI U”, and recycling cut-off. The rates for incineration, landfill, and recycling for the Plastic Over cap, as a function of its material composition, were modeled as 19.5%, 80.5%, and 0%, respectively [26]. Other process associated: (see Transportation). The recycling scenario was modeled as a process without emissions as outlined by the cut-off methodology (i.e., no emission allocated to the disposal of the material sent for recycling).
- Steel Bottom: The waste scenarios for the Steel Bottom included modeling for the Steel (identified in SimaPro) waste type for “Incineration/US US-EI U”, “Landfill/US US-EI U”, and recycling cut-off. The rates for incineration, landfill, and recycling for the Steel Bottom, as a function of its material composition, were modeled as 5.7%, 23.4%, and 70.9%, respectively [26]. Another process associated: transport (see Transportation). The recycling scenario was modeled as a process without emissions as outlined by the cut-off methodology (i.e., no emission allocated to the disposal of the material sent for recycling).
- Steel Can: The waste scenarios for the Steel Can included modeling for the Steel (identified in SimaPro) waste type for “Incineration/US US-EI U”, “Landfill/US US-EI U”, and recycling cut-off. The rates for incineration, landfill, and recycling for the Steel Can, as a function of its material composition, were modeled as 5.7%, 23.4%, and 70.9%, respectively [26]. Another process associated: transport (see Transportation). The recycling scenario was modeled as a process without emissions as outlined by the cut-off methodology (i.e., no emission allocated to the disposal of the material sent for recycling). Additional scenario analysis was conducted as explained in Scenario modeling.

Components Package 3, secondary level

- Corrugated Case: The waste scenarios for the disposal of the Corrugated Case included modeling for the Cardboard (identified in SimaPro) waste type for “Incineration/US US-EI U”, “Landfill/US US-EI U”, and recycling. The incineration, landfill, and recycling rates for the corrugated box, as a function of its material composition, were modeled as 0.7%, 2.8%, and 96.5%, respectively [26]. Another process associated: transport (see Transportation). The recycling scenario was modeled as a process without emissions.
- Tape: The waste scenarios for the disposal of the Tape included modeling for the PP and Plastics (identified in SimaPro) waste types for “Incineration/US US-EI U”, “Landfill/US US-EI U”, and recycling. The rates for incineration, landfill, and recycling for the Tape, as a function of its material composition, were modeled as 19.5%, 80.5%, and 0%, respectively [26]. Other process associated: transport (see Transportation). The recycling scenario was modeled as a process without emissions.

Components Package 3, tertiary level

- Pallet Slip Sheets: The waste scenarios for the disposal of the Pallet Slip Sheets included modeling for the Cardboard (identified in SimaPro) waste type for “Incineration/US US-EI U”, “Landfill/US US-EI U”, and recycling. The incineration, landfill, and recycling rates for the Pallet Slip Sheets, as a function of their material composition, were modeled as 0.7%, 2.8%, and 96.5%, respectively [26]. Another process associated: transport (see Transportation). The recycling scenario was modeled as a process without emissions.
- Stretch Wrap: The waste scenarios for the disposal of the Stretch Wrap included modeling for the PE and Cardboard (identified in SimaPro) waste types for “Incineration/US US-EI U”, “Landfill/US US-EI U”, and recycling. The incineration, landfill, and recycling rates for the Stretch Wrap, as a function of its material composition, were modeled as 16.9%, 69.8%, and 13.3 respectively [26]. Another process associated: transport (see Transportation). The recycling scenario was modeled as a process without emissions.
- Wood Pallet: The waste scenarios for the disposal of the Wood Pallet included modeling for the Wood (identified in SimaPro) waste type for “Incineration/US US-EI U”, “Landfill/US US-EI U”, and recycling. The incineration, landfill, and recycling rates for the Wood Pallet, as a function of its material composition, were modeled as 14.3%,

58.8%, and 26.9%, respectively [26]. Another process associated: transport (see Transportation). The recycling scenario was modeled as a process without emissions.

Scenario modeling

Package 1

- No additional models were used to perform the scenario analysis. The comparison was made, varying a parameter within the SimaPro build.

Package 2

- To model the composite bottom that replaces the steel bottom, the same type of composite material as the composite can component was used. This was modeled with three different materials, as it was a composite material with plastic, paperboard, and metal portions. The most abundant portion was the paperboard portion, modeled as “Kraft paper, unbleached, at plant/US- US-El U”. This data was a modified version of an Ecoinvent v2.2 dataset that was modified by Long Trail Sustainability for DATASMART in 2003. The data includes the European production of unbleached kraft paper in an integrated mill, which includes transportation to and from the mill, wood handling, chemical pulping, paper production, energy production on-site and internal wastewater treatment. The geography of the data was from one European producer and a Finnish database used as the European average. The second largest material portion was modeled as “Polypropylene resin, at plant NREL/RNA U”, taken from a modified US LCI data modified by Long Trail Sustainability for DATASMART in 2008. The included processes in this dataset were unspecified; however, the geography was for North America. The third material portion was modeled as “Aluminum, primary, at plant/US- US-El U”. This material was chosen in modeling from a US LCI dataset modified by Long Trail Sustainability for DATASMART in 2003. The set includes the primary aluminum ingot production, including the plant itself. It also includes transporting materials to the plant and disposing waste. The geography was North America, and the processes were updated for US data; however, some Swiss datasets were used to model European data. This component also included a processing and conversion technique, which was modeled as “Laminating, foil, with acrylic binder/US- US-EL U”. The data was chosen from a modified Ecoinvent v2.2 dataset that was modified by Long Trail Sustainability for DATASMART in 2007. The data included estimating electricity use for

the laminating and cutting of foils. Only glue from laminating processes was included, and an estimation for the waste process of glue overspray was included. The data had no specific geographic origin, and the energy values were undefined but modified to represent the US. Additionally, the process “Industrial machine, heavy, unspecified, at plant/US-/I US-EI U” was used to represent the tubing process in manufacturing. This dataset includes the most important materials and the transportation of new parts to the assembly parts. The geography includes specific elementary flows from Swiss companies. Another process added was transportation (see Transportation).

- No additional models were used to perform the scenario analysis for the full-label optimization. The comparison was made, varying a parameter within the SimaPro build.

Package 3

- No additional models were used to perform the scenario analysis. The comparison was made, varying a parameter within the SimaPro build.

3.6.2 Life Cycle Impact Assessment

Table 3. 5: *Impact categories for the selected midpoint indicator methods.*

ReCiPe 2016 Midpoint (H) V1.06			TRACI 2.1 V1.06		
Impact category	Unit	Compartment	Impact category	Unit	Compartment
Global warming	kg CO ₂ -eq	Air, soil	Global warming	kg CO ₂ eq	Air, soil
Stratospheric ozone depletion	kg CFC11 eq	Air	Ozone depletion	kg CFC-11 eq	Air
Ionizing radiation	kBq Co-60 eq	Air, water	Smog	kg O ₃ eq	Air
Ozone formation, Human health	kg NO _x eq	Air	Acidification	kg SO ₂ eq	Air
Fine particulate matter formation	kg PM2.5 eq	Air	Eutrophication	kg N eq	Air, water
Ozone formation, Terrestrial ecosystems	kg NO _x eq	Air	Carcinogens	CTUh	Air, soil, water
Terrestrial acidification	kg SO ₂ eq	Air	Non-carcinogens	CTUh	Air, soil, water
Freshwater eutrophication	kg P eq	Soil, water	Respiratory effects	kg PM2.5 eq	Air
Marine eutrophication	kg N eq	Soil, water	Ecotoxicity	CTUe	Air, soil, water
Terrestrial ecotoxicity	kg 1,4-DCB	Air, soil, water	Fossil fuel depletion	MJ surplus	Raw
Freshwater ecotoxicity	kg 1,4-DCB	Air, soil, water			
Marine ecotoxicity	kg 1,4-DCB	Air, soil, water			
Human carcinogenic toxicity	kg 1,4-DCB	Air, soil, water			
Human non-carcinogenic toxicity	kg 1,4-DCB	Air, soil, water			
Land use	m ² a crop eq	Raw			
Mineral resource scarcity	kg Cu eq	Raw			
Fossil resource scarcity	kg oil eq	Raw			
Water consumption	m ³	Raw			

Methods Used for Impact Assessment:

- Tool for the Reduction and Assessment of Chemical and other environmental Impacts (TRACI) has been developed for sustainability metrics, life cycle impact assessment, industrial ecology, and process design impact assessment for developing increasingly sustainable products, processes, facilities, companies, and communities. TRACI allows an expanded quantification of stressors that have potential effects, including ozone depletion, global warming, acidification, eutrophication, photochemical smog formation, human health particulate effects, human health cancer, human health noncancer,

ecotoxicity, and fossil fuel depletion effects. Research was ongoing to quantify land and water use in a future version of TRACI. An extensive explanation of each indicator can be found elsewhere [29].

- ReCiPe: Provides harmonized characterization factors at midpoint and endpoint levels. ReCiPe provides characterization factors that were representative of the global scale. The hierarchist perspective was based on a scientific consensus regarding impact mechanisms' time frame and plausibility [30].
- GWP100: The GWP expresses the amount of additional radiative forcing integrated over time (here 20, 50, and 100 years) caused by emission of 1 kg of GHG relative to the additional radiative forcing integrated over that same time horizon caused by the release of 1 kg of CO₂.

3.6.2.1 Assumptions and Limitations

Assumptions were made during testing to fill in gaps in the data needed for testing. These assumptions could be for individual packages in terms of ratios of materials or types of processing or could be used for the entire comparative study, such as transportation values. The assumptions used to model individual packages can be found below.

- Package 1, Plastic Package
 - Plastic Tub Component
 - Assuming that the EVOH layer can be modeled as Ethylene Vinyl Acetate, it was about 5% of the total weight of the component.
 - HDPE and EVOH were co-extruded.
 - The recycling rate of HDPE was unaffected by the EVOH layer as the layer was not large enough to contaminate the recycling stream.
 - Label (wrap-around, back, and lid) components.
 - Label was laminated with the acrylic binder, which was used to stick the label to the other components.
 - Backing for the labels was PET and needs to be considered in the overall footprint due to a lack of knowledge about scrap and recycling protocols.
 - 0% recycling due to the fact it was recycled with the components.
 - Tear-Off plastic / Formula Scoop / Plastic Lid

- Blue pigment in these components was not considered in the end-of-life scenario or the processing and conversion.
 - Tear-off plastic was assumed to be 0% recycled since it was not plausible for consumers to separate the metal foil and glue from the plastic portion before disposal.
 - Formula Scoop was modeled separately from the tear off area because it has a presumably different recycling value.
- Silver Tamper-Evident Sticker
 - 10% of total weight was the acrylic binder.
 - Kraft paper and aluminum have equal weight, and both were about 45% of the total weight.
 - No backing protocol was included in modeling.
 - 0% recycling due to mixed material
- Metal film
 - The acrylic binder was assumed to be 10% of total weight.
 - The film was sheet rolled to create the foil.
 - The lamination area was calculated assuming the glue holding the foil in place was about 1/8th of an inch thick all the way around the top of the tub.
- Glue 1
 - Case for the plastic tub was hot glued together rather than held together by tape.
- Wood Pallet 1
 - Allocation procedure was weight based.
 - Assumed to be used 5 times, so total weight/5.
 - Transportation used was provided for package 1 and assumed to be the same across all 3 cases.
- Stretch Wrap
 - Transportation used was provided for package 1 and assumed to be the same across all 3 cases.
- Package 2, Composite Package

- Steel bottom
 - Stamping process was modeled as a combination of the steel product manufacturing and metal working machine operation processes included in the modeling and was not its own processing technique.
- Plastic Over cap
 - Modeling does not include the yellow pigment of the cap.
- Full Label
 - Printing process was modeled as the use of the laser jet color printer rather than an actual processing technique.
 - An acrylic binder was assumed to stick the label to the composite can and was assumed to be 10% of the total measured weight of the label.
- Formula Scoop
 - The pigment was not included in the modeling.
- Composite Can
 - 0% recycled because of the mixed materials.
- Aluminum Ring
 - Recycling was assumed to be 0% as it will most likely not be separated from the composite can, which was also assumed as 0% recycled.
- Tape
 - The acrylic binder was assumed to be 10% of the total weight of the component.
 - Tape was used for package 2 and package 3 instead of the hot melt glue used for package 1 because the product was assumed to be shipped in formats other than DRCs for bulk stores.
- Corrugated Case
 - They were assumed to be different from the case modeled for package IF1.
- Wood Pallet 1
 - The allocation procedure was weight-based.
 - They were assumed to be used 5 times, so total weight/5.

- Transportation used was provided for package 1 and assumed to be the same across all 3 cases.
- Stretch Wrap
 - Transportation used was provided for package 1 and assumed to be the same across all 3 cases.
- Package 3, Steel Package
 - Steel bottom
 - The stamping process was modeled as a combination of the steel product manufacturing and metal working machine operation processes included in the modeling and was not its processing technique.
 - Steel Can
 - The stamping process was not explicitly included in the modeling and was assumed to be included in a combination of the steel production and the sheet rolling process; it was also assumed that the steel bottom was welded to the other component.
 - Plastic Over cap
 - Modeling did not include the yellow pigment of the cap.
 - Formula Scoop
 - The pigment was not included in modeling.
 - Composite Can
 - 0% recycled because of the mixed materials.
 - Aluminum Ring
 - Recycling was assumed to be 0% as it will most likely not be separated from the composite can, which was also assumed to be 0% recycled.
 - Tape
 - The acrylic binder was assumed to be 10% of the total weight of the component.
 - Tape was used for package 2 and package 3 instead of the hot melt glue used for package 1 because the product was assumed to be shipped in formats other than DRCs for bulk stores.
 - Corrugated Case

- They were assumed to be different from the case modeled for package 1.
- Wood Pallet 1
 - The allocation procedure was weight-based.
 - They were assumed to be used 5 times, so total weight/5.
 - Transportation used was provided for package 1 and assumed to be the same across all 3 cases.
- Stretch Wrap
 - Transportation used was provided for package 1 and assumed to be the same across all 3 cases.

3.6.2.2 Data quality assessment

Five types of data quality indicators were evaluated by the Pedigree matrix to assign uncertainty to the data modeled by using scores from 1 to 5 [31]:

1. Reliability (related to the reliability of the collected primary data).
2. Completeness (related to the completeness of the primary data).
3. Temporal correlation (related to the temporal correlation of the primary data).
4. Geographical correlation (related to the geographical correlation of the secondary data used).
5. Further technological correlation (related to the technological correlation of the secondary data used).

Each quality data indicator has an associated uncertainty factor (U_i) that was used to calculate the square geometric standard deviation, by using the following expression:

$$SD_{g95} = \sqrt{\exp[\ln(U_1)^2 + \ln(U_2)^2 + \ln(U_3)^2 + \ln(U_4)^2 + \ln(U_5)^2 + \ln(U_6)^2 + \ln(U_b)^2]}$$

Where:

U_1 : uncertainty factor of quality indicator Reliability.

U_2 : uncertainty factor of quality indicator Completeness.

U_3 : uncertainty factor of quality indicator Temporal correlation.

U_4 : uncertainty factor of quality indicator Geographical correlation.

U_5 : uncertainty factor of quality indicator Further technological correlation.

Table 3. 6: Data Quality Assessment Pedigree Matrix.

Component	Reliability		Completeness		Temporal correlation		Geographic correlation		Further technological correlation		
	Score	U1	Score	U2	Score	U3	Score	U4	Score	U5	SD
Package IF1 Assembly											
Primary level											
Plastic Tub	2	1.05	1	1.00	5	1.50	2	1.001	3	1.20	1.56
Plastic Lid	1	1.00	1	1.00	5	1.50	2	1.001	1	1.00	1.50
Tear-off plastic	1	1.00	1	1.00	5	1.50	2	1.001	1	1.00	1.50
Formula Scooper	1	1.00	1	1.00	5	1.50	1	1.000	1	1.00	1.50
Metal Film	1	1.00	1	1.00	5	1.50	2	1.001	2	1.05	1.50
Wrap around label	1	1.00	1	1.00	5	1.50	2	1.001	3	1.20	1.56
Back Label	1	1.00	1	1.00	5	1.50	2	1.001	3	1.20	1.56
Lid Label	1	1.00	1	1.00	5	1.50	2	1.001	3	1.20	1.56
Silver Tamper-Evident Sticker	2	1.05	1	1.00	5	1.50	2	1.001	2	1.05	1.51
Secondary Level											
Corrugated Case	1	1	1	1.00	4	1.20	2	1.00	2	1.05	1.21
Hot glue	2	1.05	1	1.00	1	1.00	5	1.10	3	1.20	1.24
Corrugated Dividers	1	1	1	1.00	4	1.20	2	1.00	2	1.05	1.21
Tertiary Level											
Wood Pallet	1	1.00	1	1.00	5	1.50	1	1.00	1	1.00	1.50
Pallet Slip Sheets	1	1	1	1.00	4	1.20	2	1.00	2	1.05	1.21
Stretch Wrap	1	1	1	1.00	5	1.50	2	1.00	1	1.00	1.50
Transportation level											
Transportation of raw materials	1	1	1	1	4	1.2	1	1	1	1	1.20
Transportation of final packaging system	1	1	1	1	4	1.2	1	1	1	1	1.20
Transportation End of Life Scenario	2	1.05	1	1	4	1.2	1	1	1	1	1.21
Package IF1 End of Life											
Primary level											
Plastic Tub	2	1.05	1	1.00	5	1.50	4	1.050	1	1.00	1.51
Plastic Lid	1	1.00	1	1.00	5	1.50	4	1.050	1	1.00	1.50
Tear-off plastic	1	1.00	1	1.00	5	1.50	4	1.050	1	1.00	1.50
Formula Scooper	1	1.00	1	1.00	5	1.50	4	1.050	1	1.00	1.50
Metal Film	1	1.00	1	1.00	5	1.50	4	1.050	1	1.00	1.50
Wrap around label	1	1.00	1	1.00	5	1.50	4	1.050	1	1.00	1.50
Back Label	1	1.00	1	1.00	5	1.50	4	1.050	1	1.00	1.50
Lid Label	1	1.00	1	1.00	5	1.50	4	1.050	1	1.00	1.50
Silver Tamper-Evident Sticker	1	1.00	1	1.00	5	1.50	4	1.050	1	1.00	1.50
Secondary Level											
Corrugated Case	1	1.00	1	1.00	5	1.50	4	1.050	1	1.00	1.50
Hot glue	2	1.05	1	1.00	5	1.50	4	1.050	1	1.00	1.51
Corrugated Dividers	1	1.00	1	1.00	5	1.50	4	1.050	1	1.00	1.50
Tertiary Level											
Wood Pallet	1	1.00	1	1.00	5	1.50	4	1.050	1	1.00	1.50
Pallet Slip Sheets	2	1.05	1	1.00	5	1.50	4	1.050	1	1.00	1.51
Stretch Wrap	2	1.05	1	1.00	5	1.50	4	1.050	1	1.00	1.51

Table 3.6 (cont'd):

Component	Reliability		Completeness		Temporal correlation		Geographic correlation		Further technological correlation		
	Score	U1	Score	U2	Score	U3	Score	U4	Score	U5	SD
Package IF2 Assembly											
Primary level											
Composite Can	1	1.00	1	1.00	5	1.50	2	1.05	2	1.05	1.51
Aluminum Ring	1	1.00	1	1.00	5	1.50	1	1.00	2	1.05	1.50
Steel Bottom	1	1	1	1.00	5	1.50	2	1.00	1	1.00	1.50
Formula Scooper	1	1.00	1	1.00	5	1.50	1	1.000	1	1.00	1.50
Plastic Overcap	1	1.00	1	1.00	5	1.50	2	1.05	1	1.00	1.50
Peel Off Metal Seal	1	1.00	1	1.00	4	1.20	2	1.00	2	1.05	1.21
Full Label	1	1.00	1	1.00	5	1.50	5	1.10	3	1.20	1.58
Secondary Level											
Corrugated Case	1	1	1	1.00	4	1.20	2	1.00	2	1.05	1.21
Tape	2	1.05	1	1.00	5	1.50	5	1.10	1	1.00	1.52
Tertiary Level											
Wood Pallet	1	1.00	1	1.00	5	1.50	1	1.00	1	1.00	1.50
Pallet Slip Sheets	1	1	1	1.00	4	1.20	2	1.00	2	1.05	1.21
Stretch Wrap	1	1	1	1.00	5	1.50	2	1.00	1	1.00	1.50
Transportation level											
Transportation of raw materials	1	1	1	1	4	1.2	1	1	1	1	1.20
Transportation of final packaging system	1	1	1	1	4	1.2	1	1	1	1	1.20
Transportation End of Life Scenario	2	1.05	1	1	4	1.2	1	1	1	1	1.21
Package IF2 end-of-life											
Primary level											
Composite Can	1	1.00	1	1.00	5	1.50	4	1.050	1	1.00	1.50
Aluminum Ring	1	1.00	1	1.00	5	1.50	4	1.050	1	1.00	1.50
Steel Bottom	1	1.00	1	1.00	5	1.50	4	1.050	1	1.00	1.50
Formula Scooper	1	1.00	1	1.00	5	1.50	4	1.050	1	1.00	1.50
Plastic Overcap	1	1.00	1	1.00	5	1.50	4	1.050	1	1.00	1.50
Peel Off Metal Seal	1	1.00	1	1.00	5	1.50	4	1.050	1	1.00	1.50
Full Label	1	1.00	1	1.00	5	1.50	4	1.050	1	1.00	1.50
Secondary Level											
Corrugated Case	1	1	1	1.00	5	1.50	4	1.05	2	1.05	1.51
Tape	2	1.05	1	1.00	5	1.50	4	1.05	1	1.00	1.51
Tertiary Level											
Wood Pallet	1	1.00	1	1.00	5	1.50	1	1.00	1	1.00	1.50
Pallet Slip Sheets	1	1	1	1.00	4	1.20	2	1.00	2	1.05	1.21
Stretch Wrap	1	1	1	1.00	5	1.50	2	1.00	1	1.00	1.50

Table 3.6 (cont'd):

Component	Reliability		Completeness		Temporal correlation		Geographic correlation		Further technological correlation		
	Score	U1	Score	U2	Score	U3	Score	U4	Score	U5	SD
Package IF3											
Primary level											
Steel Can	2	1.05	1	1	5	1.5	4	1.05	1	1.00	1.51
Aluminum Ring	1	1.00	1	1.00	5	1.50	1	1.00	2	1.05	1.50
Steel Bottom	1	1	1	1.00	5	1.50	2	1.00	1	1.00	1.50
Formula Scooper	1	1.00	1	1.00	5	1.50	1	1.00	1	1.00	1.50
Plastic Overcap	1	1.00	1	1.00	5	1.50	2	1.05	1	1.00	1.50
Peel Off Metal Seal	1	1.00	1	1.00	4	1.20	2	1.00	2	1.05	1.21
Secondary Level											
Corrugated Case	1	1	1	1.00	4	1.20	2	1.00	2	1.05	1.21
Tape	2	1.05	1	1.00	5	1.50	5	1.10	1	1.00	1.52
Tertiary Level											
Wood Pallet	1	1.00	1	1.00	5	1.50	1	1.00	1	1.00	1.50
Pallet Slip Sheets	1	1	1	1.00	4	1.20	2	1.00	2	1.05	1.21
Stretch Wrap	1	1	1	1.00	5	1.50	2	1.00	1	1.00	1.50
Transportation level											
Transportation of raw materials	1	1	1	1	4	1.2	1	1	1	1.00	1.20
Transportation of final packaging system	1	1	1	1	4	1.2	1	1	1	1.00	1.20
Transportation End of Life Scenario	2	1.05	1	1	4	1.2	1	1	1	1.00	1.21
Package IF3 end-of-life											
Primary level											
Steel Can	2	1.05	1	1.00	5	1.50	4	1.05	1	1.00	1.51
Aluminum Ring	1	1.00	1	1.00	5	1.50	4	1.05	1	1.00	1.50
Steel Bottom	1	1.00	1	1.00	5	1.50	4	1.05	1	1.00	1.50
Formula Scooper	1	1.00	1	1.00	5	1.50	4	1.05	1	1.00	1.50
Plastic Overcap	1	1.00	1	1.00	5	1.50	4	1.05	1	1.00	1.50
Peel Off Metal Seal	1	1.00	1	1.00	5	1.50	4	1.05	1	1.00	1.50
Secondary Level											
Corrugated Case	1	1.00	1	1.00	4	1.20	2	1.00	2	1.05	1.21
Tape	2	1.05	1	1.00	5	1.50	5	1.10	1	1.00	1.52
Tertiary Level											
Wood Pallet	1	1.00	1	1.00	5	1.50	1	1.00	1	1.00	1.50
Pallet Slip Sheets	1	1.00	1	1.00	4	1.20	2	1.00	2	1.05	1.21
Stretch Wrap	1	1.00	1	1.00	5	1.50	2	1.00	1	1.00	1.50

3.6.3 Life Cycle Interpretation

3.6.3.1 Circular Footprint Formula Modeling

In modeling the Circular Footprint Formula (CFF) End of Life methodology, SimaPro was used. Each material was remade to incorporate the various parameters and inputs that were part of the CFF. This formula can be found below in **Equation 1**.

Material $(1 - R_1)E_v + R_1 \times \left(AE_{recycled} + (1 - A)E_v \times \frac{Q_{Sin}}{Q_p} \right) + (1 - A)R_2 \times (E_{recyclingEoL} - E^*_v \times \frac{Q_{Sout}}{Q_p})$ Energy $(1 - B)R_3 \times (E_{ER} - LHV \times X_{ER,Heat} \times E_{SE,Heat} - LHV \times X_{ER,Elec} \times E_{SE,Elec})$ Disposal $(1 - R_2 - R_3) \times E_D$
--

Equation 1: Circular Footprint Formula [32].

The 6 materials modeled included Aluminum, Steel, Polypropylene (PP), High Density Polyethylene (HDPE), Linear Low-Density Polyethylene (LLDPE), Corrugated Board and Wood. The inputs for the variables as well as the parameter values used in modeling for each material were listed below. The modeling of these materials were based on several assumptions from various sources available [17], [33–38].

- CFF Aluminum – The inputs from nature for this material include E_v , E^*_v , $E_{recyclingEoL}$, $E_{recycled}$, E_v , and E_D . Inputs from the technosphere include E_{ER} , E_{SE} , Heat, and $E_{SE, Electric}$. **Table 3. 7** below shows the parameter values used in final modeling.
 - Aluminum Waste - This material was modeled as 1 ton of “Aluminum scrap, post-consumer GLO, recycled content cut off U”.
 - Erecycled – The inputs for this parameter includes 1.1 tons of the “Aluminum Waste” mentioned above. It also includes 1 ton of "metal working average for aluminum product manufacturing GLO cut off U” and 250 tkm of “Transport lorry EURO4 US U”.

- E*v – This parameter was modeled as 1 ton of “Aluminum, primary, at plant/US- US-El U”.
- Ed – This parameter was modeled as 1 ton of “Aluminum scrap, post-consumer GLO, recycled content cut off U”.
- Eer – The input for this parameter includes 1 ton of the “Aluminum Waste” mentioned above. It also includes 1 MJ of "Heat, natural gas, at industrial furnace >100kW US U”.
- ErecyclingEoL - The inputs for this parameter include the “Aluminum Waste” mentioned above. It also includes "metal working average for aluminum product manufacturing GLO cut off U” and “Transport lorry EURO4 US U”.
- Ese Elec – The input for this parameter was 1 kWh of "electricity high certified electricity at grid US U”
- Ese Heat – The input for this parameter was 1 MJ of "Heat, natural gas, at industrial furnace >100kW US U”.
- Ev – This parameter was modeled as 1 ton of “Aluminum, primary, at plant/US- US-El U”.

Table 3. 7: *Value of CFF parameters for the CFF Aluminum Material.*

Value of Parameters	
R1	0
A	0.2
Fqsin	0.9
R2	0.6
FQSout	0.9
R3	0.15705
B	0
LHV	0.7
XERheat	0.4
XERelec	0.47

- CFF Corrugated – The inputs from nature for this material include Ev, E*v, ErecyclingEoL, E recycled, Ev, and ED. Inputs from the technosphere include Eer, Ese, Heat, and Ese, Electric. **Table 3. 8** below shows the parameter values used in final modeling.

- Corrugated Waste - This material was modeled as 1 ton of “Waste paper, mixed, from public collection, for further treatment/US* US-EI U”.
- Erecycled – The inputs for this parameter includes 1.1 tons of the “Corrugated Waste” mentioned above. It also includes 1 ton of "Production of carton board boxes, offset printing, at plant/US* US-EI U” and 250 tkm of “Transport lorry EURO4 US U”.
- E*v – This parameter was modeled as 1 ton of “Corrugated board, mixed fibre, single wall, at plant/US- US-EI U”
- Ed – This parameter was modeled as 1 ton of “Waste paper, mixed, from public collection, for further treatment/US* US-EI U”.
- Eer – The input for this parameter includes 1 ton of the “Corrugated Waste” mentioned above. It also includes 1 MJ of "Heat, natural gas, at industrial furnace >100kW US U”.
- ErecyclingEoL - The inputs for this parameter includes 1.1 tons of the “Corrugated Waste” mentioned above. It also includes 1 ton of "Production of carton board boxes, offset printing, at plant/US* US-EI U” and 250 tkm of “Transport lorry EURO4 US U”.
- Ese Elec – The input for this parameter was 1 kWh of "electricity high certified electricity at grid US U”
- Ese Heat – The input for this parameter was 1 MJ of "Heat, natural gas, at industrial furnace >100kW US U”.
- Ev – This parameter was modeled as 1 ton of “Corrugated board, mixed fibre, single wall, at plant/US- US-EI U”

Table 3. 8: *Value of CFF parameters for the CFF Corrugated Material.*

Value of Parameters	
R1	0.88
A	0.2
Fqsin	0.85
R2	0.75
FQSout	1
R3	0.432
B	0
LHV	17.5
XERheat	0.41
XERelec	0.47

- CFF HDPE – The inputs from nature for this material include E_v , E^*_v , $E_{recyclingEoL}$, $E_{recycled}$, E_v , and E_D . Inputs from the technosphere include E_{er} , E_{se} , $Heat$, and E_{se} , Electric. **Table 3. 9** below shows the parameter values used in final modeling.
 - HDPE Waste - This material was modeled as 1 kg of “Waste polyethylene, for recycling, sorted {US} | market for waste polyethylene, for recycling, sorted | Cut-off, U”.
 - Erecycled – The inputs for this parameter includes 1.1 tons of the “HDPE Waste” mentioned above. It also includes 120 kg of "Tap water {GLO}| market group for | Cut-off, U” and 250 tkm of “Transport lorry EURO4 US U”. As well as 485 kWh of “Electricity, high voltage, certified electricity, at grid/US* US-EI U”.
 - E^*_v – This parameter was modeled as 1 ton of “Polyethylene, HDPE, granulate, at plant/US- US-EI U”
 - E_d – This parameter was modeled as 1 ton of “Waste polyethylene, for recycling, sorted {US} | market for waste polyethylene, for recycling, sorted | Cut-off, U”.
 - E_{er} – The input for this parameter includes 0.03 kg of the “HDPE Waste” mentioned above. It also includes 0.0072 MJ of "Heat, natural gas, at industrial furnace >100kW US U”.
 - $E_{recyclingEoL}$ - The inputs for this parameter includes 1.1 tons of the “HDPE Waste” mentioned above. It also includes 120 kg of "Tap water {GLO}| market group for | Cut-off, U” and 250 tkm of “Transport lorry EURO4 US U”. As well as 485 kWh of “Electricity, high voltage, certified electricity, at grid/US* US-EI U”.
 - $E_{se Elec}$ – The input for this parameter was 1 kWh of "electricity high certified electricity at grid US U”
 - $E_{se Heat}$ – The input for this parameter was 1 MJ of "Heat, natural gas, at industrial furnace >100kW US U”.
 - E_v – This parameter was modeled as 1 ton of “Polyethylene, HDPE, granulate, at plant/US- US-EI U”

Table 3. 9: Value of CFF parameters for the CFF HDPE Material.

Value of Parameters	
R1	0
A	0.5
Fqsin	0.9
R2	0.29
FQSout	1
R3	0.081
B	0
LHV	41.8
XERheat	0.42
XERelec	0.47

- CFF LLDPE – The inputs from nature for this material include Ev, E*v, ErecyclingEoL, E recycled, Ev, and ED. Inputs from the technosphere include Eer, Ese, Heat, and Ese, Electric. **Table 3. 10** below shows the parameter values used in final modeling.
 - LLDPE Waste - This material was modeled as 1 kg of “Waste polyethylene, for recycling, sorted {US} | market for waste polyethylene, for recycling, sorted | Cut-off, U”.
 - Erecycled – The inputs for this parameter includes 1.1 tons of the “LLDPE Waste” mentioned above. It also includes 120 kg of "Tap water {GLO}| market group for | Cut-off, U” and 250 tkm of “Transport lorry EURO4 US U”. As well as 485 kWh of “Electricity, high voltage, certified electricity, at grid/US* US-EI U”.
 - E*v – This parameter was modeled as 1 ton of “Polyethylene, LLDPE, granulate, at plant/US- US-EI U”
 - Ed – This parameter was modeled as 1 ton of “Waste polyethylene, for recycling, sorted {US} | market for waste polyethylene, for recycling, sorted | Cut-off, U”.
 - Eer – The input for this parameter includes 0.03 kg of the “LLDPE Waste” mentioned above. It also includes 0.0072 MJ of "Heat, natural gas, at industrial furnace >100kW US U”.
 - ErecyclingEoL - The inputs for this parameter includes 1.1 tons of the “LLDPE Waste” mentioned above. It also includes 120 kg of "Tap water {GLO}| market group for | Cut-off, U” and 250 tkm of “Transport lorry EURO4 US U”. As well as 485 kWh of “Electricity, high voltage, certified electricity, at grid/US* US-EI U”.

- Ese Elec – The input for this parameter was 1 kWh of "electricity high certified electricity at grid US U"
- Ese Heat – The input for this parameter was 1 MJ of "Heat, natural gas, at industrial furnace >100kW US U".
- Ev – This parameter was modeled as 1 ton of "Polyethylene, HDPE, granulate, at plant/US- US-EI U"

Table 3. 10 : *Value of CFF parameters for the CFF LLDPE Material.*

Value of Parameters	
R1	0
A	0.5
Fqsin	0.75
R2	0.29
FQSout	1
R3	0.05985
B	0
LHV	41.3
XERheat	0.42
XERelec	0.47

- CFF PP – The inputs from nature for this material include Ev, E*v, ErecyclingEoL, E recycled, Ev, and ED. Inputs from the technosphere include Eer, Ese, Heat, and Ese, Electric. **Table 3. 11** below shows the parameter values used in final modeling.
 - PP Waste - This material was modeled as 1 kg of "Polypropylene scrap, from PP injection molding, at plant/kg/RNA".
 - Erecycled – The inputs for this parameter includes 1.1 tons of the "PP Waste" mentioned above. It also includes 120 kg of "Tap water {GLO}| market group for | Cut-off, U" and 250 tkm of "Transport lorry EURO4 US U". As well as 485 kWh of "Electricity, high voltage, certified electricity, at grid/US* US-EI U".
 - E*v – This parameter was modeled as 1 ton of "Polypropylene resin, at plant NREL/RNA U".
 - Ed – This parameter was modeled as 1 ton of "Polypropylene scrap, from PP injection molding, at plant/kg/RNA".
 - Eer – The input for this parameter includes 0.03 kg of the "PP Waste" mentioned above. It also includes 0.0072 MJ of "Heat, natural gas, at industrial furnace >100kW US U".

- ErecyclingEoL - The inputs for this parameter includes 1.1 tons of the “PP Waste” mentioned above. It also includes 120 kg of "Tap water {GLO}| market group for | Cut-off, U” and 250 tkm of “Transport lorry EURO4 US U”. As well as 485 kWh of “Electricity, high voltage, certified electricity, at grid/US* US-EI U”.
- Esec Elec – The input for this parameter was 1 kWh of "electricity high certified electricity at grid US U”
- Esec Heat – The input for this parameter was 1 MJ of "Heat, natural gas, at industrial furnace >100kW US U”.
- Ev – This parameter was modeled as 1 ton “Polypropylene resin, at plant NREL/RNA U”.

Table 3. 11: Value of CFF parameters for the CFF PP Material.

Value of Parameters	
R1	0
A	0.5
Fqsin	0.9
R2	0.29
FQSout	1
R3	0.0135
B	0
LHV	46
XERheat	0.43
XERelec	0.47

- CFF Steel – The inputs from nature for this material include Ev, E*v, ErecyclingEoL, Erecycled, Ev, and ED. Inputs from the technosphere include Eer, Esec, Heat, and Esec Electric. **Table 3. 12** below shows the parameter values used in final modeling.
 - Steel Waste - This material was modeled as 1 ton of “Steel waste, value of scrap/GLO”.
 - Erecycled – The inputs for this parameter includes 1.1 tons of the “Steel Waste” mentioned above. It also includes 1 ton of "metal working average for steel product manufacturing GLO cut off U” and 250 tkm of “Transport lorry EURO4 US U”.
 - E*v – This parameter was modeled as 1 ton of “Steel, low alloyed, at plant/US- US-EI U”.
 - Ed – This parameter was modeled as 1 ton of “Steel waste, value of scrap/GLO”.

- Eer – The input for this parameter includes 1 ton of the “Steel Waste” mentioned above. It also includes 1 MJ of "Heat, natural gas, at industrial furnace >100kW US U”.
- ErecyclingEoL - The inputs for this parameter includes 1.1 tons of the “Steel Waste” mentioned above. It also includes 1 ton of "metal working average for steel product manufacturing GLO cut off U” and 150 tkm of “Transport lorry EURO4 US U”.
- Ese Elec – The input for this parameter was 1 kWh of "electricity high certified electricity at grid US U”
- Ese Heat – The input for this parameter was 1 MJ of "Heat, natural gas, at industrial furnace >100kW US U”.
- Ev – This parameter was modeled as 1 ton of “Steel, low alloyed, at plant/US- US-EI U”.

Table 3. 12: Value of CFF parameters for the CFF Steel Material.

Value of Parameters	
R1	0.58
A	0.2
Fqsin	0.9
R2	0.8
FQSout	0.9
R3	0.3645
B	0
LHV	0.7
XERheat	0.4
XERelec	0.47

- CFF Wood – The inputs from nature for this material include Ev, E*v, ErecyclingEoL, E recycled, Ev, and ED. Inputs from the technosphere include Eer, Ese, Heat, and Ese, Electric. **Table 3. 13** below shows the parameter values used in final modeling.
 - Wood Waste - This material was modeled as 1 ton of “Wood waste, at MDF mill/kg/RNA”.
 - Erecycled – The inputs for this parameter includes 1.1 tons of the “Wood Waste” mentioned above. It also 250 tkm of “Transport lorry EURO4 US U”.
 - E*v – This parameter was modeled as 1 ton of “Pallet(22 kg)/US- US-EI U”.
 - Ed – This parameter was modeled as 1 ton of “Wood waste, at MDF mill/kg/RNA”.
 - Eer – The input for this parameter includes 1 ton of the “Wood Waste” mentioned above. It also includes 1 MJ of "Heat, natural gas, at industrial furnace >100kW US U”.

- ErecyclingEoL - The inputs for this parameter includes 1.1 tons of the “Wood waste, at MDF mill/kg/RNA” and 150 tkm of “Transport lorry EURO4 US U”.
- Ese Elec – The input for this parameter was 1 kWh of "electricity high certified electricity at grid US U”
- Ese Heat – The input for this parameter was 1 MJ of "Heat, natural gas, at industrial furnace >100kW US U”.
- Ev – This parameter was modeled as 1 ton of “Pallet(22 kg)/US- US-El U”.

Table 3. 13: *Value of CFF parameters for the CFF Wood Material.*

Value of Parameters	
R1	0
A	0.8
Fqsin	1
R2	0.3
FQSout	1
R3	0.12105
B	0
LHV	17.2
XERheat	0.41
XERelec	0.47

3.6.4 LCA Results

3.6.4.1 Contribution Analysis

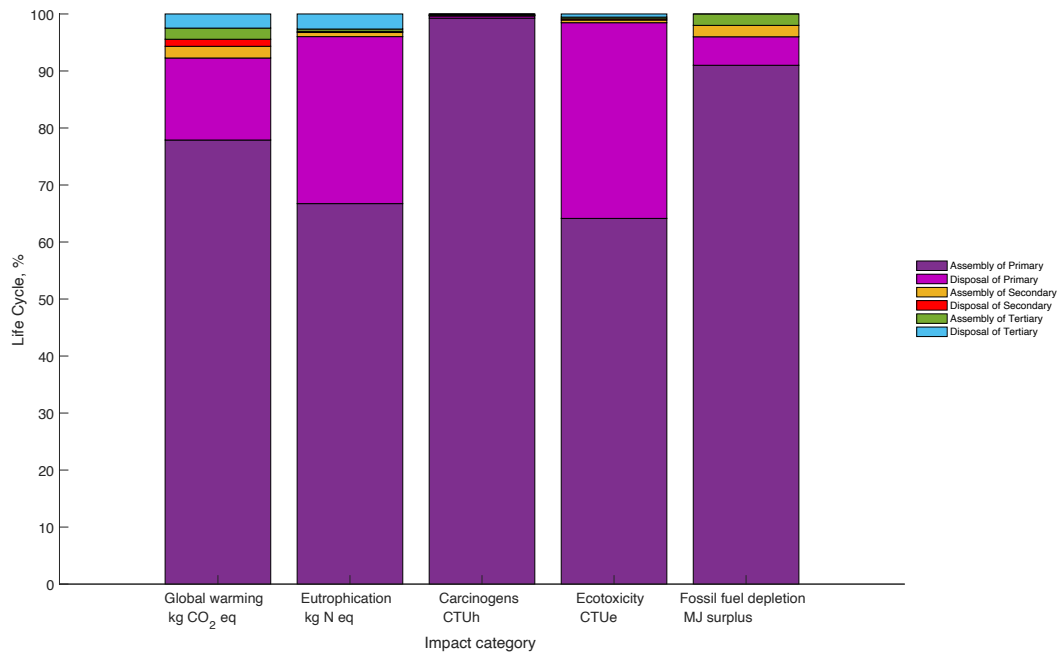


Figure 3. 11: Main contributions to midpoint indicators global warming, eutrophication, carcinogens, ecotoxicity, and fossil fuel depletion of assemblies and disposal scenarios for the composite container package system according to TRACI 2.1 V1.06.

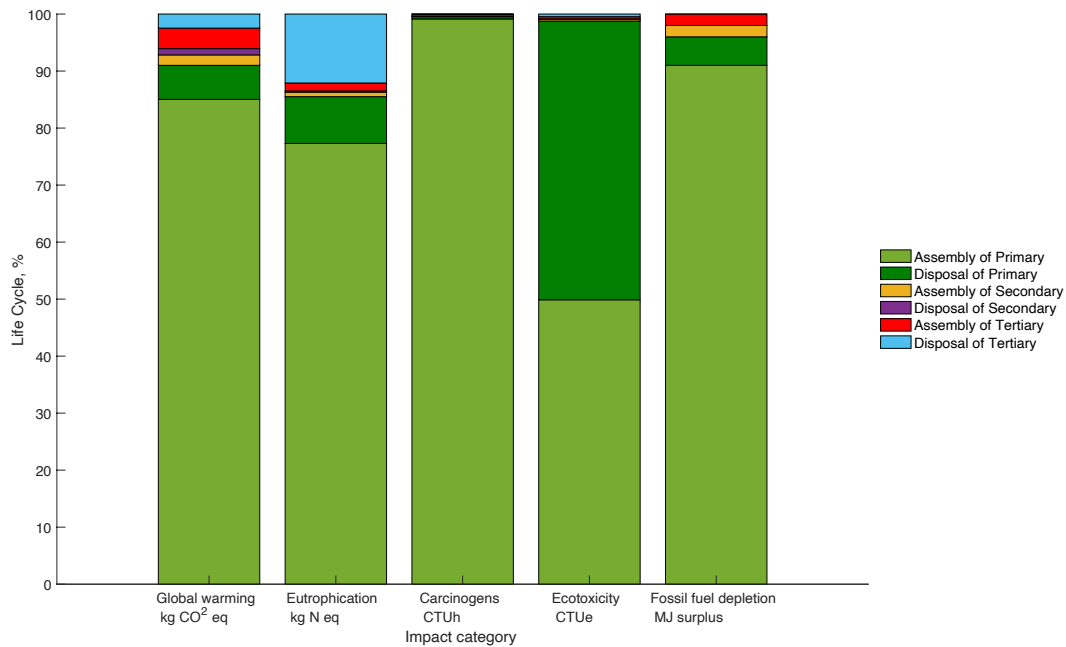


Figure 3. 12: Main contributions to midpoint indicators global warming, eutrophication, carcinogens, ecotoxicity, and fossil fuel depletion of assemblies and disposal scenarios for the steel can package system according to TRACI 2.1 V1.06.

3.6.4.2 Comparative Results in ReCiPe

When the environmental footprint was analyzed using the ReCiPe 2016 Midpoint (H) V1.06 comparative analysis as depicted in **Figure 3. 13**. For both categories, the package IF2 has the highest contribution. The highest contribution of Package 2 in terms of land use and water consumption was associated with the use of more materials derived from biobased resources and the conversion process to the composite can.

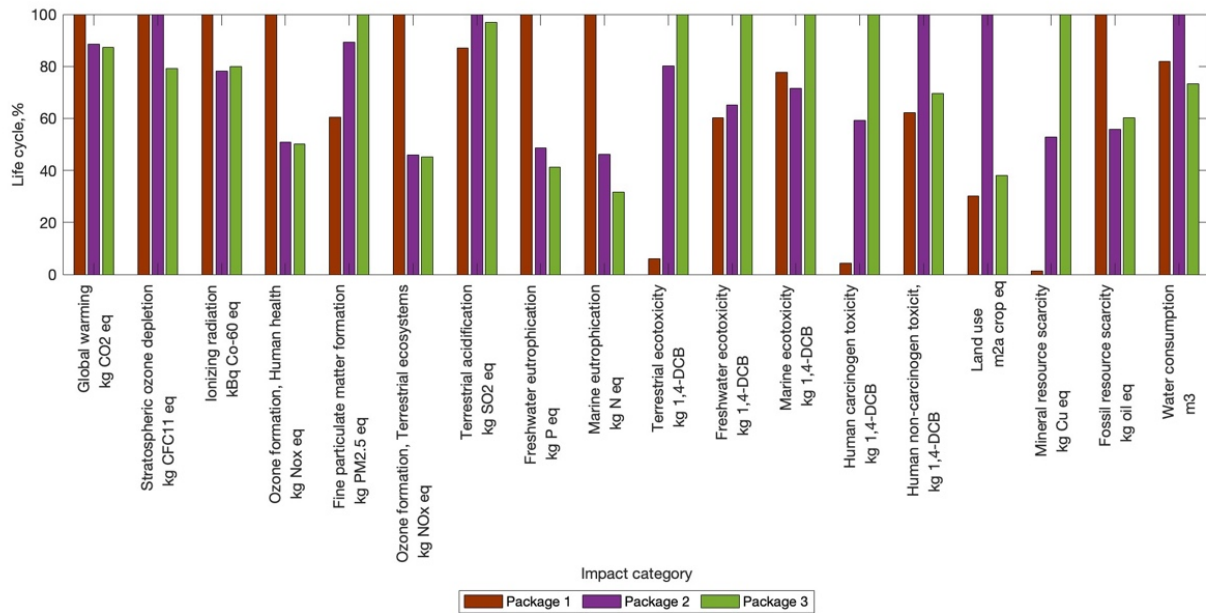


Figure 3. 13: Comparative impact assessment for the life cycle of packages Packages 1, 2, and 3 according to ReCiPe 2016 Midpoint (H) V1.06.

3.6.4.3 Scenario Analysis

The lightweighting scenario analysis performed for the steel can package, was lightweighting of the steel can component by 30%, as presented in **Figure 3. 14**.

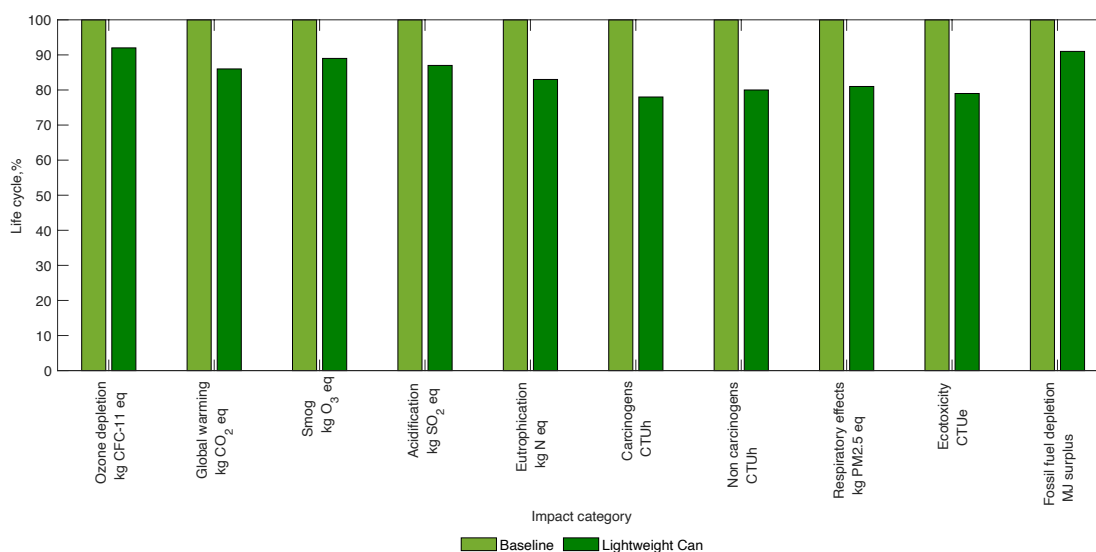


Figure 3. 14: Package 3 Scenario analysis – Lightweighting of the steel can component.
Reduction of weight of the steel can primary component by 30% according to TRACI 2.1 V1.06.

3.6.4.4 Keeping it in perspective scenario.

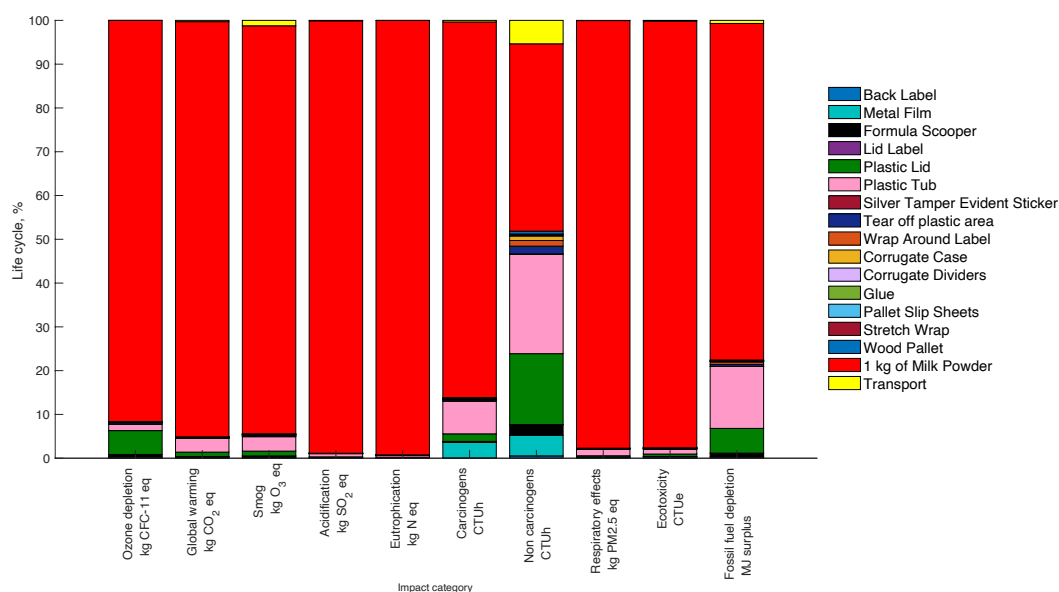


Figure 3. 15: Contribution breakdown of the Assembly portion of the Plastic package, Package 1, with the addition of 1 kg of Milk Powder.

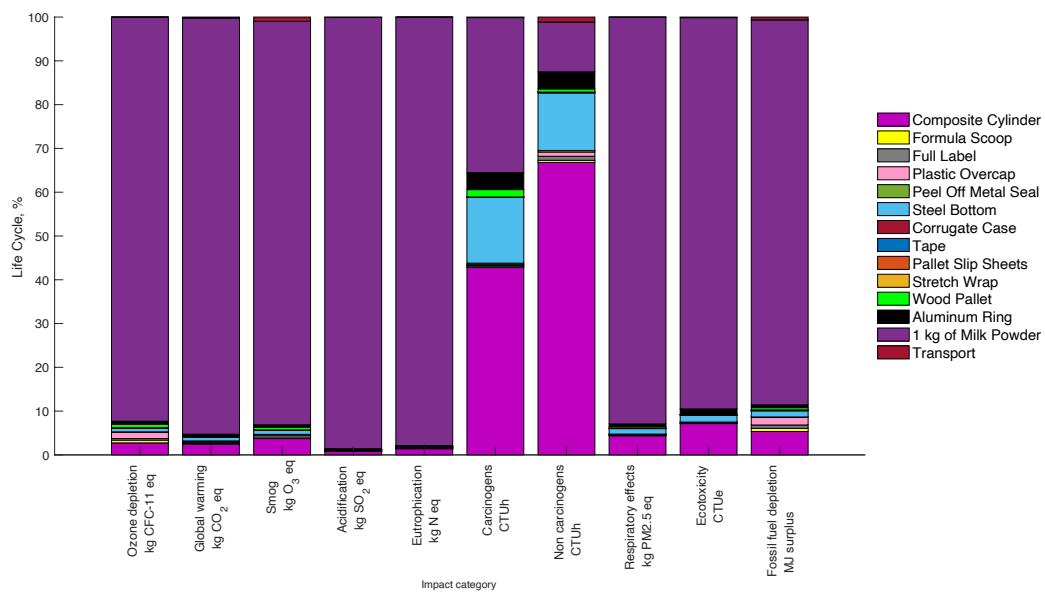


Figure 3. 16: Contribution breakdown of the Assembly portion of the Composite package, Package 2, with addition of 1 kg of Milk Powder.

REFERENCES

- [1] A. Zabaniotou and E. Kassidi, “Life cycle assessment applied to egg packaging made from polystyrene and recycled paper,” *J Clean Prod*, vol. 11, no. 5, pp. 549–559, Aug. 2003, doi: 10.1016/S0959-6526(02)00076-8.
- [2] D. H. Kang, R. Auras, and J. Singh, “Life cycle assessment of non-alcoholic single-serve polyethylene terephthalate beverage bottles in the state of California,” *Resour Conserv Recycl*, vol. 116, pp. 45–52, Jan. 2017, doi: 10.1016/j.resconrec.2016.09.011.
- [3] S. Humbert, V. Rossi, M. Margni, O. Jolliet, and Y. Loerincik, “Life cycle assessment of two baby food packaging alternatives: Glass jars vs. plastic pots,” *International Journal of Life Cycle Assessment*, vol. 14, no. 2, pp. 95–106, Mar. 2009, doi: 10.1007/s11367-008-0052-6.
- [4] J. Cleary, “Life cycle assessments of wine and spirit packaging at the product and the municipal scale: A Toronto, Canada case study,” *J Clean Prod*, vol. 44, pp. 143–151, 2013, doi: 10.1016/j.jclepro.2013.01.009.
- [5] K. L. Whittingham, A. G. Earle, D. I. Leyva-de la Hiz, and A. Argiolas, “The impact of the United Nations Sustainable Development Goals on corporate sustainability reporting,” *BRQ Business Research Quarterly*, vol. 26, no. 1, pp. 45–61, Jan. 2023, doi: 10.1177/23409444221085585.
- [6] United Nations DESA, “The Sustainable Development Goals Report 2022,” 2022. Accessed: Aug. 21, 2023. [Online]. Available: <https://unstats.un.org/sdgs/report/2022/>
- [7] Nike Inc., “Sustainable Development Goals (SDGs).” Accessed: Aug. 21, 2023. [Online]. Available: <https://about.nike.com/en/newsroom/resources/sustainable-development-goals-sdgs>
- [8] Nike Inc., “Breaking Barriers,” 2021. Accessed: Aug. 21, 2023. [Online]. Available: <https://about.nike.com/en/newsroom/reports/fy21-nike-inc-impact-report-2>
- [9] J. Broadbent, “Abbott Laboratories to set up new factory amid infant-formula shortage plaguing US parents.” Accessed: Aug. 16, 2023. [Online]. Available: <https://search-ebscohost-com.proxy2.cl.msu.edu/login.aspx?direct=true&db=edsinc&AN=edsinc.A723601166&site=eds-live>.
- [10] Food & Beverage Close-Up, “Research and Markets Adds Report: Baby Food and Infant Formula Market,” Feb. 2020. [Online]. Available: www.researchandmarkets.com/r/p2aag7
- [11] K. Cadwell, A. Blair, C. Turner-Maffei, M. Gabel, and K. Brimdyr, “Powdered Baby Formula Sold in North America: Assessing the Environmental Impact,” *Breastfeeding Medicine*, vol. 15, no. 10, pp. 671–679, Oct. 2020, doi: 10.1089/bfm.2020.0090.

- [12] Perrigo, “Perrigo Pediatrics .” Accessed: May 10, 2023. [Online]. Available: <https://www.perrigopediatrics.com/>
- [13] United States Environmental Protection Agency, “Greenhouse Gas Equivalencies Calculator.” Accessed: Aug. 21, 2023. [Online]. Available: <https://www.epa.gov/energy/greenhouse-gas-equivalencies-calculator>
- [14] E. Romano, R. Roma, F. Tidona, G. Giraffa, and A. Bragaglio, “Dairy Farms and Life Cycle Assessment (LCA): The Allocation Criterion Useful to Estimate Undesirable Products,” *Sustainability*, vol. 13, no. 8, p. 4354, Apr. 2021, doi: 10.3390/su13084354.
- [15] M. Yan and N. M. Holden, “Life cycle assessment of multi-product dairy processing using Irish butter and milk powders as an example,” *J Clean Prod*, vol. 198, pp. 215–230, Oct. 2018, doi: 10.1016/j.jclepro.2018.07.006.
- [16] M. Krokida, M. Taxiarchou, A. Peppas, and K. Kyriakopoulou, “Life Cycle Assessment (LCA) on European skimmed milk powder processing production plant,” *Scientific Bulletin. series F. Biotechnologies*, vol. XX, pp. 280–285, 2016, [Online]. Available: <https://www.researchgate.net/publication/347444515>
- [17] T. Ekvall, A. Björklund, G. Sandin, K. Jelse, J. Lagergren, and M. Rydberg, “Modeling recycling in life cycle assessment,” 2020. Accessed: Aug. 20, 2023. [Online]. Available: <https://www.diva-portal.org/smash/record.jsf?pid=diva2%3A1549446&dswid=-9963>
- [18] K. Joachimiak-Lechman, D. Garstecki, M. Konopczyński, and A. Lewandowska, “Implementation of Life Cycle Based Tools in the Circular Economy Context—Case Study of Plastic Waste,” *Sustainability*, vol. 12, no. 23, p. 9938, Nov. 2020, doi: 10.3390/su12239938.
- [19] A. C. Farrapo, T. T. Matheus, R. M. Lagunes, R. Filleti, F. Yamaji, and D. A. Lopes Silva, “The Application of Circular Footprint Formula in Bioenergy/Bioeconomy: Challenges, Case Study, and Comparison with Life Cycle Assessment Allocation Methods,” *Sustainability*, vol. 15, no. 3, p. 2339, Jan. 2023, doi: 10.3390/su15032339.
- [20] V. Prado-Lopez, T. P. Seager, M. Chester, L. Laurin, M. Bernardo, and S. Tylock, “Stochastic multi-attribute analysis (SMAA) as an interpretation method for comparative life-cycle assessment (LCA),” *International Journal of Life Cycle Assessment*, vol. 19, no. 2, pp. 405–416, Feb. 2014, doi: 10.1007/s11367-013-0641-x.
- [21] S. Kim and J. Park, “Comparative Life Cycle Assessment of Multiple Liquid Laundry Detergent Packaging Formats,” *Sustainability*, vol. 12, no. 11, p. 4669, Jun. 2020, doi: 10.3390/su12114669.
- [22] V. Prado and R. Heijungs, “Implementation of stochastic multi attribute analysis (SMAA) in comparative environmental assessments,” *Environmental Modelling and Software*, vol. 109, pp. 223–231, Nov. 2018, doi: 10.1016/j.envsoft.2018.08.021.

- [23] N. Rajagopalan, R. Venditti, S. Kelley, and J. Daystar, “Multi-attribute uncertainty analysis of the life cycle of lignocellulosic feedstock for biofuel production,” *Biofuels, Bioproducts and Biorefining*, vol. 11, no. 2, pp. 269–280, Mar. 2017, doi: 10.1002/bbb.1737.
- [24] SimaPro, “SimaPro.” Accessed: Jan. 11, 2022. [Online]. Available: <https://simapro.com/>
- [25] R. A. Auras and S. E. M. Selke, “Life Cycle Assessment,” in *Life Cycle of Sustainable Packaging: From Design to End-of-Life*, First., R. Auras and S. Selke, Eds., Hoboken, New Jersey: John Wiley & Sons, Inc., 2023 , 2022, pp. 179–215.
- [26] United States Environmental Protection Agency, “Advancing Sustainable Materials Management: 2018 Tables and Figures Assessing Trends in Materials Generation and Management in the United States,” 2018. Accessed: Aug. 20, 2023. [Online]. Available: https://www.epa.gov/sites/default/files/2021-01/documents/2018_ff_fact_sheet_dec_2020_fnl_508.pdf
- [27] B. P. Weidema and M. S. Wesnæs, “Data quality management for life cycle inventories—an example of using data quality indicators,” *J Clean Prod*, vol. 4, no. 3–4, pp. 167–174, Jan. 1996, doi: 10.1016/S0959-6526(96)00043-1.
- [28] J. O. Karlsson, T. Garnett, N. C. Rollins, and E. Röö, “The carbon footprint of breastmilk substitutes in comparison with breastfeeding,” *J Clean Prod*, vol. 222, pp. 436–445, Jun. 2019, doi: 10.1016/j.jclepro.2019.03.043.
- [29] United States Environmental Protection Agency, “Tool for the Reduction and Assessment of Chemical and Other Environmental Impacts (TRACI) TRACI version 2.1 User’s Guide,” 2012. [Online]. Available: www.epa.gov/research
- [30] M. A. J. Huijbregts *et al.*, “ReCiPe2016: a harmonised life cycle impact assessment method at midpoint and endpoint level,” *International Journal of Life Cycle Assessment*, vol. 22, no. 2, pp. 138–147, Feb. 2017, doi: 10.1007/s11367-016-1246-y.
- [31] B. P. Weidema and M. S. Wesnæs, “Data quality management for life cycle inventories-an example of using data quality indicators,” *J Clean Prod*, vol. 4, no. 3–4, pp. 167–174, 1996, doi: 10.1016/S0959-6526(96)00043-1.
- [32] J. Rickert and A. Ciroth, “Application of the Circular Footprint Formula in Product Environmental Footprint (PEF) 1 APPLICATION OF THE CIRCULAR FOOTPRINT FORMULA (CFF) IN PRODUCT ENVIRONMENTAL FOOTPRINT (PEF) Illustrated through a case study on intermediate paper products,” 2020. [Online]. Available: <https://ec.europa.eu/environment/eussd/videos/2019-10->
- [33] W. Graus and E. Worrell, “Trend in efficiency and capacity of fossil power generation in the EU,” *Energy Policy*, vol. 37, no. 6, pp. 2147–2160, Jun. 2009, doi: 10.1016/j.enpol.2009.01.034.

- [34] N. Vukovic and E. Makogon, “Waste-to-Energy Generation: Complex Efficiency Analysis of Modern Technologies,” *Sustainability*, vol. 14, no. 21, p. 13814, Oct. 2022, doi: 10.3390/su142113814.
- [35] O. Eriksson and G. Finnveden, “Energy Recovery from Waste Incineration—The Importance of Technology Data and System Boundaries on CO2 Emissions,” *Energies (Basel)*, vol. 10, no. 4, p. 539, Apr. 2017, doi: 10.3390/en10040539.
- [36] M. Pavlas, M. Touš, P. Klimek, and L. Bébar, “Waste incineration with production of clean and reliable energy,” *Clean Technol Environ Policy*, vol. 13, no. 4, pp. 595–605, Aug. 2011, doi: 10.1007/s10098-011-0353-5.
- [37] R. Gemmer and K. Paulsen, “2022 Combined Heat and Power/District Energy System Portfolio Meeting: Summary Report,” San Antonio, Jun. 2022.
- [38] US Department of Energy, “Chapter 6: Innovating Clean Energy Technologies in Advanced Manufacturing,” in *Quadrennial Technology Review*, 2015. Accessed: Aug. 21, 2023. [Online]. Available: <https://www.energy.gov/quadrennial-technology-review-2015>

4.0 Comparing LCA Software

Various software tools capable of performing streamlined and full LCAs for all industries have been developed over the years. Each software has pros and cons, especially regarding data availability and manipulation, modeling capabilities, and user-friendliness. Full LCA software often has more flexibility in modeling as practitioners can manipulate existing data or create their own for any stage in LCA, from raw material acquisition to EoL. Streamlined LCA software is often used when stakeholders are interested in evaluating environmental performance in a timely and cost-effective manner, as is needed in most business cases [1]. Several different software's have been developed for this very reason; however, utilizing this type of software raises concerns over accuracy and reliability of results as users may not be able to model the chosen systems precisely. For instance, streamlined LCA software PIQET, draws data from the full LCA software SimaPro but only includes “typical” data used in processing, materials, transportation, filling, and disposal; therefore, it is limited in the fact that certain designs and processes may not be accurately modeled [2].

Most industries, companies, and stakeholders now need help determining whether the Full or Streamlined LCA software will better fit their needs. Similarly, more entities are starting to use LCA to evaluate footprints; more companies are developing or updating LCA software to be used by the masses. For instance, Greenly, openLCA, SimaPro, Life Cycle Assessment for Experts (formally GaBi), and Umberto are all widely advertised to many companies looking to perform LCA without the help of outside consultants [3-8]. However, determining which software to use may be more complex when considering factors other than price. Data availability of these various software can impact the results of an LCA for any product or process, which leads stakeholders to wonder if results from an LCA software are skewed simply because of the software chosen to perform the study.

The following chapter compares the results of an LCA study done for comparing the EF of three package systems in two software, one a streamlined software specializing in packaging LCA, and the other being a generalized full LCA software. Results are compared to investigate how the software chosen to model all three systems can influence the results obtained.

4.1 Software Overview

The streamlined LCA software chosen for this research was PackageSmart, launched in 2011 by EarthShift Global in the U.S. [9]. This software was chosen specifically for its capability in packaging specific LCA as well as its ease of use for potential business applications. This software features EcoInvent database Version 3 data as well as US LCI database data and utilizes the EoL model “Waste scenario packaging 2015/US US-EI S”.

The full LCA software chosen was SimaPro Analyst V9.3.03, as mentioned in **Section 3.3 Materials and Methods**. All modeling for this portion of research is outlined in the previous section. This consists of the system boundaries of the study including cradle-to-gate plus EoL, the functional unit is the delivery of 1000 g of infant formula to the consumer, and the packaging system involves a primary (plastic - package 1, paperboard - package 2, and steel-package 3), secondary (corrugated case), and tertiary (pallet) levels.

4.2 Methods and Modeling

To compare results of a full LCA (Chapter 3) and streamlined LCA, two different software programs were used. The full LCA was performed with SimaPro Analyst version 9.3.03, developed by PRé Sustainability and accessed through a license purchased by Michigan State University. The streamlined LCA was performed with PackageSmart, developed by Earth Shift Global and accessed on a web browser through a license provided by the company. The methodology used to perform the LCA in both software were fully ISO 14040/14044 compliant. In addition, the LCA in both software shared the same goal and scope definitions, system boundaries, and functional unit as described in Chapter 3.

Due to the fact that the two software programs being compared are developed by different companies, have different capabilities, and utilize different databases, modeling the three infant formula packages introduced into the software programs are slightly different. This includes assumptions, EoL modeling of each component, and input data such as materials or processes. The models utilize similar modeling for transportation when possible. When the same data was possible to be used, it was done. The most similar data was used if the same data was unavailable between software. For example, in Package 2, the composite cylinder component is modeled in SimaPro using “Industrial machine, heavy, unspecified, at plant/US-/I US-EI U” to represent the actual production of the component. This exact data is not available in PackageSmart; therefore, this production was modeled as “folding boxes (includes board)/US”,

as the process was added to indicate production of the full composite material cylinder and the paperboard material is the most prominent in the material.

Chapter 3 above includes the modeling of the full LCA study in detail, including the various assumptions used to model, the end-of-life inputs and breakdowns, and all data included in the models of each component. This following section includes all the same information used for the streamlined LCA.

4.2.1 Streamline LCA modeling, assumptions, and end-of-life

PackageSmart Modeling:

The data used to model the various packaging components is detailed below in the same way it was reported in **Section 3.6.1.1 Data Used in Modeling**. The data information obtained from PackageSmart is less specific than that can be obtained from SimaPro, therefore the geography, exact database and year of modification, and background processes are not reported. All data used in modeling is taken from the EcoInvent or US LCI databases, as that is what is available to software users; however, the software does not specify the database for each specific material or process.

Package 1, Plastic Package

Components Package 1, primary level

- Back Label: This component was modeled with four different materials, the first being “Polypropylene resin, at plant NREL/RNA S”. Additionally, the process “Printing Colour, Offset, 47.5% solvent, at plant/US- US-EL S” was used to model the printing of the label. The processing and conversion process chosen for the Back Label was “Extrusion, plastic film/US- US-El S”. In addition, “Laminating, foil, with acrylic binder/US- US-EL S” was used in modeling. Another process added was transportation (see **TRANSPORT**).
- Metal Film: This component was modeled as two materials, the first being “Aluminum, primary, at plant/US- US-EL S”. The second material chosen was “Acrylic Binder, 34% in H₂O, at plant/US- US EL S”. The component also involved two converting processes, the first being “Laminating, foil, with acrylic binder/US- US-EL S”. The other converting process used in modeling was “Sheet Rolling, Aluminum/US- US-EL S”. Another process added was transportation (see **TRANSPORT**).

- Formula Scooper: This component was modeled as “Polypropylene resin, at plant NREL/RNA S”. The component also included a converting process of “Injection Moulding/US US-El S”. Another process added was transportation (see **TRANSPORT**).
- Lid Label: This component was modeled with four different materials, the first being “Polypropylene resin, at plant NREL/RNA S”. Additionally, the process “Printing Colour, Offset, 47.5% solvent, at plant/US- US-EL S” was used to model the printing of the label. The processing and conversion process chosen for the Back Label was “Extrusion, plastic film/US- US-El S”. In addition, “Laminating, foil, with acrylic binder/US- US-EL S” was used in modeling. Another process added was transportation (see **TRANSPORT**).
- Plastic Lid: This component was modeled as “Polypropylene resin, at plant NREL/RNA S”. The component also included a converting process of “Injection Moulding/US US-El S”. Another process added was transportation (see **TRANSPORT**).
- Plastic Tub: The plastic tub was modeled with two different materials, the first being “High Density Polyethylene resin, at plant NREL/RNA S”. The second material used to model was “Ethylene Vinyl Acetate copolymer, at plant/US- US-EL S”. This component was also modeled with two main processing and conversion techniques, the first being “Blow moulding/US- US-EL S”. The second conversion process used was “Extrusion, plastic film/US- US-El S”. Another process added was transportation (see **TRANSPORT**).
- Silver Tamper-Evident Sticker: This component was modeled as “Kraft paper, unbleached, at plant/US- US-El S”. Another material used to model this component was “Aluminum, primary, at plant/US- US-El S”. The binder between the Kraft Paper and Aluminum was “Acrylic Binder, 34% in H₂O, at plant/US- US EL S”. In addition, the process “Laminating, foil, with acrylic binder/US- US-EL S” was used in modeling. Another process added was transportation (see **TRANSPORT**).
- Tear-Off Plastic Area: This component was modeled as “Polypropylene resin, at plant NREL/RNA S”. The component also included a converting process of “Injection Moulding/US US-El S”. Another process added was transportation (see **TRANSPORT**).
- Wrap Around Label: This component was modeled with four different materials, the first being “Polypropylene resin, at plant NREL/RNA S”. Additionally, the process “Printing

Colour, Offset, 47.5% solvent, at plant/US- US-EL S” was used to model the printing of the label. The processing and conversion process chosen for the Back Label was “Extrusion, plastic film/US- US-El S”. In addition, “Laminating, foil, with acrylic binder/US- US-EL S” was used in modeling. Another process added was transportation (see **TRANSPORT**).

Components Package 1, secondary level

- Corrugated Case: This component was modeled as “Corrugated board, mixed fibre, single wall, at plant/US- US-El S”. Another process added was transportation (see **TRANSPORT**).
- Dividers: This component was modeled as “Corrugated board, mixed fibre, single wall, at plant/US- US-El S”. Another process added was transportation (see **TRANSPORT**).
- Hot Melt Glue: This component was modeled as "Dummy_Glue-adhesive(30-50% terpene,30-50% polybutene,5-10% polyolefin), at plant". Another process added was transportation (see **TRANSPORT**).

Components Package 1, tertiary level

- Pallet Slip Sheets: This component was modeled as “Corrugated board, mixed fibre, single wall, at plant/US- US-El S”. Another process added was transportation (see **TRANSPORT**).
- Stretch Wrap: This component was modeled as two components, the first being the stretch wrap itself as “Stretch Wrap, LLDPE film, at plant/US S”. The second component was the core board in which the stretch wrap was stored, which was modeled as “Core Board, at plant/US- US-El S”. Another process added was transportation (see **TRANSPORT**).
- Wood Pallet: This component was modeled as “Pallet (22kg)/US- US-El S”. Another process added was transportation (see **TRANSPORT**).

Package 2, Composite Package

Components Package 2, primary level

- Aluminum Ring: This component was modeled as “Aluminum, primary, at plant/US- US-El U”. This component also includes a processing and conversion portion of the modeling, named “Metal working, average for aluminum production manufacturing

{GLO}| market for | Cut-Off S”. Another process added was transportation (see **TRANSPORT**).

- Composite Can: This component was modeled with three different materials as it was a composite material with plastic, paperboard, and metal portions. The most abundant portion was the paperboard portion, modeled as “Kraft paper, unbleached, at plant/US-US-El S”. The second largest material portion was modeled as “Polypropylene resin, at plant NREL/RNA S”. The third material portion was modeled as “Aluminum, primary, at plant/US-US-El S”. This component also included two processing and conversion techniques, one of which was modeled as “Laminating, foil, with acrylic binder/US-US-El S”. Additionally, the process “folding boxes (includes board)/US” was used to represent the tubing process in manufacturing. Another process added was transportation (see **TRANSPORT**).
- Formula Scooper: This component was modeled as “Polypropylene resin, at plant NREL/RNA S”. The component also included a converting process of “Injection Moulding/US US-El S”. Another process added was transportation (see **TRANSPORT**).
- Full Label: This component was modeled as two materials, the first being “Kraft paper, bleached, at plant/US-US-El S”. The second material was “Acrylic Binder, 34% in H₂O, at plant/US-US-El S”. No additional processes were used to model printing, as no available data was deemed accurate enough to include in modeling. Another process added was transportation (see **TRANSPORT**).
- Peel Off Metal Seal: This component was modeled as “Steel, low-alloyed, at plant/US-US-El S”. The processing portion of this component was “Steel product manufacturing, average metalworking/US-US-El S”. Another process added was transportation (see **TRANSPORT**).
- Plastic Over cap: This component was modeled as “Linear low density polyethylene resin, at plant NREL/RNA S”. The processing portion of this component was modeled as “Injection Moulding/US US-El S. Another process added was transportation (see **TRANSPORT**).
- Steel Bottom: This component was modeled as “Steel, low-alloyed, at plant/US-US-El S”. The processing portion of this component was "Steel product manufacturing, average metalworking/US-US-El S”. A second processing and converting technique used to

model this component was “Sheet Rolling, Steel/US- US-EL S”. Another process added was transportation (see **TRANSPORT**).

Components Package 2, secondary level

- Corrugated Case: This component was modeled as “Corrugated board, mixed fibre, single wall, at plant/US- US-El S”. Another process added was transportation (see **TRANSPORT**).
- Tape: This component was modeled as “Polypropylene resin, at plant NREL/RNA S”. In addition, the material, “Ethyl vinyl acetate copolymer, at plant/US- US-El S” was used to model the adhesive of the tape. The conversion and processing modeling chosen was “Extrusion, plastic film/US- US-El S”. Another process added was transportation (see **TRANSPORT**).

Components Package 2, tertiary level

- Pallet Slip Sheets: This component was modeled as “Corrugated board, mixed fibre, single wall, at plant/US- US-El S”. Another process added was transportation (see **TRANSPORT**).
- Stretch Wrap: This component was modeled as two components, the first being the stretch wrap itself as “Stretch Wrap, LLDPE film, at plant/US S”. The second component was the core board in which the stretch wrap was stored, which was modeled as “Core Board, at plant/US- US-El S”. Another process added was transportation (see **TRANSPORT**).
- Wood Pallet: This component was modeled as “Pallet (22kg)/US- US-El S”. Another process added was transportation (see **TRANSPORT**).

Package 3, Steel Package

Components Package 3, primary level

- Aluminum Ring: This component was modeled as “Aluminum, primary, at plant/US- US-El U”. This component also includes a processing and conversion portion of the modeling, named “Metal working, average for aluminum production manufacturing {GLO}| market for | Cut-Off S”. Another process added was transportation (see **TRANSPORT**).

- Formula Scooper: This component was modeled as “Polypropylene resin, at plant NREL/RNA S”. The component also included a converting process of “Injection Moulding/US US-El S”. Another process added was transportation (see **TRANSPORT**).
- Peel Off Metal Seal: This component was modeled as “Steel, low-alloyed, at plant/ US- US-El S”. The processing portion of this component was “Steel product manufacturing, average metalworking/US- US-El S”. Another process added was transportation (see **TRANSPORT**).
- Plastic Over cap: This component was modeled as “Linear low density polyethylene resin, at plant NREL/RNA S”. The processing portion of this component was modeled as “Injection Moulding/US US-El S. Another process added was transportation (see **TRANSPORT**).
- Steel Bottom: This component was modeled as “Steel, low-alloyed, at plant/ US- US-El S”. The processing portion of this component was "Steel product manufacturing, average metalworking/US- US-El S”. A second processing and converting technique used to model this component was “Sheet Rolling, Steel/US- US-EL S”. Another process added was transportation (see **TRANSPORT**).
- Steel Can: This component was modeled as “Steel, low-alloyed, at plant/ US- US-El S”. Processing and converting techniques were used to model this component, which were “Sheet Rolling, Steel/US- US-EL S”. Another processing and converting technique used to model this component was “Welding, arc, steel/US- US-El S”. Another process added was transportation (see **TRANSPORT**).

Components Package 3, secondary level

- Corrugated Case: This component was modeled as “Corrugated board, mixed fibre, single wall, at plant/US- US-El S”. Another process added was transportation (see **TRANSPORT**).
- Tape: This component was modeled as “Polypropylene resin, at plant NREL/RNA S”. In addition, the material, “Ethyl vinyl acetate copolymer, at plant/US- US-El S” was used to model the adhesive of the tape. The conversion and processing modeling chosen was “Extrusion, plastic film/US- US-El S”. Another process added was transportation (see **TRANSPORT**).

Components Package 3, tertiary level

- Pallet Slip Sheets: This component was modeled as “Corrugated board, mixed fibre, single wall, at plant/US- US-EI S”. Another process added was transportation (see **TRANSPORT**).
- Stretch Wrap: This component was modeled as two components, the first being the stretch wrap itself as “Stretch Wrap, LLDPE film, at plant/US S”. The second component was the core board in which the stretch wrap was stored, which was modeled as “Core Board, at plant/US- US-EI S”. Another process added was transportation (see **TRANSPORT**).
- Wood Pallet: This component was modeled as “Pallet (22kg)/US- US-EI S”. Another process added was transportation (see **TRANSPORT**).

Transport

- Transportation for each component of every packaging level (primary, secondary, and tertiary) was modeled as "Transport, combination truck, average fuel mix NREL/US S". The same data was used for transportation of the entire packaging system.

Electricity

- No specified Electricity data used to model.

Ink

- Environmental burdens of ink were selectively included with some processes and described when included. Otherwise, inks were not included in the inventory since they represent a small amount of the weight and environmental footprint.

Filling of product

- The product and the burdens of filling the containers with a product were not considered.

Assumptions in Modeling

- All assumptions detailed in **Section**
- 3.6.2.1 Assumptions and Limitations above remain valid for the PackageSmart modeling.

End of Life

EoL modeling in PackageSmart was done to replicate that specified by **Table 3. 4** above. This modeling is equivalent to the cut-off methodology, which was the primary EoL methodology represented in the previous chapter. Breakdowns between Recycling, Landfill, and Incineration are identical for each component between the two software programs. Default

values for landfill and incineration were 80.5% and 19.5% respectively. Recycling rates of each component were manually input into the PackageSmart build to reflect recycling rates used in SimaPro.

- The waste scenario chosen in PackageSmart was “Waste scenario packaging 2015/US US-EI S”, the most recent scenario available in modeling.
- The Landfill data chosen to model was “Landfill/US US-EI S”.
- The Incineration data chosen to model was “Incineration/US US-EI S”.

4.2.2 Notable Differences between the two models

Some major differences should be taken into consideration when comparing the results of the two software, as discrepancies in inputs would presumably lead to the software’s outputs to be different. Below are the notable differences.

- Specific Component differences
 - Package 1 – Hot melt glue
 - In SimaPro, this component is modeled as the material “Polyurethane adhesive {GLO}|market for polyurethane”.
 - In PackageSmart it is modeled as "Dummy_Glue-adhesive(30-50% terpene,30-50% polybutene,5-10% polyolefin), at plant".
 - Package 2 – Composite Tube
 - In SimaPro, this component is modeled using the process “Industrial machine, heavy, unspecified, at plant/US-/I US-EI U”.
 - In PackageSmart, therefore this was modeled as “folding boxes (includes board)/US”.
 - Package 2 – Full Label
 - In SimaPro, this component is modeled using the process “Use, printer, laser jet, colour, per kg printed paper/US- US-EI U”.
 - In PackageSmart, there is no modeling data available to represent the printing of the full label, therefore the component is only modeled as a material.
- Unit versus System Processes in modeling
 - When modeling in SimaPro, the Unit process data was chosen for modeling. The unit process data is the smallest possible unit in which inputs and outputs are

quantified in LCI. System processes are aggregated versions, coming from a compilation of various inputs and outputs of a products life cycle [10]. Although SimaPro can model these packaging systems using System process, the modelling of the three packaging systems was done before modeling in SimaPro and is much more time-consuming to change from U to S. This was also not changed to match because this classification is not supposed to influence LCA results since system process is an aggregation of unit process, therefore the classification between Unit and System data should not be the difference driving result discrepancies [11].

4.2.3 Comparison of Results

The TRACI 2.1 impact method was used for both SimaPro and PackageSmart to compare the results between the software, allowing for the ten impact categories to be compared directly with the same units. The LCIA for each separate analysis was run individually in the respective software; then, the values obtained in the analysis were compared. Results that can be compared between software are shown below; not all analyses capable of each software can be compared to each other; hence, **Section 3.4 Results and Discussion** may show different types of results.

4.3 Results and Discussion

4.3.1 Contribution Analysis

The SimaPro and PackageSmart software can provide a component contribution breakdown to determine which components are explicitly contributing to the environmental impact of the package. **Figure 4. 1** below shows the results of the component breakdown for the Primary Package Level of Package 1. **Figure 4. 1a** are the results from SimaPro, while **Figure 4. 1b** are the results from PackageSmart.

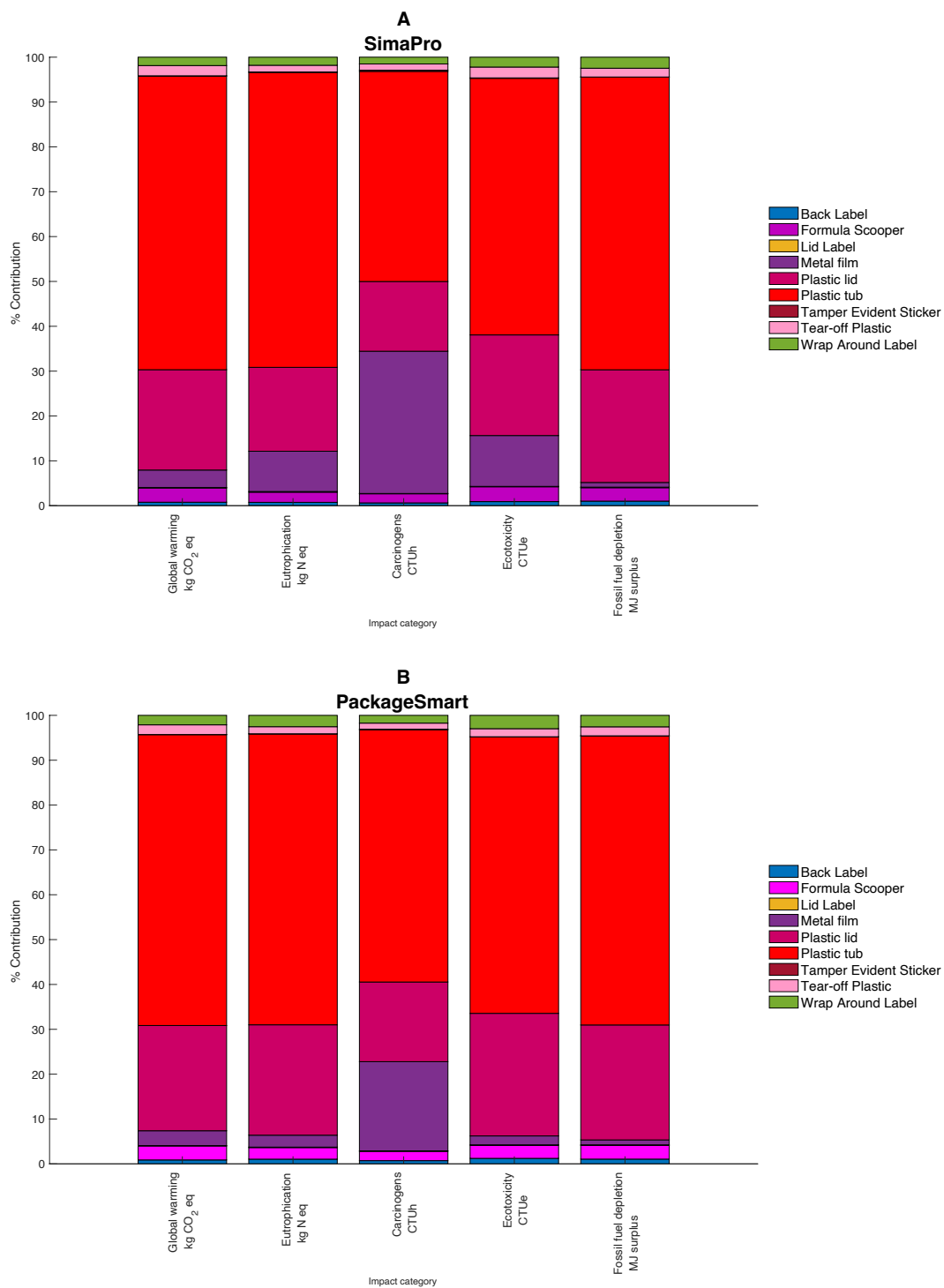


Figure 4. 1: Component Contribution Breakdown for Package 1, the plastic container according to a) SimaPro and b) PackageSmart for the five TRACI 2.1 Impact Categories.

Table 4. 1: Values for each primary package component contribution for all three packages from both SimaPro and PackageSmart.

Component	Impact Category	Units	SimaPro Value	PackageSmart Value	Difference
Back Label	Global Warming	kg CO ₂ eq	4.31E-03	6.15E-03	35%
	Eutrophication	kg N eq	5.14E-06	2.89E-05	140%
	Carcinogens	CTUh	1.04E-10	2.09E-10	67%
	Ecotoxicity	CTUe	1.72E-02	1.64E-01	162%
	Fossil Fuel				
	Depletion	MJ surplus	2.15E-02	2.14E-02	1%
Formula Scoop	Global Warming	kg CO ₂ eq	1.77E-02	2.18E-02	21%
	Eutrophication	kg N eq	1.56E-05	7.09E-05	128%
	Carcinogens	CTUh	3.40E-10	6.03E-10	56%
	Ecotoxicity	CTUe	6.25E-02	3.87E-01	144%
	Fossil Fuel				
	Depletion	MJ surplus	6.31E-02	6.18E-02	2%
Lid Sicker	Global Warming	kg CO ₂ eq	5.23E-04	7.66E-04	38%
	Eutrophication	kg N eq	1.01E-06	3.00E-06	99%
	Carcinogens	CTUh	1.14E-11	3.12E-11	93%
	Ecotoxicity	CTUe	1.63E-03	1.42E-02	159%
	Fossil Fuel				
	Depletion	MJ surplus	2.68E-03	2.41E-03	11%
Metal Film	Global Warming	kg CO ₂ eq	2.17E-02	2.31E-02	6%
	Eutrophication	kg N eq	6.18E-05	7.31E-05	17%
	Carcinogens	CTUh	5.30E-09	5.79E-09	9%
	Ecotoxicity	CTUe	2.14E-01	2.65E-01	21%
	Fossil Fuel				
	Depletion	MJ surplus	2.20E-02	2.22E-02	1%
Plastic Lid	Global Warming	kg CO ₂ eq	1.25E-01	1.65E-01	28%
	Eutrophication	kg N eq	1.29E-04	6.77E-04	136%
	Carcinogens	CTUh	2.60E-09	5.17E-09	66%
	Ecotoxicity	CTUe	4.23E-01	3.64E+00	158%
	Fossil Fuel				
	Depletion	MJ surplus	5.30E-01	5.17E-01	2%
Plastic Tub	Global Warming	kg CO ₂ eq	3.65E-01	4.55E-01	22%
	Eutrophication	kg N eq	4.53E-04	1.78E-03	119%
	Carcinogens	CTUh	7.83E-09	1.64E-08	71%
	Ecotoxicity	CTUe	1.08E+00	8.21E+00	154%
	Fossil Fuel				
	Depletion	MJ surplus	1.38E+00	1.30E+00	6%
Tamper Evident Sticker	Global Warming	kg CO ₂ eq	1.87E-04	2.15E-04	14%
	Eutrophication	kg N eq	5.39E-07	6.49E-07	18%
	Carcinogens	CTUh	4.32E-11	4.77E-11	10%
	Ecotoxicity	CTUe	1.77E-03	2.27E-03	24%
	Fossil Fuel				
	Depletion	MJ surplus	2.00E-04	1.99E-04	1%
Tear off Plastic	Global Warming	kg CO ₂ eq	1.27E-02	1.51E-02	17%
	Eutrophication	kg N eq	1.03E-05	4.34E-05	123%
	Carcinogens	CTUh	2.34E-10	3.91E-10	50%
	Ecotoxicity	CTUe	4.56E-02	2.40E-01	136%
	Fossil Fuel				
	Depletion	MJ surplus	4.13E-02	4.05E-02	2%
Wrap around label	Global Warming	kg CO ₂ eq	1.04E-02	1.48E-02	35%
	Eutrophication	kg N eq	1.24E-05	6.96E-05	139%
	Carcinogens	CTUh	2.52E-10	5.05E-10	67%
	Ecotoxicity	CTUe	4.15E-02	3.96E-01	162%
	Fossil Fuel				
	Depletion	MJ surplus	5.20E-02	5.16E-02	1%

As seen in **Figure 4. 1**, the two software programs provide similar component breakdowns, concluding that the Plastic Lid and Plastic Tub components contribute the most to the overall environmental impact of the system. Similarly, in **Figure 4. 2** and **Figure 4. 3**, the two software provide similar component breakdowns for Packages 2 and 3, respectively. For Package 2, the two components that contribute the most in almost impact categories is the composite cylinder and the steel bottom; however, the actual contribution percentages differ quite a bit. For instance, in the Carcinogens impact category for SimaPro, the composite cylinder and steel bottom contribute 64% and 24%, respectively whereas in PacakgeSmart these contributions shift to 27% and 57%, respectively. Breakdowns for Package 3 are nearly identical, with the steel can and steel bottom being the top two contributors in each category. Actual values generated by the software tools, however, show rather large discrepancies when looking at **Table 4. 1**. Between impact categories and packages, differences in values obtained by SimaPro and PackageSmart differ from anywhere between 1% and 162%, meaning that although the conclusions as to which package components contribute the most to the packaging system impact are the same, the values of those impacts vary tremendously between software. The same trend is also seen for Package 2 in **Figure 4. 2** with a range of 2% and 166% difference and for Package 3 in **Figure 4. 3** with a 1% to 167% difference. The exact drivers for these range of differences are unknown, which may leave potential for future work investigating this however it is presumed by this author that the differences may be due to data manipulation in SimaPro that is unable to be replicated in PackageSmart.

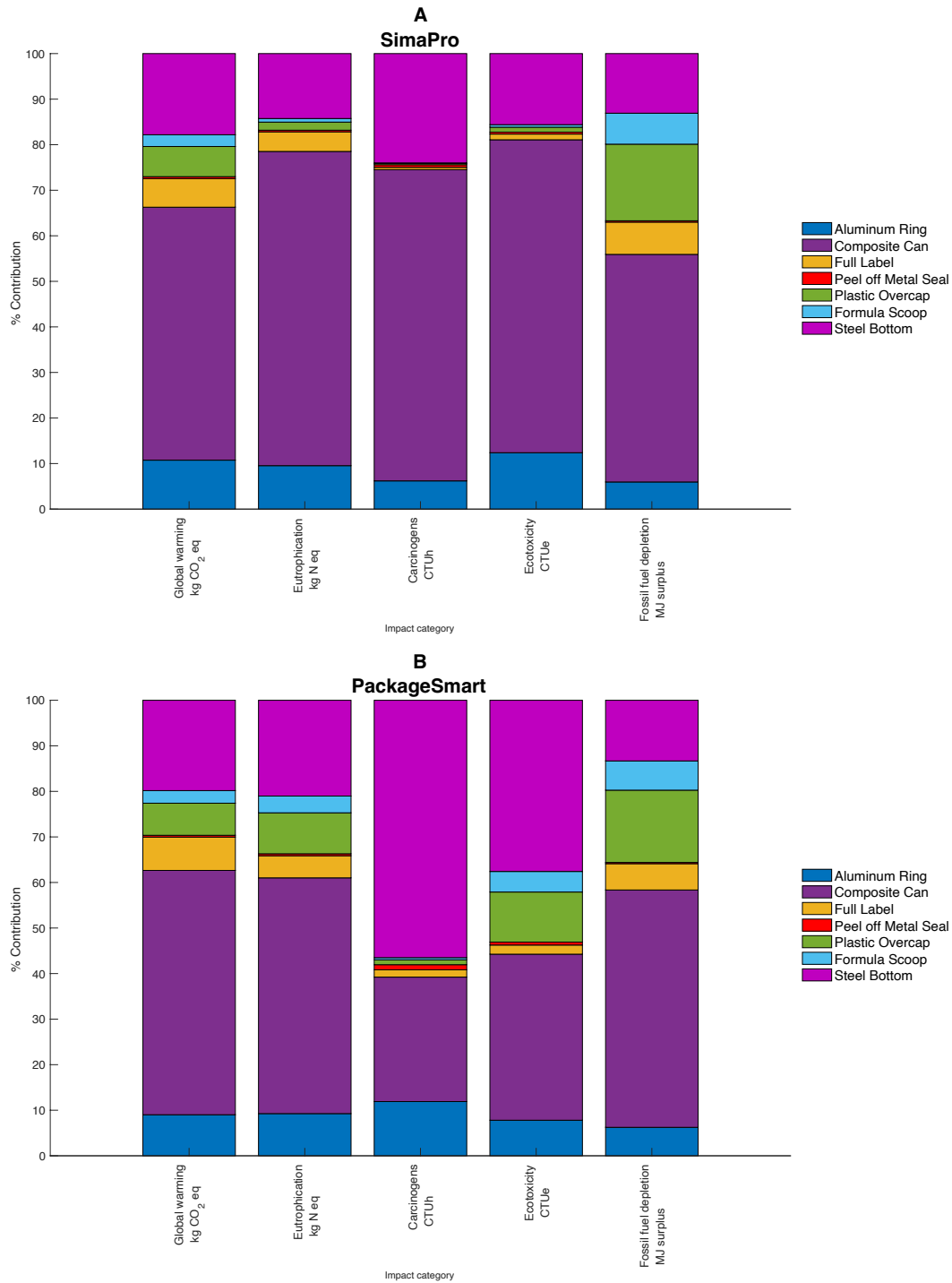


Figure 4. 2: Component Contribution Breakdown for Package 2, the composite container according to a) SimaPro and b) PackageSmart for the five TRACI 2.1 Impact Categories.

Table 4. 2: Values for each primary package component contribution for all Package 2 from both SimaPro and PackageSmart.

Contribution Table					
Component	Impact Category	Units	SimaPro Value	PackageSmart Value	Difference
Composite Can	Global Warming	kg CO ₂ eq	3.01E-01	3.59E-01	18%
	Eutrophication	kg N eq	1.27E-03	1.07E-03	17%
	Carcinogens	CTUh	1.56E-07	3.36E-08	129%
	Ecotoxicity	CTUe	5.89E+00	3.32E+00	56%
	Fossil Fuel Depletion	MJ surplus	4.39E-01	4.73E-01	8%
Formula Scooper	Global Warming	kg CO ₂ eq	1.40E-02	1.85E-02	28%
	Eutrophication	kg N eq	1.45E-05	7.65E-05	136%
	Carcinogens	CTUh	2.92E-10	5.83E-10	66%
	Ecotoxicity	CTUe	4.74E-02	4.11E-01	159%
	Fossil Fuel Depletion	MJ surplus	5.97E-02	5.82E-02	2%
Full Label	Global Warming	kg CO ₂ eq	3.40E-02	4.89E-02	36%
	Eutrophication	kg N eq	7.94E-05	1.01E-04	24%
	Carcinogens	CTUh	1.18E-09	1.99E-09	50%
	Ecotoxicity	CTUe	1.08E-01	1.82E-01	51%
	Fossil Fuel Depletion	MJ surplus	6.22E-02	5.24E-02	17%
Plastic Overcap	Global Warming	kg CO ₂ eq	3.58E-02	4.71E-02	27%
	Eutrophication	kg N eq	3.28E-05	1.87E-04	140%
	Carcinogens	CTUh	6.21E-10	1.33E-09	72%
	Ecotoxicity	CTUe	9.33E-02	1.00E+00	166%
	Fossil Fuel Depletion	MJ surplus	1.48E-01	1.44E-01	2%
Peel Off Metal Seal	Global Warming	kg CO ₂ eq	2.31E-03	2.65E-03	14%
	Eutrophication	kg N eq	6.68E-06	8.82E-06	28%
	Carcinogens	CTUh	1.30E-09	1.37E-09	5%
	Ecotoxicity	CTUe	3.59E-02	5.88E-02	48%
	Fossil Fuel Depletion	MJ surplus	2.64E-03	2.38E-03	10%
Steel Bottom	Global Warming	kg CO ₂ eq	9.64E-02	1.33E-01	32%
	Eutrophication	kg N eq	2.63E-04	4.37E-04	50%
	Carcinogens	CTUh	5.49E-08	6.95E-08	23%
	Ecotoxicity	CTUe	1.34E+00	3.42E+00	88%
	Fossil Fuel Depletion	MJ surplus	1.15E-01	1.21E-01	5%
Aluminum Ring	Global Warming	kg CO ₂ eq	5.82E-02	6.03E-02	4%
	Eutrophication	kg N eq	1.76E-04	1.92E-04	9%
	Carcinogens	CTUh	1.42E-08	1.46E-08	3%
	Ecotoxicity	CTUe	1.06E+00	7.11E-01	40%
	Fossil Fuel Depletion	MJ surplus	5.23E-02	5.67E-02	8%

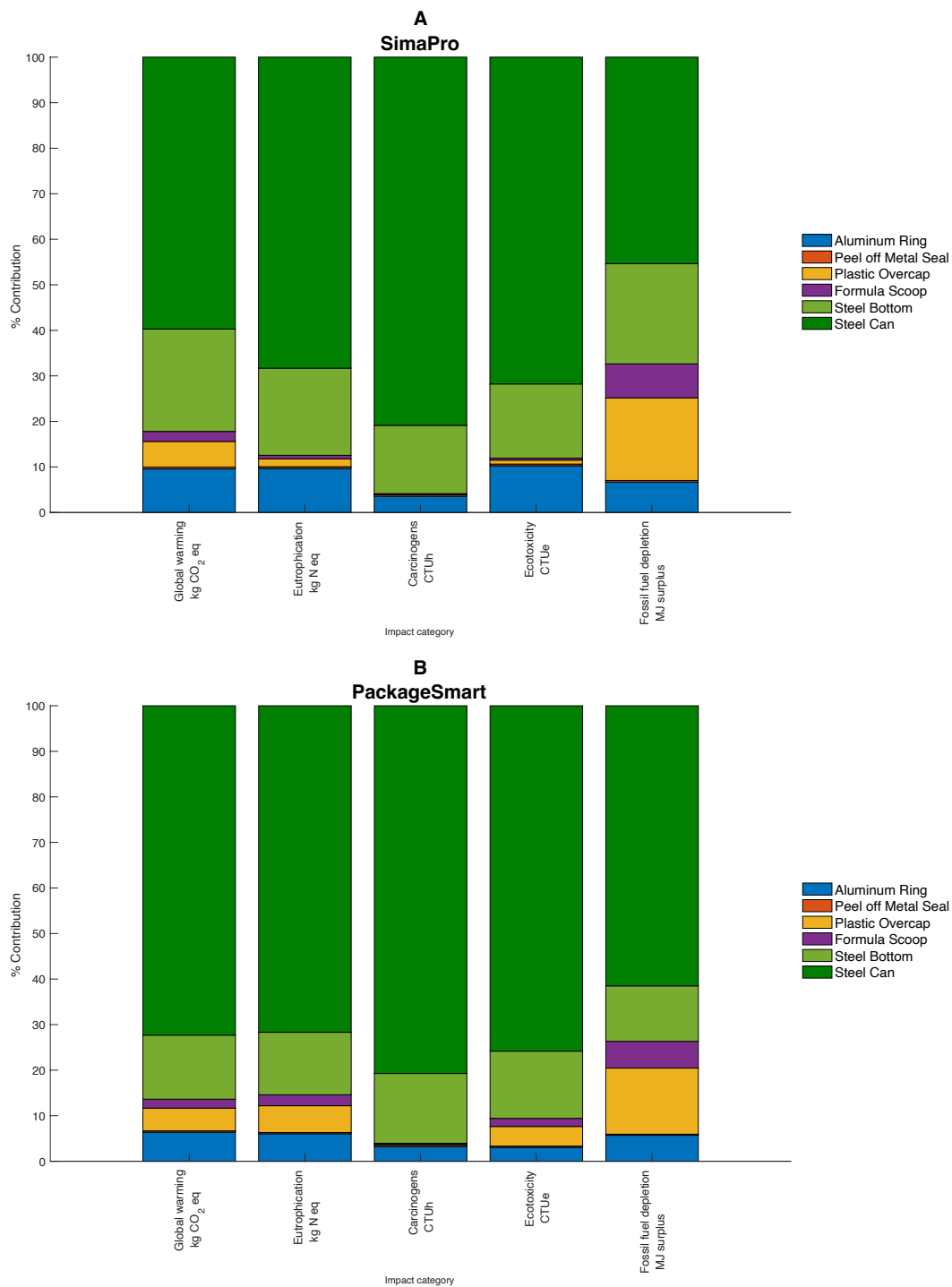


Figure 4. 3: Component Contribution Breakdown for Package 3, the steel container according to a) SimaPro and b) PackageSmart for the five TRACI 2.1 Impact Categories.

Table 4. 3: Values for each primary package component contribution for all Package 3 from both SimaPro and PackageSmart.

Contribution Table					
Component	Impact Category	Units	SimaPro Value	PackageSmart Value	Difference
Steel Can	Global Warming	kg CO ₂ eq	3.67E-01	6.82E-01	60%
	Eutrophication	kg N eq	1.25E-03	2.28E-03	58%
	Carcinogens	CTUh	3.22E-07	3.66E-07	13%
	Ecotoxicity	CTUe	7.44E+00	1.76E+01	81%
	Fossil Fuel Depletion	MJ surplus	3.57E-01	6.10E-01	52%
Aluminum Ring	Global Warming	kg CO ₂ eq	5.88E-02	6.03E-02	2%
	Eutrophication	kg N eq	1.77E-04	1.92E-04	8%
	Carcinogens	CTUh	1.42E-08	1.46E-08	3%
	Ecotoxicity	CTUe	1.06E+00	7.11E-01	40%
	Fossil Fuel Depletion	MJ surplus	5.26E-02	5.67E-02	8%
Peel Off Metal Seal	Global Warming	kg CO ₂ eq	2.42E-03	2.65E-03	9%
	Eutrophication	kg N eq	7.00E-06	8.82E-06	23%
	Carcinogens	CTUh	1.36E-09	1.37E-09	0%
	Ecotoxicity	CTUe	3.75E-02	5.88E-02	44%
	Fossil Fuel Depletion	MJ surplus	2.76E-03	2.38E-03	15%
Plastic Overcap	Global Warming	kg CO ₂ eq	3.46E-02	4.71E-02	30%
	Eutrophication	kg N eq	3.17E-05	1.87E-04	142%
	Carcinogens	CTUh	6.00E-10	1.33E-09	75%
	Ecotoxicity	CTUe	9.02E-02	1.00E+00	167%
	Fossil Fuel Depletion	MJ surplus	1.43E-01	1.44E-01	1%
Formula Scooper	Global Warming	kg CO ₂ eq	1.35E-02	1.85E-02	31%
	Eutrophication	kg N eq	1.42E-05	7.65E-05	137%
	Carcinogens	CTUh	2.85E-10	5.83E-10	69%
	Ecotoxicity	CTUe	4.55E-02	4.11E-01	160%
	Fossil Fuel Depletion	MJ surplus	5.88E-02	5.82E-02	1%
Steel Bottom	Global Warming	kg CO ₂ eq	1.38E-01	1.33E-01	4%
	Eutrophication	kg N eq	3.51E-04	4.37E-04	22%
	Carcinogens	CTUh	5.99E-08	6.95E-08	15%
	Ecotoxicity	CTUe	1.69E+00	3.42E+00	68%
	Fossil Fuel Depletion	MJ surplus	1.73E-01	1.21E-01	36%

4.3.2 Comparative Analysis

When comparing the three packages' systems against one another using the aforementioned functional unit of the delivery of 1000 g of infant formula to the consumer, both software programs can provide a total environmental impact for each package. Therefore, this was compared. **Figure 4. 4** below shows the comparative analysis among the three packages. **Figure 4. 4a** is the comparison from SimaPro and **Figure 4. 4b** is the comparison from PackageSmart.

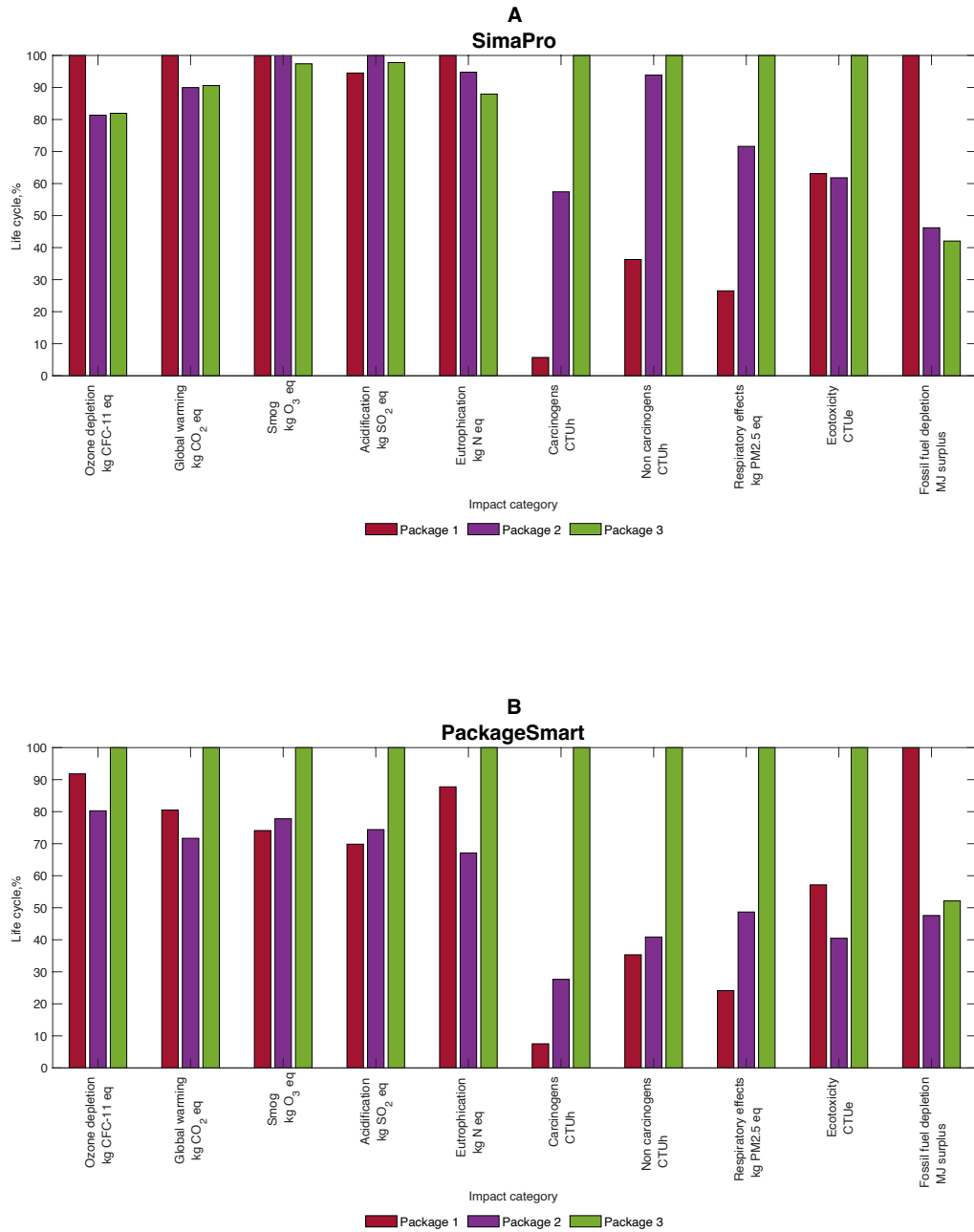


Figure 4. 4: Overall Comparison of comparative results for the three package systems using TRACI 2.1 Impact method.

Table 4. 4: Overall Comparison of comparative results for the three package systems using TRACI 2.1 Impact method.

		SimaPro	PackageSmart	% Difference	
Package 1	Impact category	Units	Package 1 (Plastic)	Package 1 (Plastic)	
	Ozone depletion	kg CFC-11 eq	5.08E-08	5.41E-08	6%
	Global warming	kg CO ₂ eq	8.01E-01	8.51E-01	6%
	Smog	kg O ₃ eq	4.40E-02	4.07E-02	8%
	Acidification	kg SO ₂ eq	2.73E-03	3.07E-03	12%
	Eutrophication	kg N eq	2.39E-03	2.97E-03	22%
	Carcinogenics	CTUh	2.30E-08	3.45E-08	40%
	Non carcinogenics	CTUh	1.35E-07	1.85E-07	31%
	Respiratory effects	kg PM2.5 eq	1.77E-04	1.98E-04	11%
	Ecotoxicity	CTUe	1.29E+01	1.32E+01	2%
	Fossil fuel depletion	MJ surplus	2.32E+00	2.27E+00	2%
Package 2	Impact category	Unit	Package 2 (Composite)	Package 2 (Composite)	
	Ozone depletion	kg CFC-11 eq	4.13E-08	4.73E-08	14%
	Global warming	kg CO ₂ eq	7.20E-01	7.58E-01	5%
	Smog	kg O ₃ eq	4.41E-02	4.27E-02	3%
	Acidification	kg SO ₂ eq	2.89E-03	3.27E-03	12%
	Eutrophication	kg N eq	2.27E-03	2.27E-03	0%
	Carcinogenics	CTUh	2.31E-07	1.26E-07	58%
	Non carcinogenics	CTUh	3.48E-07	2.14E-07	48%
	Respiratory effects	kg PM2.5 eq	4.79E-04	3.99E-04	18%
	Ecotoxicity	CTUe	1.27E+01	9.38E+00	30%
	Fossil fuel depletion	MJ surplus	1.07E+00	1.08E+00	1%
Package 3	Impact category	Unit	Package 3 (Steel)	Package 3 (Steel)	
	Ozone depletion	kg CFC-11 eq	4.16E-08	5.89E-08	34%
	Global warming	kg CO ₂ eq	7.25E-01	1.06E+00	37%
	Smog	kg O ₃ eq	4.29E-02	5.49E-02	25%
	Acidification	kg SO ₂ eq	2.82E-03	4.39E-03	43%
	Eutrophication	kg N eq	2.10E-03	3.38E-03	47%
	Carcinogenics	CTUh	4.02E-07	4.57E-07	13%
	Non carcinogenics	CTUh	3.71E-07	5.22E-07	34%
	Respiratory effects	kg PM2.5 eq	6.69E-04	8.20E-04	20%
	Ecotoxicity	CTUe	2.05E+01	2.32E+01	12%
	Fossil fuel depletion	MJ surplus	9.78E-01	1.18E+00	19%

When looking at **Figure 4. 4**, the two software generate different results when running a LCIA for the same three packages. The SimaPro results indicate that Package 1 has the highest impact in 4 out of the 10 impact categories, Package 2 has the highest impact in 2 out of the 10 impact categories, and Package 3 has the highest impact in the remaining 4 out of 10 impact categories. The PackageSmart results on the other hand show that Package 1 has the highest impact in just 1 of the impact categories, Package 2 does not have the highest impact in any impact categories, and Package 3 has the highest impact in 9 out of the 10 impact categories.

When looking at **Table 4. 4**, however, it can be seen that the actual values for each indicator within the three respective packages are relatively similar. Except for Carcinogens category for Package 2, the differences between values obtained by each software are less than 50% difference, which when the units are so small, may only be an absolute value difference of 0.01 units. Statistical significance of these values is not determined in this particular research.

4.3.3 Scenario Analysis

As mentioned in Chapter 3, some scenarios were run to investigate the change in impact when lightweighting primary package components within all three systems. Both software have the capability of running this type of analysis with the use of the parameter function. **Figure 4. 5** below shows the lightweighting scenario for Package 1. This scenario involved lightweighting the Plastic Lid and Plastic Tub components by 30%, an arbitrary number used in modeling to ensure a trend could be found, it is understood, however, that this amount of reduction is not necessarily feasible for the company to actually model. **Figure 4. 5a** shows the results from SimaPro and **Figure 4. 5b** shows the results from PackageSmart.

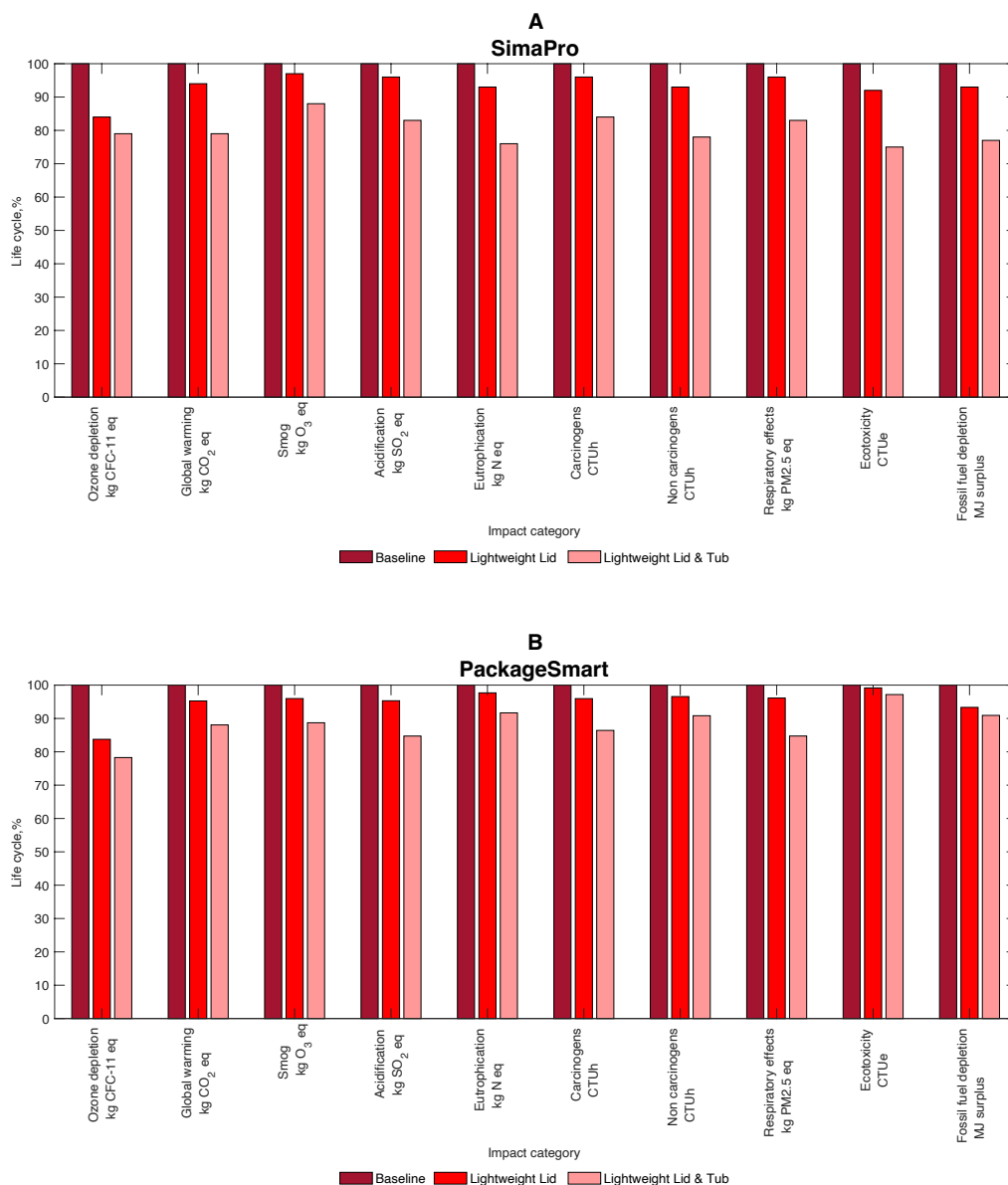


Figure 4. 5: Scenario analysis for Package 1 using TRACI 2.1 impact assessment method. Lightweighting the lid and tub components for Package 1 by 30%.

Table 4. 5: Value Comparison for the Scenario analysis for Package 1 using TRACI 2.1 impact assessment method. Lightweighting the lid and tub components for Package 1 by 30%.

	SimaPro		PackageSmart		% Difference
	Impact category	Units	Baseline	Baseline	
Baseline	Ozone depletion	kg CFC-11 eq	5.23E-08	5.41E-08	3%
	Global warming	kg CO2 eq	0.78626712	8.51E-01	8%
	Smog	kg O3 eq	0.041347494	4.07E-02	2%
	Acidification	kg SO2 eq	0.002510739	3.07E-03	20%
	Eutrophication	kg N eq	0.00246732	2.97E-03	18%
	Carcinogenics	CTUh	1.96E-08	3.45E-08	55%
	Non carcinogenics	CTUh	1.53E-07	1.85E-07	19%
	Respiratory effects	kg PM2.5 eq	0.000145596	1.98E-04	30%
	Ecotoxicity	CTUe	13.130155	1.32E+01	1%
	Fossil fuel depletion	MJ surplus	2.3769767	2.27E+00	5%
Lightweight Lid	Impact category	Unit	Lightweight Lid	Lightweight Lid	
	Ozone depletion	kg CFC-11 eq	4.37E-08	4.53E-08	4%
	Global warming	kg CO2 eq	0.7428268	8.11E-01	9%
	Smog	kg O3 eq	0.040072989	3.90E-02	3%
	Acidification	kg SO2 eq	0.002400356	2.92E-03	20%
	Eutrophication	kg N eq	0.002289978	2.90E-03	23%
	Carcinogenics	CTUh	1.87E-08	3.31E-08	56%
	Non carcinogenics	CTUh	1.43E-07	1.78E-07	22%
	Respiratory effects	kg PM2.5 eq	0.000140078	1.90E-04	30%
	Ecotoxicity	CTUe	12.089886	1.31E+01	8%
	Fossil fuel depletion	MJ surplus	2.2209866	2.12E+00	5%
Lightweight Lid and Tub	Impact category	Unit	Lightweight Lid and Tub	Lightweight Lid and Tub	
	Ozone depletion	kg CFC-11 eq	4.12E-08	4.24E-08	3%
	Global warming	kg CO2 eq	0.62321746	7.50E-01	18%
	Smog	kg O3 eq	0.036566166	3.61E-02	1%
	Acidification	kg SO2 eq	0.002080323	2.60E-03	22%
	Eutrophication	kg N eq	0.001869427	2.72E-03	37%
	Carcinogenics	CTUh	1.64E-08	2.98E-08	58%
	Non carcinogenics	CTUh	1.19E-07	1.68E-07	34%
	Respiratory effects	kg PM2.5 eq	0.000120776	1.68E-04	32%
	Ecotoxicity	CTUe	9.8415902	1.29E+01	27%
	Fossil fuel depletion	MJ surplus	1.8279383	2.06E+00	12%

Table 4. 6: Value Comparison for the Scenario analysis for Package 1 using TRACI 2.1 impact assessment method. Lightweighting the lid and tub components for Package 1 by 30%.

		SimaPro	PackageSmart	% Difference
Baseline	Impact category	Units	Baseline	Baseline
	Ozone depletion	kg CFC-11 eq	100%	100%
	Global warming	kg CO2 eq	100%	100%
	Smog	kg O3 eq	100%	100%
	Acidification	kg SO2 eq	100%	100%
	Eutrophication	kg N eq	100%	100%
	Carcinogenics	CTUh	100%	100%
	Non carcinogenics	CTUh	100%	100%
	Respiratory effects	kg PM2.5 eq	100%	100%
	Ecotoxicity	CTUe	100%	100%
	Fossil fuel depletion	MJ surplus	100%	100%
Lightweight Lid	Impact category	Unit	Lightweight Lid	Lightweight Lid
	Ozone depletion	kg CFC-11 eq	84%	84%
	Global warming	kg CO2 eq	94%	95%
	Smog	kg O3 eq	97%	96%
	Acidification	kg SO2 eq	96%	95%
	Eutrophication	kg N eq	93%	98%
	Carcinogenics	CTUh	96%	96%
	Non carcinogenics	CTUh	93%	97%
	Respiratory effects	kg PM2.5 eq	96%	96%
	Ecotoxicity	CTUe	92%	99%
	Fossil fuel depletion	MJ surplus	93%	93%
Lightweight Lid and Tub	Impact category	Unit	Lightweight Lid and Tub	Lightweight Lid and Tub
	Ozone depletion	kg CFC-11 eq	79%	78%
	Global warming	kg CO2 eq	79%	88%
	Smog	kg O3 eq	88%	89%
	Acidification	kg SO2 eq	83%	85%
	Eutrophication	kg N eq	76%	92%
	Carcinogenics	CTUh	84%	86%
	Non carcinogenics	CTUh	78%	91%
	Respiratory effects	kg PM2.5 eq	83%	85%
	Ecotoxicity	CTUe	75%	97%
	Fossil fuel depletion	MJ surplus	77%	91%

When looking at **Figure 4. 5**, the two software programs generate similar results when running a lightweighting scenario for Package 1 in which the lid and tub components are lightweight by 30%. These components are chosen because these are the two heaviest components in the primary package system and were deemed to be contributing the most according to **Figure 4. 1**. Both results indicate that when lightweighting the lid component by 30%, a reduction in impact for each TRACI impact category can be seen. Both sets of results also show that when lightweighting both the lid and tub components will result in an even larger reduction of impact across all TRACI impact categories.

When looking at **Table 4. 5** **Table 4. 4**, however, it can be seen that the actual values for each indicator vary anywhere between 1% and 58%, indicating that values between software programs do not end up being the same despite the fact that the same conclusions can be reached. When looking at **Table 4. 6**, the percentage decreases are compared, which show that that even though the same trend is seen, reported decrease in impact across categories is different, varying between 0% and 26%, which may impact decision making in the long run.

4.4 Conclusions

This chapter compared the results between two LCA software tools using almost the same LCI data. One software, SimaPro V9.0.3, is a full LCA software that can be used to model various products and services in many industries. The other software, PackageSmart, is a streamlined LCA tool designed to evaluate packaging-related environmental impacts. Both software programs were used to model three different package systems for infant formula delivery, including a primary (plastic - package 1, paperboard - package 2, and steel-package 3), secondary (corrugated case), and tertiary (pallet) levels. When modeling, data for inputs and outputs of the system were chosen to best match for both software, with slight differences when exact replicate data was unavailable.

Based on the results shown above, it can be concluded that similar results are obtained with both software when looking at one package, specifically primary packages. The results about which packaging components contribute the most environmental impact are very similar. For instance, in Package 1, the two highest contributing components were the Plastic lid and Plastic tub for both software results. However, the two software show different results when comparing the three packages. When modeling with SimaPro, it is found that Package 1 has the highest impact in 4 out of the 10 categories, Package 2 has the highest impact in 2 out of 10

categories, and Package 3 has the highest impact in the remaining 4 out of 10 categories. When modeling with PackageSmart, Package 1 has the highest impact in 1 out of 10 categories, Package 2 does not have the highest impact in any category, and Package 3 has the highest impact in the remaining 9 of 10 categories. This means that different conclusions will be reached depending on which software is used to make a comparative assessment among these three package systems.

Conclusions drawn from this chapter include that when modeling the same LCA study in different software, results will not be the same. Differences in data availability and software capability is most likely the cause of this discrepancy, as it is known that streamlined LCA software does not provide the same opportunities for data manipulation as full LCA. The full LCA software, SimaPro, allows LCA practitioners to manipulate data to best represent the three package systems, however, modeling involves much more time and monetary investment. The streamlined LCA software, PackageSmart, is much easier to use for modeling due to its simplistic structure, smaller data availability as well as analysis capability, and requires much less input for each component.

Differences in results between the software are rather dramatic, as the results with SimaPro do not provide clear cut answers as to highest or lowest EF, while results with PackageSmart heavily skew to decide that Package 3 has the highest EF. This indicates that choosing the software to use in LCA modeling can greatly impact the results and should be taken into consideration when interpreting comparative LCA results.

Results between these two software programs were only compared because the studies utilize the same goal and scope, system boundaries, functional unit, assumptions and LCI data. Had any of these factors changed the results between software would not allow for direct comparison. Additionally, the comparison of results may not translate to other studies; for instance, if the studied system was a different product or had different parameters, the software may have generated more similar results. Comparing the results of SimaPro and PackageSmart was done in this research because of access; conclusions that these two software programs are not generating the same results for this LCA study does not translate if one of the software chosen is changed, such as if we compared results from SimaPro and PIQET.

It is recommended that when considering performing an LCA, a practitioner should consider, which software or tool to use based on the needs of the goal and scope. For instance, if

a practitioner wants to manipulate EoL models or discover the exact process driving the environmental impact of a component, a full LCA software such as SimaPro should be used. If the practitioner is looking for a simpler, less time and money-consuming, answer to which component may be driving the impact of a package, a streamlined LCA software such as PackageSmart should be sufficient. However, we still do not have an answer to the absolute question of what package has the lowest environmental footprint.

REFERENCES

- [1] N. M. P. Bocken, J. M. Allwood, A. R. Willey, and J. M. H. King, “Development of a tool for rapidly assessing the implementation difficulty and emissions benefits of innovations,” *Technovation*, vol. 32, no. 1, pp. 19–31, Jan. 2012, doi: 10.1016/j.technovation.2011.09.005.
- [2] K. L. Verghese, R. Horne, and A. Carre, “PIQET: the design and development of an online ‘streamlined’ LCA tool for sustainable packaging design decision support,” *Int J Life Cycle Assess*, vol. 15, no. 6, pp. 608–620, Jul. 2010, doi: 10.1007/s11367-010-0193-2.
- [3] Greenly, “Greenly.” Accessed: Oct. 03, 2023. [Online]. Available: <https://greenly.earth/en-us/why-greenly>
- [4] GreenDelta, “openLCA.” Accessed: Oct. 03, 2023. [Online]. Available: <https://www.openlca.org/>
- [5] SimaPro, “SimaPro.” Accessed: Jan. 11, 2022. [Online]. Available: <https://simapro.com/>
- [6] Trayak, “EcoImpact Sustainability Platform.” Accessed: Oct. 03, 2023. [Online]. Available: <https://trayak.com/ecosustainability-platform/>
- [7] iPoint, “Umberto.” Accessed: Oct. 03, 2023. [Online]. Available: <https://www.ifu.com/umberto/lca-software/>
- [8] Sphera, “LCA for Experts (GaBi).” Accessed: Oct. 03, 2023. [Online]. Available: <https://sphera.com/life-cycle-assessment-lca-software/>
- [9] PR Newswire, “EarthShift Launches PackageSmart: A Highly Effective Sustainable Package Design Software,” *PR Newswire Association LLC*, Huntington, VT, Jun. 09, 2011. [Online]. Available: <https://apps.earthshift.com/PackageSmart/Account/TrialAccount.aspx>
- [10] SimaPro Help Center, “What are unit and system processes?” Accessed: Oct. 16, 2023. [Online]. Available: <https://support.simapro.com/s/article/What-are-unit-and-system-processes>
- [11] SimaPro Help Center, “How do I chose between Unit and System Libraries? .” Accessed: Oct. 16, 2023. [Online]. Available: <https://support.simapro.com/s/article/How-do-I-choose-between-unit-and-system-libraries>

5.0 Conclusion and Recommendations for Future Work

This thesis was conducted to evaluate the environmental footprint of three package systems designed to deliver infant formula. Additionally, the research was used to investigate how modeling choices can affect the results of LCA. A comparative LCA study was performed to do this, both in Full LCA software and Streamlined LCA software, with the Full LCA also being used to evaluate three different EoL methodologies. A summary of results is found in **Table 5. 1**.

Table 5. 1: Summary analysis results. Values for Package 1, 2, and 3 for Full and Streamlined LCA, as well as all EoL methodologies.

		Package 1			Package 2			Package 3		
Impact Category		Cut-off	50/50	CFF	Cut-off	50/50	CFF	Cut-off	50/50	CFF
Full LCA (SimaPro)	Ozone depletion kg CFC-11 eq	5.08E-08	5.33E-08	5.94E-08	4.13E-08	4.18E-08	4.97E-08	4.16E-08	4.38E-08	4.20E-08
	Global warming kg CO2 eq	8.01E-01	8.08E-01	9.33E-01	7.20E-01	7.28E-01	9.33E-01	7.25E-01	7.48E-01	7.29E-01
	Smog kg O3 eq	4.40E-02	4.28E-02	5.42E-02	4.41E-02	4.47E-02	5.27E-02	4.29E-02	4.52E-02	4.35E-02
	Acidification kg SO2 eq	2.73E-03	2.63E-03	3.70E-03	2.89E-03	2.94E-03	3.56E-03	2.82E-03	2.96E-03	2.82E-03
	Eutrophication kg N eq	2.39E-03	2.52E-03	1.16E-03	2.27E-03	2.28E-03	2.44E-03	2.10E-03	2.14E-03	2.11E-03
	Carcinogenics CTUh	2.30E-08	2.06E-08	4.31E-08	2.31E-07	2.31E-07	2.85E-07	4.02E-07	4.05E-07	4.02E-07
	Non carcinogenics CTUh	1.35E-07	1.58E-07	1.33E-07	3.48E-07	3.49E-07	3.98E-07	3.71E-07	3.74E-07	3.72E-07
	Respiratory effects kg PM2.5 eq	1.77E-04	1.53E-04	2.60E-04	4.79E-04	4.83E-04	5.97E-04	6.69E-04	6.86E-04	6.74E-04
	Ecotoxicity CTUe	1.29E+01	1.34E+01	1.02E+01	1.27E+01	1.27E+01	1.58E+01	2.05E+01	2.05E+01	2.05E+01
	Fossil Fuel Depletion MJ surplus	2.32E+00	2.41E+00	2.54E+00	1.07E+00	1.08E+00	1.17E+00	9.78E-01	1.03E+00	1.00E+00
Streamlined LCA (PackageSmart)	Ozone depletion kg CFC-11 eq	5.41E-08	-	-	4.73E-08	-	-	5.89E-08	-	-
	Global warming kg CO2 eq	8.51E-01	-	-	7.58E-01	-	-	1.06E+00	-	-
	Smog kg O3 eq	4.07E-02	-	-	4.27E-02	-	-	5.49E-02	-	-
	Acidification kg SO2 eq	3.07E-03	-	-	3.27E-03	-	-	4.39E-03	-	-
	Eutrophication kg N eq	2.97E-03	-	-	2.27E-03	-	-	3.38E-03	-	-
	Carcinogenics CTUh	3.45E-08	-	-	1.26E-07	-	-	4.57E-07	-	-
	Non carcinogenics CTUh	1.85E-07	-	-	2.14E-07	-	-	5.22E-07	-	-
	Respiratory effects kg PM2.5 eq	1.98E-04	-	-	3.99E-04	-	-	8.20E-04	-	-
	Ecotoxicity CTUe	1.32E+01	-	-	9.38E+00	-	-	2.32E+01	-	-
	Fossil Fuel Depletion MJ surplus	2.27E+00	-	-	1.08E+00	-	-	1.18E+00	-	-

In the full LCA performed to compare environmental footprint of three package systems, the results were presented using SimaPro software and cut-off allocation EoL. For the TRACI 2.1 V1.06 midpoint method, the plastic package, Package 1, has the highest impact in the ozone depletion, global warming, eutrophication, and fossil fuel depletion categories. The composite package, Package 2, has the highest impact in the smog and acidification categories. The remaining categories of carcinogens, non-carcinogens, respiratory effects, and ecotoxicity show the highest impact from the steel package, Package 3. Results vary only slightly when using the 50/50 recycling allocation method. For the TRACI 2.1 V1.06 midpoint method, the plastic package, Package 1, has the highest impact on the ozone depletion, global warming, eutrophication, and fossil fuel depletion categories. The composite package, Package 2, has a low impact in all categories. The remaining categories of smog, acidification, carcinogens, non-carcinogens, respiratory effects, and ecotoxicity show the highest impact from the steel package, Package 3. A different conclusion was reached with the CFF method for modeling EoL. The difference in results among these methods occurs due to the various assumptions used; for instance, the CFF incorporates primary and secondary materials and energy recovery, while the cut-off method assumes that none of the environmental impacts from recycling are included in the EF. For the TRACI 2.1 V1.06 midpoint method, Package 1 has the highest impact in the fossil fuel depletion category; Package 2 does not have the highest impact in any category; and the remaining categories of ozone depletion, global warming, smog, acidification, eutrophication, carcinogens, non-carcinogens, respiratory effects, and ecotoxicity show the highest impact from Package 3.

Because all three EoL methodologies do not provide clear-cut results indicating which package systems have the highest or lowest impact, trade-offs must be analyzed to reach conclusions on the impact of EoL methodology. When using the SMAA methodology for addressing trade-offs within each set of comparative results, it was found that the final ranking of each package from lowest to highest overall environmental footprint remains the same. In all three cases, Package 1 (plastic) ranks as having the lowest environmental footprint compared to the others, and Package 2 (composite) ranks as the second lowest environmental footprint compared to the other packages. Package 3 (steel can) has the highest probability of having the largest environmental footprint for the cut-off and CFF EoL methodologies. In the 50/50 methodology, Package 1 (plastic) has the highest probability of being ranked with the highest

environmental footprint. Still, the probability is lower than that, ranking the plastic package as having the lowest environmental footprint. This finding indicates that all three EoL methodologies result in the same conclusions when addressing trade-offs using SMAA. The results of this comparative LCA for infant formula packages show that Package 1 is the option with the lowest environmental footprint and Package 3 is the option with the highest environmental footprint, with Package 2 being between the two.

Different results were obtained when performing this same LCA study in a different software, PackageSmart. In this software, comparative results indicate that Package 1 has the highest impact in 1 out of 10 categories, Package 2 does not have the highest impact in any category, and Package 3 has the highest impact in the remaining 9 of 10 categories.

When comparing the results obtained from SimaPro and PackageSmart, there can be two conclusions drawn, First, the environmental impacts among components within the same package are very similar, leading to results indicating the same component contributing the most to the system. This is also true when performing scenario analysis with each package. However, when doing an analysis directly comparing the impacts associated with each package, very different conclusions will be reached between software.

When comparing the results from both software, it can be concluded that similar results are obtained with both software when looking at one package, specifically primary packages. The results about which packaging components contribute the most environmental impact are similar. For instance, in Package 1, the two highest contributing components were the Plastic lid and Plastic tub for both software results. However, when comparing the three packages, the two software show different results. When modeling with SimaPro, it was found that Package 1 has the highest impact in 4 out of the 10 categories, Package 2 has the highest impact in 2 out of 10 categories, and Package 3 has the highest impact in the remaining 4 out of 10 categories. When modeling with PackageSmart, Package 1 has the highest impact in 1 out of 10 categories, Package 2 does not have the highest impact in any category, and Package 3 has the highest impact in the remaining 9 of 10 categories. This means that different conclusions will be reached depending on which software is used to make a comparative assessment among these three package systems.

Overall, conclusions that can be drawn from the research discussed in this thesis relate strictly to the performance and results of the comparative LCA of three packages designed for

infant formula delivery. When performing the LCA using SimaPro, a full LCA software, three EoL scenarios can be modeled, changing the disposal impacts of the three packaging systems. Among the cut-off allocation, 50/50 allocation, and CFF EoL methods modeled, all three EoLs presented different comparative results. All three results however involved trade-offs which need to be properly addressed before using the results to make any final conclusions about which packages may have the highest or lowest EF. When statistically analyzing the results to address these trade-offs using the SMAA methodology, it can be found that adjusting the EoL methodology does not influence final rankings of highest and lowest EF. On the other hand, when changing the software tool that is used to evaluate the EF, comparative results among the three packages are not the same. Therefore, it can be concluded for this LCA study, the EoL methodology used to model the system has little impact on final results when using SMAA to evaluate trade-offs. The software used to model the LCA however does have influence on the final results, indicating that choosing the right software to model is a key decision needed to be made by LCA practitioners.

5.1 Recommendations for Future Work

This research can be extended by evaluating the effect of EoL scenarios and software tools with a different product or package system. Other decisions such as the outlining of system boundaries, definition of functional unit, or key assumptions in modeling could influence final results and therefore could provide opportunity for research informing the importance of those decisions and how those parameters affect results obtained in LCA. Further research could also validate the results found in this study by potentially comparing LCA results in the same methodology but using different LCA software tools, different EoL models, or using a different LCI dataset. In general, performing more LCA studies in the packaging industry can broaden the depth of knowledge about packaging related materials and processes and assist packaging engineers in designing environmentally conscious package systems.