A COMPARATIVE ANALYSIS OF COMMERCIALLY AVAILABLE LIFE CYCLE ASSESSMENT SOFTWARE

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ABSTRACT

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Against a backdrop of increasing demand for products, the packaging industry is continually searching for ways to meet the needs of consumers while simultaneously improving the environmentally sustainability of packaging. This requires making informed decisions based at least in part on knowledge of the environmental impacts attributable to the different packaging options being considered. Many companies have turned to using Life Cycle Assessment (LCA) to obtain the necessary environmental impact information. To support this effort, several software programs have been developed to aid in doing an LCA. These programs vary considerably in complexity and focus, leading to questions of how similar are the results they provide.

To study the consistency of results across LCA software programs, nine common packaging systems were modeled in each of five different programs: GaBi, SimaPro, openLCA, COMPASS, and Package Modeling. Comparison of the LCA information provided by these programs for the packaging systems showed several significant differences. To better understand why the differences occurred, four simplified systems were created with the intent of minimizing the number of variables involved in the system models. Each of these systems consisted of obtaining and disposing of a single basic packaging material: aluminum, glass, corrugated board, and polyethylene terephthalate (PET). Once again a comparison of results showed significant differences.

Using information from these basic material comparisons, and making use of the transparency in LCA calculations provided by GaBi and SimaPro, a study was done that traced the causes of the inconsistencies in results back to how implementations of assessment methods differed between the two programs. A comparison of 14 combinations of basic materials and impact categories involving 3 different assessment methods found 98 instances of characterization factors differing between GaBi and SimaPro. These differences in characterization factors accounted for all the discrepancies in results between the two programs. No errors in calculations were found with either program, and there were no significant differences in the type or amount of inputs and emissions in the life cycle inventories from the two programs.

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1. INTRODUCTION

The world's natural resources are under intense pressure to meet the growing needs and desires of its inhabitants. World population continues to increase, while at the same time demand for goods of all types increases as undeveloped regions become more modernized. Over the years conservation efforts have pushed their way to the forefront of product and packaging development in an attempt to reach a balance between resources and demands. For the packaging industry this has become an effort to provide packaging that is environmentally sustainable while still meeting all of the performance requirements needed to package a given product.

A key requirement in creating sustainable packaging is being able to compare the environmental impacts of different packaging options. Without a common basis of comparison there is no credible means of determining that any option is more environmentally sustainable than the others available. An approach to estimating environmental impact that is seeing increasing use in packaging is Life Cycle Assessment (LCA). In conducting an LCA the contribution of each step in a product/package life cycle, from getting the raw materials all the way through to disposal at end of useful life, can be looked at and combined to give a picture of the overall environmental impact.

While LCA can provide a clearer picture of the environmental impact of a product/package, the task of conducting an LCA can be difficult and time consuming. It is often impractical for individuals and companies to obtain first hand all the pertinent data needed for an LCA on a package design, and the effort required increases proportionally when looking at multiple packaging options utilizing different materials and processes. To overcome this difficulty several software systems have become available with the intent of reducing the amount of effort needed to do an LCA, or some subset of a full LCA that the software creators deem appropriate for packaging applications.

The advent of multiple LCA software systems, while offering the promise of expedited LCA, also creates questions about their use. Foremost is the question of consistency in results between software systems; are the results from different software similar, or does the choice of software affect the results in some manner? As LCA is becoming a key tool in package design, it is important to know if the selection of software affects the analysis in ways that can impact the decision making process. This research is intended to aid in determining if the choice of LCA software may affect results, and thereby influence decisions based on these results.

2. PACKAGING GROWTH CONSIDERATIONS

Packaging is tied to environmental concerns by the immense amount of resources required to provide packaging for the distribution of products throughout the world, and by the makeup of the packaging materials. There are other ties between packaging and the environment, a key function of a package can be to protect the environment from the package contents, but it is generally the volume and content of material going into packaging that creates the larger environmental concerns.

One of the driving factors for the volume of packaging material being used is the size of the population being served. Figure 1 shows the estimated population of the world since 1804 based on United States (U..S.) Census Bureau data (U.S. Census 2002). There were approximately one billion people in the world in 1804; 118 years later the number had doubled to 2 billion in 1922; 52 years after that the population had doubled again to 4 billion in 1974; and it is estimated the population will double again to 8 billion people by 2028. With the increase in population comes an increase in demand for products to support the population. Unfortunately, the earth's resources have not increased, so as population grows there is increased strain on the environment.

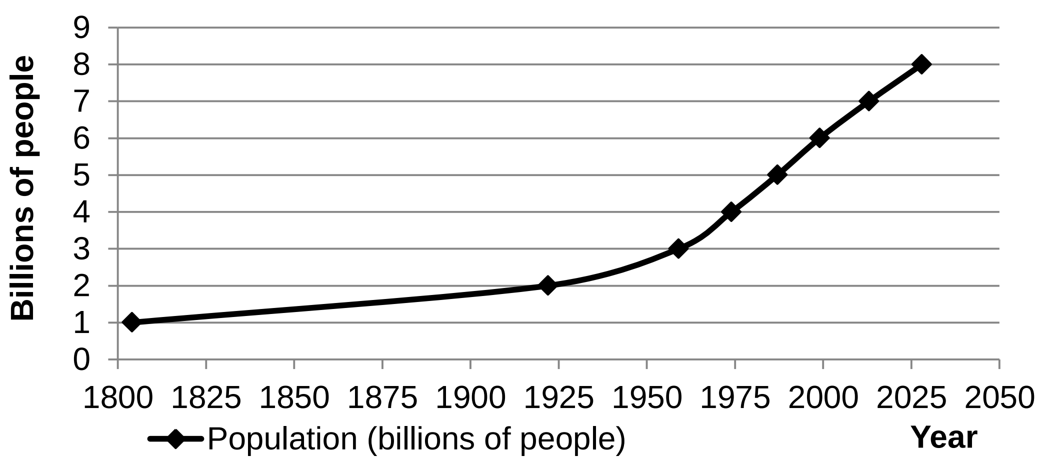


Figure 1: Estimate of world population from 1804 to 2028. Data Source: U.S. Census Bureau (U.S. Census 2002).

Trends in U.S. population and waste generation over several decades provide an example of how increasing population can impact the amount of packaging material required. Figure 2 shows how U.S. population, annual municipal solid waste (MSW) generation, and annual packaging waste generation have changed since 1960, based on U.S. Census Bureau and U.S. Environmental Protection Agency (EPA) data (U.S. Census 2012, 2013; EPA 2011). U.S. population increased 71% over the 50 year time period shown, while annual MSW generation increased 184% and packaging waste generation increased 176%. Clearly MSW waste generation and packaging waste generation have increased with population in the U.S., and at rates significantly greater than the rate of population increase. Please note that the waste material being discussed here is the total material entering the waste stream; this includes compostable, recyclable, and non recyclable material.

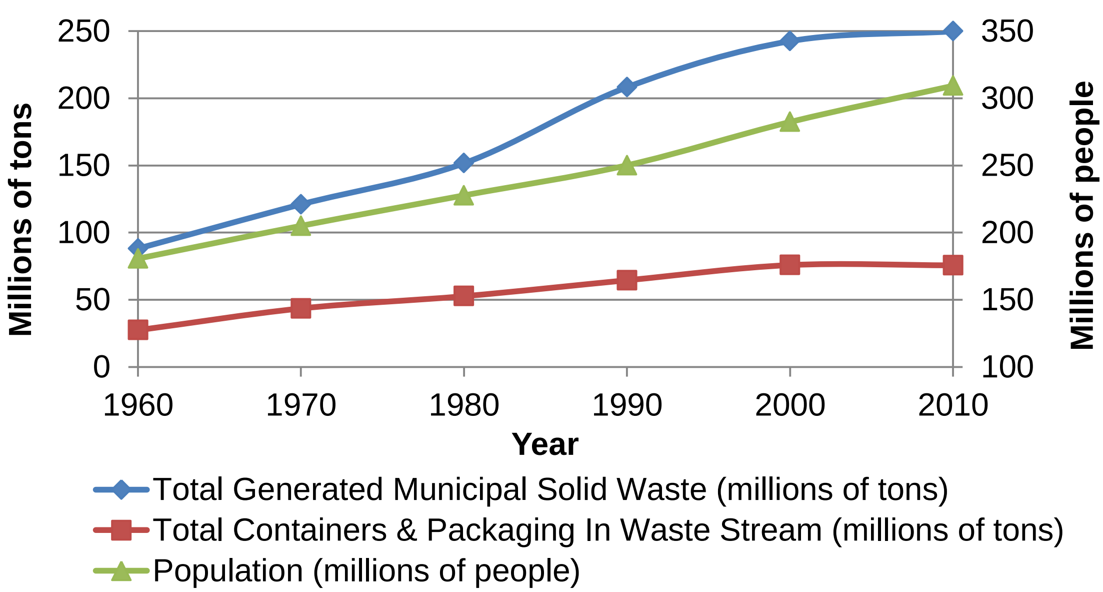


Figure 2: Population and waste material generation in U.S. from 1960 to 2010. Data Sources: U.S. Census Bureau and U.S. EPA (U.S. Census 2012, 2013; EPA 2011). For interpretation of the references to color in this and all other figures, the reader is referred to the electronic version of this dissertation.

Another factor that can influence the volume of packaging material being used is demand for products from countries with emerging industrial economies. As incomes increase, more consumers can afford items that were previously too expensive for them to purchase. In these situations it is not just the increase in population driving increased use of natural resources, there is also the pent-up demand of the existing population that now expects to be satisfied.

New car sales in China is an excellent example of how pent-up demand that is released by economic growth can affect product demand, and thereby increase stress on available resources. China's economic growth has resulted in the Chinese market for new cars surpassing the U.S. market in sales in 2009 (Lin 2012), a position it is expected to retain. With this growth in car sales go all the items needed to produce, maintain, and operate the vehicles. These items in turn need some form of packaging to enable them to reach the end user in acceptable condition.

An example of how economic growth impacts resource utilization can be seen in the changes that have occurred in China's consumption of oil. Figure 3 shows oil consumption in China and the U.S. over 3 decades as reported by the U.S. Energy Information Administration (EIA 2013). While China's total daily oil usage in 2010 was approximately half that of the U.S., China had a 429% increase in oil consumption over the 30 year period from 1980 to 2010, compared to a 12.5% increase for the U.S. Furthermore, while oil consumption in the U.S. may be stabilizing, the rate of increase for China appears to be accelerating. This implies that increasing demand for oil and other resources to fuel Chinese economic growth will cause more strain on the environment in years to come.

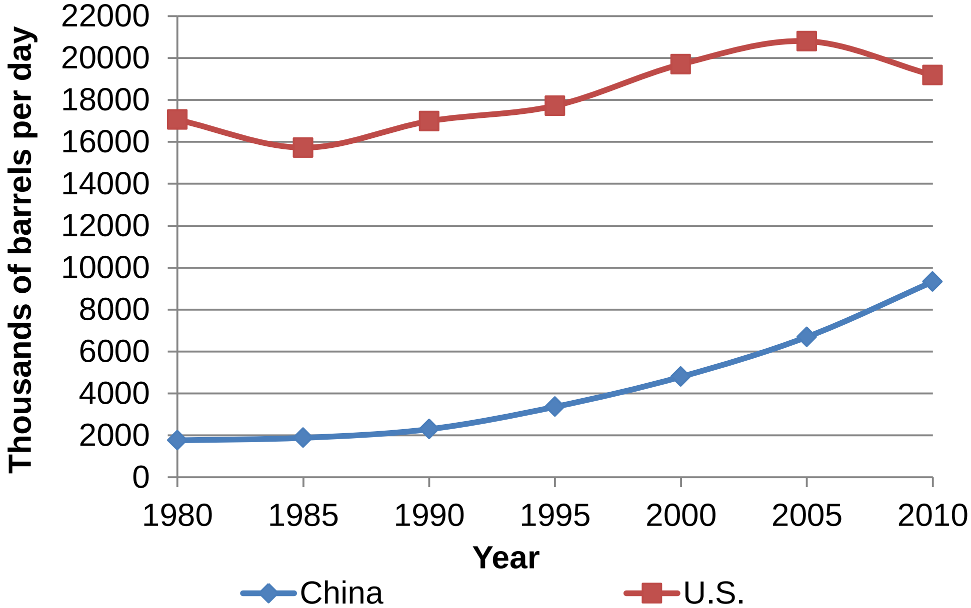


Figure 3: Oil consumption for China and the U.S. from 1980 to 2010.
Data Source: U.S. EIA (EIA 2013).

China is not the only economy expected to see significant sustained growth. Table 1 provides a list of the top 20 emerging markets (Bloomberg Markets 2013) combined with the 2010 estimates of their populations (UN ESA 2013). All of these countries are expected to have gross domestic product (GDP) growth over the next 4 years of 15.6% to 45.9%. While China is clearly the biggest emerging market in terms of both expected GDP growth and population, the other 19 countries identified in the table represent another 1.25 billion people in markets expected to see significant GDP growth. As these markets mature they will likely drive the demand for products, and therefore packaging, even higher.

Table 1: Emerging markets

Rank	Country	Percent GDP Growth, 2013 to 2017 [1]	Population Estimate, 2010 [2]
1	China	45.9	1,341,335,000
2	South Korea	22.9	48,184,000
3	Thailand	25.9	69,122,000
4	Peru	27.4	29,077,000
5	Czech Republic	21.1	10,493,000
6	Malaysia	21.8	28,401,000
7	Turkey	21.2	72,752,000
8	Chile	24.2	17,114,000
9	Russia	26.6	142,958,000
10	Indonesia	31.3	239,871,000
11	Colombia	21.9	46,295,000
12	Poland	21.2	38,277,000
13	Namibia	22.3	2,283,000
14	Zambia	31.3	13,089,000
15	South Africa	19.9	50,133,000
16	Mexico	17.5	113,423,000
17	Brazil	22.3	194,946,000
18	Hungary	15.6	9,984,000
19	Morocco	27.7	31,951,000
20	Philippines	20.4	93,261,000

[1] Data Source: Bloomberg (Bloomberg Markets 2013)

[2] Data Source: United Nations, Department of Economic and Social Affairs (UN ESA 2013)

3. SUSTAINABILITY and LIFE CYCLE ASSESSMENT

Given that increasing demand for products will drive the need for more product packaging, and given that the earth's resources are finite, it is clear that packaging must evolve to a state where it is sustainable by the earth's resources. What is meant by saying something is "sustainable"? The EPA (2013) states that "Sustainability creates and maintains the conditions under which humans and nature can exist in productive harmony, that permit fulfilling the social, economic and other requirements of present and future generations." An alternate definition comes from the World Commission on Environment and Development (WCED 1987): "Sustainable development is development that meets the needs of the present without compromising the ability of future generations to meet their own needs." To put it simply, packaging must be able to meet the needs of the present without compromising the ability to meet the needs of the future.

There are several approaches to improving package sustainability: material reduction, reuse, recycling, and composting, to name a few. Each approach has merit and in some cases the approaches can be combined, but how can their effectiveness be determined in a given situation? The environmental impact of different packaging options must be quantified to provide a true understanding of the benefits and/or costs associated with each option. Without such an understanding it is possible for design changes to do more harm than good.

One of the simplest concepts in packaging sustainability is to use less material, the rationale being that less packaging material means less environmental impact. Even this simple concept has caveats; the overall environmental impact cannot always be judged by the weight or volume of the packaging material alone. Different types of material can have different environmental impacts, and the effects of reuse and recycling need to be taken into account. For instance, a glass container intended to be refilled may need to be stronger, and therefore heavier, than a single-use version, but being used multiple times can result in a more environmentally friendly option. As an example, while single-use beer bottles are common in the U.S., refillable glass bottles are common in Canada. With an average return rate of 97%, Canadian brewers claim the refillable bottle system is responsible for an annual reduction of 187,000 metric tons in greenhouse gas emissions (CNW 2005).

Wever (2009) proposed that environmental sustainability of packaging is tied to the transportation efficiency of the product. In essence, improving the cube utilization for transporting a given product results in less packaging material and energy being required per item shipped. This is another simple concept that has merit, but also has the same caveats as using less material. Cube utilization as an indication of sustainability does not by itself take into account that different materials can have different environmental impacts, nor does it account for the effects of reuse and recycling.

If the type of packaging material is not being changed, and reuse or recycling is not affected, then the amount of material being used or the cube utilization obtained can give an indication of a relative change of environmental impact, but not an absolute magnitude of the impact. Furthermore, neither approach takes into account any change in the amount of product damage that can occur due to the reduction of packaging. A small increase in product damage can cause more environmental impact than what is avoided by using less packaging. Material reduction and cube utilization improvement are viable relative improvement indicators when used in proper context, but something more is needed to address comparisons of different types of packaging materials and processing methods.

Sand (2010) recommends incorporating sustainability as part of the packaging value chain. In this context sustainability is looked at in terms of added value provided to customers at each stage in the packaging cycle. While this may be a useful business model for evaluating different packaging alternatives, it does not provide the means of obtaining the necessary information on sustainability. Sand does note that decisions regarding sustainability require environmental impact information from raw materials through to disposal, a reflection of the cradle-to-grave philosophy that has become a cornerstone of sustainability.

The idea of estimating the environmental impact of a product or package by looking at its entire life cycle, from obtaining raw materials (the "cradle"), through manufacturing, distribution, end use, and disposal (the "grave") has been around at least since the 1960s (ALCAS 2013). Harry E. Teasley, Jr. is credited with conceiving the concept of doing a study covering the entire life cycle of a package when he worked for The Coca-Cola Company managing their packaging function in 1969 (Hunt and Franklin 1996). At the time the company was looking at issues related to packaging beverages that included whether to self-manufacture cans, use plastic bottles (new at the time), or use refillable bottles. Teasley envisioned a study that would quantify the energy, material, and environmental impacts of the very different container options being considered. The study was carried out, becoming the first life cycle assessment of packaging on record, though at the time it was referred to as a Resource and Environmental Profile Analysis (REPA). A similar resource and environmental release quantification method practiced in Europe was called Ecobalance (EPA 2006). According to Hunt and Franklin (1996), it was not until 1990 that the term Life Cycle Assessment (LCA) was first used in the U.S.

The Coca-Cola study was not published in full due to the proprietary nature of its contents, but was used by the company to aid packaging and business decisions in the early 1970s. One aspect to come out of the study was that the poor environmental image plastics had at the time was not supported by the findings; thus this first study showed the power of LCA to dispute an accepted notion. It is interesting that even today plastics often have a bad environmental reputation that may not be justified in a given situation. A recent occurrence of this can be found in the carry bag debate where local governments are banning the use of plastic bags (Lin 2010; Karp 2011). One of the arguments often used to support such a ban is that plastic is less environmentally friendly than paper, yet LCA shows the opposite (Lewis et al 2010).

Another study setting ground work for what would later become LCA was done in the United Kingdom in 1972 by Ian Boustead (EEA 1996). Boustead's work involved estimating the total energy used in production of glass, plastic, steel, and aluminum beverage containers. In this early work the emphasis was on the single issue of energy; looking at wastes and other emissions was not a priority. Over the years other environmental concerns besides energy have come to the spotlight. As each new concern came to prominence, the concept of estimating a product's contribution to environmental impacts by looking at the entire life cycle of the product found growing acceptance.

One reason LCA has grown in use is that it offers more than just knowing the total contribution, or impact, a product has regarding an environmental issue. The ability of LCA to show where in a product life cycle environmental contributions occur is of significant value, too. Armed with this information, efforts to reduce environmental impacts can be concentrated in the areas that will yield the greatest benefit. LCA can also be used to identify burden shifting, which occurs when a design change reduces impact in one stage of the product's life cycle at the expense of increasing it as much, or more, in another stage. Thus LCA can provide both a guide for improving the environmental impact of a product and a check on the results. The practice of reviewing a product's life cycle for ways to optimize overall environmental performance has come to be referred to as Life Cycle Thinking, or LCT (EC-JRC 2013).

The systematic approach provided by LCA for estimating environmental impacts has been found useful in supporting informed decision making across a broad range of products and issues. Whether it is looking at the production of biodiesel (Gonzalez-Garcia et al. 2013), determining the carbon footprint for honey production (Kendall et al 2013), or debating the environmental benefit of buying locally produced food (Saunders et al. 2006), LCA has become a method of choice for environmental sustainability analysis. The use of LCA is expanding in the packaging industry as well. With the focus on reducing the environmental impacts of packaging in today's world, LCA is being turned to increasingly as a support tool to aid in evaluation of packaging designs (Sonneveld 2000).

4. PUBLICATIONS ON LIFE CYCLE ASSESSMENT

In 1997 the International Organization for Standards (ISO) released the first version of ISO 14040 in an attempt to bring consistency to the methodology of conducting an LCA. An updated version of ISO 14040, in combination with the more recent ISO 14044, provides the general framework for conducting an LCA today (ISO 2006). While these standards provide the basis for doing an LCA, there are many publications available that seek to explain, expand on, or aid in the use of these standards. Such publications can be useful in understanding the fundamentals of LCA; however, they can quickly seem redundant since they are often covering very similar material. This sense of redundancy can be viewed as an indication of the success ISO 14040 and 14044 have had in standardizing the approach to LCA.

4.1 Introductions To Life Cycle Assessment

A useful introduction to LCA can be found in *Environmental Life Cycle Analysis* (Ciambrone, 1997). The book is easy to read and relatively short, allowing it to hold a reader's attention from start to end. Readers gain insight into the basic principles of inventory analysis (gathering data), impact analysis (translating data into environmental impact categories), and improvement analysis (how LCA results can be used to improve the product). Setting boundary conditions to define what will be included and excluded from analysis, developing flow diagrams and process diagrams to identify the data that will be needed, and how the quality of the data can affect the LCA results are all covered. While a useful starting point in obtaining a general understanding of LCA, this book is limited on application examples and may not be suited to someone looking for detailed information on a specific topic. As a side note, the author did try to coin the term “MANPRINT” to refer to the impact of a product on the environment, something which thankfully did not catch on.

Another publication that is a good starting point for learning about LCA is *Life Cycle Assessment: Principles and Practice* (SAIC 2006). Created by an EPA funded research project, it is now available as an EPA document. Again this is a short document, 80 pages total, that gives a straightforward presentation of the basic tenets of LCA. This publication is newer than the first book mentioned, allowing it to reference more recent information covering LCA development. It does share a similar limitation of application examples, so it too may not be suitable for anyone looking for something beyond an introduction to LCA. One advantage of this publication is that it is available for free on line from the EPA website.

4.2 Life Cycle Assessment Procedural References

For a general reference on LCA one choice is the *Handbook on Life Cycle Assessment: An Operational Guide to the ISO Standards*, commissioned by the Dutch Government Ministry of Housing (Guinée 2002). The book provides a short discussion of the background and purpose of LCA, a guide to creating an LCA, an operational annex that provides support information, and a section on the scientific background supporting LCA. It is in the last two sections that this book extends beyond being just an introduction to LCA. Supplying practical support information regarding issues that come up in conducting an LCA, along with background information on the science behind LCA, makes this book a useful application reference. Of particular note is the example provided for creating a PEDIGREE MATRIX to aid in determining the quality of data being used in an LCA. The other publications mentioned so far talk about the importance of data quality, but do not discuss in any detail a method for determining it.

An alternative reference for LCA practitioners is *International Reference Life Cycle Data System (ILCD) Handbook – General Guide for Life Cycle Assessment – Detailed Guidance* (EC JRC-IES 2010). This publication provides step by step guidance in understanding how to perform an LCA. Its purpose is to bring consistency to the practical implementation of LCA methodology based on accepted best practices. Recommendations are provided for conducting an LCA from initial planning all the way through to reporting results. The annex (appendix) on data quality is one of many useful features. Another good feature is the discussion of frequent errors that have occurred in doing the various steps of an LCA, an attempt to help people learn from the mistakes made by others in the past. The guidance provided, while detailed, is not focused on any specific product or service; it is a general reference with concepts that are easily adaptable. One thing this publication is not intended to be is an introduction to LCA, people should first read one of the introductory publications already mentioned before attempting to use this one.

People who are interested in the efficient performance of LCA calculations may want to read *The Computational Structure of Life Cycle Assessment* (Heijungs and Suh 2002). The authors go into great detail about performing LCA calculations using matrix arithmetic. Solutions to problems such as how to handle cutoff of flows or closed loop recycling with matrix arithmetic are covered. While not for everyone, this book is worth considering if a spreadsheet, or similar program, is being used to do LCA calculations.

Spreadsheets generally have standard matrix arithmetic functions built in, and the savings in computation time over a more linear calculation approach are reported to be significant. When using software programs specifically developed to assist in LCA, such as the ones looked at in this paper, the LCA calculations are performed by the software.

For an overall picture of how LCA and sustainability can affect packaging decisions, a useful reference is *Packaging for Sustainability* (Verghese et al. 2012). With only a single chapter on LCA, one that is geared toward an executive overview, this book is not about how to do an LCA. Instead, a much broader look is taken at how sustainability impacts business decisions, and how LCA is a tool that provides information that can influence these decisions. Emphasis is put on companies needing to include sustainability as part of their corporate strategy. Marketing, regulatory compliance, consumer perceptions, and infrastructure availability are all shown to play a part in how a company includes sustainability in its thinking. Among the many subjects discussed are that consumers do not necessarily support sustainability with their purchasing habits, and that a recyclable package will only get recycled if there is infrastructure in place to handle the task. A section on packaging materials is included with information covering representative life cycles, general environmental impact considerations, and recovery and disposal options. This is a worthwhile book to read for anyone involved in packaging sustainability, which should be anyone involved in packaging design and decision making.

4.3 Impact Methodologies

One area where there are many differing publications is in impact assessment methodologies. ISO 14040 and 14044 provide a framework for doing LCA, but purposely leave out specifics on identifying impact categories. It has been left to the LCA practitioner to identify what impacts are significant to the study being done, and how best to map inputs and emissions to these impact categories. In order to help fill this void, work groups of scientists and LCA practitioners have created various impact methodologies for many common environmental issues. Individual methods are based on available scientific information and best practices, and are peer reviewed. However, this does not mean that two methods will agree. In order for LCA practitioners to understand how an impact assessment methodology works, papers are published describing the impact categories provided, the conversion of inputs and emissions to these categories, and the scientific basis behind it all. While there are many different assessment methods available, the three that are pertinent to this work are Impact 2002+, ReCiPe, and TRACI 2.

The Impact 2002+ assessment method is described in *IMPACT 2002+: A New Life Cycle Impact Assessment Methodology* (Jolliet et al. 2003). Impact 2002+ converts inputs and emissions into 15 midpoint environmental impact categories, and then maps combinations of midpoint indicators into 4 damage (endpoint) categories. The 4 damage categories are Human Health, Ecosystem Quality, Climate Change, and Resources (mineral and non-renewable energy use). Some midpoint categories map into multiple damage categories. Each midpoint category is expressed in terms of a reference substance. For instance, an emission that affects global warming is converted into the amount of CO_2 emissions to air that produces an equivalent impact. All the inputs and emissions that affect a midpoint impact category can be converted to an equivalent amount of the reference substance for that category, and then added together to determine the midpoint indicator value. For each damage category, midpoint values that map into the category are multiplied by damage characterization factors to convert them into a common unit, allowing the midpoint values to be summed into a single value representing the impact of the damage category. In an attempt to further aid analysis of the results, normalization factors are provided that convert damage category values into ratios referenced to the emissions associated with one person for one year, based on Western Europe.

An interesting side note about Impact 2002+ is that while the authors recommend considering the 4 damage categories separately, which is in line with ISO 14044, they also state the categories can be aggregated into a single result with proper weighting factors. This is a departure from ISO 14044 which states “It should be recognized that there is no scientific basis for reducing LCA results to a single overall score or number” (ISO 2006). While not supported by ISO 14044 due to the lack of scientific basis, coming up with a single LCA score is in essence what companies are doing when they make decisions based on more than one environmental impact category. Whether it is applying a formal set of weighting factors, or informally deciding that one impact category is more important than another, companies implicitly aggregate category results when setting the course they will follow for a product or service.

The ReCiPe assessment method is covered in *ReCiPe 2008: A life cycle assessment method which comprises harmonized category indicators at the midpoint* *and the endpoint level, First edition (revised), Report I: Characterization* (Goedkoop et al. 2013). ReCiPe has 18 environmental midpoint categories and 3 endpoint categories, most of which are similar to those found in Impact 2002+, but that does not mean they are identical. While using more than one assessment method to verify trends is advisable when performing an LCA, variation in the methodologies used to determine indicators can be a source of differences in the values obtained from multiple methods. Another reason for using multiple assessment methods is that one method may not cover all the environmental impact categories of interest for a given project. One midpoint indicator pertinent to this paper that ReCiPe supplies, and for which there is no counterpart in Impact 2002+, is water depletion (usage).

One feature of ReCiPe is that three different scenarios are provided for grouping assumptions that can affect the analysis of data. Each scenario provides a distinct perspective on time-frame and other issues that contribute to uncertainty in the LCA results. The individualist (I) perspective is based on short-term interest, where impacts are not being disputed. The hierarchist (H) perspective assumes that the most common policy principles are followed, and is viewed as the default model to use when a specific perspective has not been chosen. The egalitarian (E) perspective looks at the longest time-frame and considers impacts that may not be fully understood yet, but that do have some basis for characterization. Clearly the egalitarian perspective is likely to have the greatest uncertainty in analysis results, while the individualist perspective provides a limited time over which any analysis can be considered valid. The hierarchist perspective falls somewhere in between, trying to strike a balance between uncertainty, available knowledge, and useful time-frame. While these different scenarios add some flexibility to using ReCiPe, one must be careful to ensure comparisons are done using a common scenario.

One interesting part of the discussion of architecture for ReCiPe deals with the variations that can occur on a regional basis when trying to quantify potential damage from emissions. Hygienic conditions, weather conditions, background concentrations, and population density are all examples of issues with significant regional variability that can influence the effect of emissions on the environment. ReCiPe often uses environmental models based on Europe, and although attempts have been made to generalize these models within ReCiPe, the authors do note that “the ReCiPe method has limited validity for all regions that cannot be defined as well-developed temperate regions” (Goedkoop et al. 2013). This is an excellent cautionary note for any assessment method; the validity of the results are only as good as the assessment model being used, which in turn is dependent upon the appropriateness of the information the model is based on.

The TRACI 2 assessment method is an updated version of the original TRACI method developed by the EPA in 2002, with TRACI 2.0 released in 2011 and TRACI 2.1 released in 2012. The TRACI methodology is discussed in the paper *TRACI: The Tool for the Reduction and Assessment of Chemical and Other Environmental Impacts* (Bare et al. 2002). TRACI differs from Impact 2002+ and ReCiPe in that it was developed specifically for use in the U.S., coming after the conclusion was reached that no tool in existence at that time was sufficiently applicable to the U.S. to meet the EPA’s needs. TRACI also differs in that it deals only with category midpoints, leaving it to the user to convert the midpoint information into desired endpoints. Information provided in the referenced paper does show examples of how different endpoints can be affected by the impact category midpoints provided. The updated TRACI 2 methodology is covered in the paper *TRACI 2.0: the tool for the reduction and assessment of chemical and other environmental impacts 2.0* (Bare 2011). TRACI 2 covers 9 impact categories, with 3 of these (Particulate, Cancer, and Non Cancer) being sub categories listed under Human Health. The user's manual for TRACI 2.1 (Bare 2012) does list Fossil Fuel Use as a tenth impact category; however, the implementations of TRACI 2 found in the commercial LCA software used for this paper did not include this category.

4.4 Journals and Other Publications

The publications discussed so far are only a small sample of what is available. Books, papers, and journal articles on LCA abound. Several articles from the *International Journal of Life Cycle Assessment* are referenced in this paper, as are articles from the journal *Packaging Technology and Science*. Another source of LCA information is the *Journal of Industrial Ecology*, which has recently tightened its policy on what is expected in an LCA paper submitted for publication (Lifset 2013). This has been done because the editors believe LCA has evolved to the point where there is now widespread use and that basic case studies are now common. For a paper to be accepted by the journal now, it must advance the practice of LCA by providing new and important data that challenges established views, use a novel methodology, or provide new information on a topic of significance. This change in policy reflects the success that has been achieved in the development of LCA under ISO 14040 and 14044.

A general discussion of LCA publications would not be complete without mentioning the ongoing publication of research papers that contribute to debates on how best to model various substance flows within an LCA. One example is the paper *Critical aspects in the life cycle assessment (LCA) of bio-based materials – Reviewing methodologies and deriving recommendations* (Pawelzik et al. 2013). The authors of this paper are concerned that current LCA standards do not adequately address biogenic carbon storage associated with bio-based materials, and that failing to do so can have a significant effect on estimating greenhouse gas emissions for products using these materials. Papers like this are intended to widen the scope of thought on an environmental impact issue, in this case the effect of carbon sequestration when accounting for greenhouse gas emissions, and over time can result in changes being made to what is considered accepted best practices for performing an LCA. The research presented in these papers is what drives the continued evolution of LCA.

5. REVIEW OF BASIC LIFE CYCLE ASSESSMENT PRINCIPLES

LCA is a method by which environmental impacts can be identified, quantified, and evaluated to provide information for guiding decision making about a product, process, or service. The information from an LCA may be used for various purposes including comparison of design options, product improvement, monitoring environmental regulatory compliance, and providing a basis for product environmental claims. An LCA will not provide information on parameters such as production costs, product performance ratings, marketing considerations, and consumer acceptance, to name a few. Thus LCA is one of many sources that feed information into the decision making process for businesses today, and the information niche it fills is that of aiding in understanding the environmental consequences associated with a decision.

An LCA is divided into four phases: goal definition and scope, inventory analysis, impact assessment, and interpretation. While these phases are laid out to be performed sequentially, LCAs often become iterative in nature, with information from a later phase getting fed back to reevaluate the work done in an earlier phase. For example, it may be that data from the inventory phase is not as specific as originally desired and the goal or scope of the LCA has to be modified accordingly. The interpretation phase may reveal more questions that need to be answered, requiring additional inventory data and impact assessment. Newer or more product specific data may become available that replaces older or estimated data, requiring another pass through the LCA to see if results are affected. In essence, an LCA does not have a flat one dimensional flow; instead the flow through an LCA is dynamic in nature, with review and updates occurring for the different phases as new information becomes available.

5.1 Goal Definition and Scope

Adequately defining the goal and scope of an LCA is key to having an efficient LCA process and a useful result. The goals of the LCA determine what information is needed to fulfill the purpose of the LCA, the information needed drives the type of assessments that have to be made, which in turn defines the type and quality of the data that must be acquired. Having clearly defined goals serves to focus effort in subsequent LCA phases onto what is needed, minimizing wasted effort.

The first step in performing an LCA is to understand who the LCA is being performed for and how they are going to use the information that is provided. An LCA can be initiated by various parties for different reasons; one may want information to support a public policy decision, another may need guidance on selection of the best option for a new product, someone else may want to know how an existing product compares to others for a specific type of environmental impact. Trying to do everything for everyone can result in an overly complex, time consuming, and expensive LCA. Recognizing what information is actually needed by the stakeholders who initiated the LCA, how specific that information has to be to meet their needs, their expectations on the timeliness of the information, and how best to report the information to them can significantly streamline the LCA process.

After the goals of the LCA are sufficiently defined to insure the information expectations of the stakeholders will be met, the functional unit and system boundaries the LCA will be based on must be set. The functional unit is simply a quantifiable amount of a product, service, or process that can serve as a basis of reference for comparing the environmental impacts of different options. For example, laundry detergent can be powder or liquid, so kilograms of powder detergent or liters of liquid detergent are not good units to use for evaluating these options since they cannot be directly compared to each other. Even when comparing just powder detergents, weight would not be an appropriate functional unit if the detergents being considered require differing amounts to be used. A better choice for a functional unit would be to use a fixed number of loads of laundry. This can then be related back to the amount of detergent, powder or liquid, needed to do the loads of laundry. Once an appropriate functional unit has been selected, then the environmental impacts of the different options being considered can be scaled to reflect the amount of impacts associated with producing one functional unit, thus allowing comparison of dissimilar options.

System boundaries define the limits of what will be included in an LCA. An LCA can be an all inclusive cradle-to-grave study, extending from the acquisition of raw materials for a product all the way through to disposal at end-of-life, or it can be the “gate-to-gate” contribution of one or more processes in producing a product. The needs of the stakeholders are what drive the setting of system boundaries. If someone wants to know the total environmental impact of a product, say a glass bottle filled with beer, then a cradle-to-grave LCA is called for. On the other hand, if the intent of the LCA is to help select a cleaning method for the bottles before filling them with beer, then it is the contribution of the cleaning process options that need to be looked at, not the entire life cycle of a bottle of beer.

System boundaries may have to be expanded to account for production of co-products. When dealing with multiple products produced from a common process, it is necessary to fairly allocate the inputs and emissions associated with the process among the resulting co-products. Since allocation based on characteristics such as weight, volume, or monetary value of the co-products do not necessarily reflect the true distribution of environmental burdens, it is preferable to find a way to separate the co-products. One way to achieve this separation is to subdivide the common process into sub-processes associated with the various co-products. Where this is not practical, the principle of avoided burden can be used to separate the environmental burdens of a co-product from the product of interest. To do this, the co-product is viewed as reducing the need for the same item generated by more direct means, so the system boundary is expanded to include production of an equivalent amount of the undesired co-product, and the environmental burdens associated with this generation are subtracted from the process that produces the co-products. Ideally this leaves only the burdens associated with the product of interest; however, care must be taken when applying this method. Any type of emission associated with equivalent production of an undesired co-product that does not have an offsetting emission in the original multi-product process will result in a negative emission being reported.

Assumptions, rules, and methodologies guiding the implementation of the LCA, such as the use of system expansion, should be stated as part of the scope of the LCA. Anything that affects what data is collected, how the data is collected, and how the data is analyzed should be included and updated as needed. Everyone involved with the LCA, whether it be with implementation, reviewing, or using the results, must work from a common reference point.

5.2 Life Cycle Inventory (LCI)

Performing an LCI amounts to collecting and quantifying all of the inputs and emissions associated with the product, process, or service being studied. It is from this inventory that the environmental burdens associated with the product, process, or service will be determined. In its simplest form, an LCI produces a list of all the substances involved with the production, use, and disposal of a product, along with the amount required of each substance. In practice, a product is made from components, which may have several levels of subcomponents, which are made from materials, which are comprised of substances. Added to this is that each step of the way from obtaining raw materials to disposal at end-of-life involves more energy and material usage for transportation and processing, resulting in additional environmental burden. Performing an LCI from cradle-to-grave can be a very daunting task; fortunately there are ways to minimize the effort.

The starting point for an LCI is to generate a flow diagram of the processes within the system being studied. You must know a system before you can perform an LCA on it, and if you cannot diagram the system, then you do not know the system well enough. The system boundaries are established when defining the goal and scope of the LCA study. The flow diagram then builds on this by linking the input and emissions of the system to the individual unit processes within the system, and by showing how the unit processes interconnect to produce the product.

Once a system flow diagram is in place, the next step is to create a plan for collecting data. What data will be needed and where the data will come from is driven by the data requirements set down when defining the goal and scope of the LCA. Some data may be generic in nature and found in commercially available databases such as Ecoinvent (Ecoinvent Center 2013), or government sponsored databases such as the U.S. Life Cycle Inventory (NREL 2013). Other data may be in the form of industry averages for the region of interest and found in industry or government publications. Product or process specific data may require that time and effort be allocated to field surveys. Each of these sources has advantages and disadvantages. The generic database approach is relatively easy and fast, but will lack specific information about the product being studied, and the generic information may not be sufficiently timely. Industry averages may be more specific and timely than generic information, but will require more time to locate and evaluate. Product specific information is the most relevant, but can require substantial effort to obtain.

When collecting data for an LCA, a practical approach to balancing cost versus data quality involves using a combination of product specific, industry, and generic data. Product specific data may be collected for key information that differentiates the product, industry averages may be used for common processes, and generic data used to fill in data gaps. One way to minimize the data collection effort in comparing multiple alternatives for a product is to do an initial LCA based on generic data to look for the most promising options, then gather industry and product specific data only for those options. In this way the effort associated with data collection becomes more focused on the better possibilities.

Another aspect of data collection that must be addressed is when to exclude processes because they do not make a significant contribution to the environmental burden. Ideally, an LCA includes all processes no matter how small their contribution, but realistically it is not cost effective to spend valuable time collecting data for something that has little bearing on the final results. Furthermore, as an LCA becomes cluttered with insignificant processes, it may detract from the analysis of significant contributions. If it is clear that a process does not make a significant contribution to the LCA results, then it should be excluded; however, the reasons for excluding it should be documented. If it is not clear that a process contribution is insignificant, then the process should be included at least through a first pass of the LCA with generic data.

5.3 Life Cycle Impact Assessment (LCIA)

The LCIA phase of an LCA can be thought of as the processing phase, where the raw inventory data collected during the LCI phase is converted into estimates of environmental impact. There are many ways in which the environment can be affected: global warming, ozone depletion, acidification, eutrophication, and nonrenewable energy use, to name a few. Each of these environmental issues represents an impact category that has been studied, and for which there is reasonable scientific basis to establish a quantifiable causal relationship between human activities and the severity of the impact to the environment. An LCIA employs impact assessment methodologies consisting of agreed upon models of quantifiable relationships to convert the inputs and emissions involved with producing a product, process, or service into indicators representing the estimated levels of impact that will occur in the environmental categories of concern.

Conversion of input and emission substances starts with applying characterization factors, conversion values developed from scientific study, that relate the effect a substance has on an impact category to the amount of a reference substance required to produce an equivalent effect. Multiplying the input and emission substances in the inventory by the appropriate characterization factors, and then summing the results for an impact category, produces the impact indicator for that category. Midpoint indicators generally represent impact categories directly related to specific environmental mechanisms, such as global warming or ozone depletion. Endpoint indicators often represent damage to systems, such as human health or marine life, and may be based on multiple midpoint indicators, making the models the endpoint calculations are based on more complex. This increase in complexity, and the associated increase in assumptions and simplifications that have to be made, can cause greater uncertainty in the results for endpoints versus midpoints (SAIC 2006).

Impact category indicators initially have units that are based on the reference substance for each category. It may be desirable for comparison purposes to modify this to something else. Normalization can be used to change the indicators to be a ratio relative to a desired reference point. One reference point might be an original base line LCA for a product, allowing subsequent LCAs for new versions to have their impact indicators expressed as being more than, or less than, the original version. Another common reference point is to express an indicator as relative to the amount of emission one person generates in a specific area over a specific amount of time, such as the amount associated with one European over one year of time. Using, or not using, normalization depends on the requirements for analyzing and communicating the LCA results back to the stakeholders in a manner they find useful, something that should be determined when the goal and scope of the LCA is being defined.

Weighting is another means by which the results of an LCA can be adjusted to aid interpretation or improve communication. Weighting is simply a formal way to apply a ranking of importance to different impact categories. Each impact category indicator is multiplied by a weight factor representing its relative importance, and then the weighted results are summed together into a single value representing the total environmental impact of the product, process, or service. Weighting is what a company effectively does when it decides on one product option over another based on multiple impact categories. The problem with weighting is that there is generally no scientific basis for saying that one impact category is more important than another. This makes weighting a judgment call, and something that is significantly more open to questioning than category indicators. If weighting is used, it should be applied in a consistent manner and the basis of the weighting must be documented.

5.4 Life Cycle Interpretation

Understanding the results of an LCA is not as simple as saying one option is better than another. Even if the relative performance of options show a consistent pattern favoring one option across all the impact categories being considered, there are still questions about assumptions, uncertainties, and the significance of results that must be considered. An LCA generally involves a set of assumptions, as well as limits on the availability, timeliness, and applicability of data used, all of which must be reviewed to ascertain what affect they may have on the results.

The starting point for life cycle interpretation is to identify where the greatest contributions to impact categories are coming from. If a few processes account for the majority of an impact in a category, then these are the processes that should be focused on in the interpretation phase. For example, if one process contributes 90% of the impact in a category, then any variations in this process caused by changes in assumptions or issues with data quality will likely produce more pronounced changes in the impact category result than variations in all the other processes combined. LCAs generate a lot of data, so being able to focus effort on major areas of contribution is important to an efficient and cost effective LCA. Identifying the major contributors to an impact category also provides guidance on where future effort to reduce the impact should be concentrated.

The next task is to review the LCI and LCIA results to verify they are consistent with the scope of the study and that they are sufficient to allow the goals of the study to be met. The quality of the data collected should be verified against the expectations set forth at the beginning of the LCA. The extent to which LCI data measurement error affects the inherent uncertainty associated with LCIA results should be checked, as well as the sensitivity of LCIA results to small changes in data. Anomalies in the data and results should be identified and explained. How well the collection and assessment of data meets the needs of the study should be documented, along with the course of action taken to deal with any deficiencies that were found. Each deficiency must be addressed as to how it will affect the LCA, and whether more data collection and analysis is warranted.

Once it is established that the LCI and LCIA results meet the needs of the LCA, they should be reported along with any caveats, conclusions, and recommendations required. The report should include all assumptions, limitations, methods, data, and an adequate discussion of the analysis being done. Reporting the assumptions and limitations of the LCA are just as important as reporting the results, as these define the context under which the results can be viewed. The report must take into account the expectations of the stakeholders in regard to the type of information expected, as covered when defining the goals and scope of the LCA. While the needs of the stakeholders may dictate a summary form of report be presented to them, this should always be backed up by a complete report that is intended to go through a peer review process.

6. LIFE CYCLE ASSESSMENT SOFTWARE

The complex and time consuming nature of LCA has prompted the development of several software programs aimed at reducing the effort involved in performing an LCA. While general purpose software such as MS Excel, Matlab, or Mathematica can be set up to do LCA calculations, software specifically designed for LCA facilitates assembling the LCI data as well as coming preconfigured to do LCIA calculations. These programs simplify initial modeling of products by providing access to databases of generic LCA material and process information. Having the product models then flow as input to the assessment methodologies included with the software eliminates the effort normally associated with entering and verifying an assessment method in a spreadsheet or math program.

LCA software programs can be broad-based fully ISO 14040/14044 compliant packages, or they can be simplified versions geared toward specific applications. The broad-based packages allow access to multiple databases and impact assessment methods, allowing them to be more general purpose. The simplified programs are streamlined versions of LCA, often having only a single database and assessment method available. Some LCA software is proprietary, others are commercially available. The LCA software programs discussed in this paper are all commercially available.

6.1 SimaPro

SimaPro (PRé Consultants 2011) is a general purpose LCA software program that is fully compliant with ISO 14040/14044, providing complete LCI and LCIA capabilities. A product life cycle is modeled as a collection of assemblies, processes, and waste or disposal scenarios. An assembly is made up of a collection of substances (minerals, chemicals), materials, processes, and other assemblies (subassemblies). Disposal scenarios can include reuse, disassembly, and waste scenarios. Multiple libraries (databases) containing predefined substances, materials, processes, and waste treatments for modeling products can be installed. Various impact assessment methodologies can be installed, modified, or created. A high degree of flexibility and visibility is provided in doing LCA calculations, with all impact characterization factors accessible, and contributions to an impact category traceable down to a substance level. This flexibility does make SimaPro more complex than the streamlined LCA software offerings. SimaPro versions 7.2.4 and 7.3.3 were used for this paper.

6.2 GaBi

GaBi (PE International 2011) is another general purpose LCA software program that is fully compliant with ISO 14040/14044, providing complete LCI and LCIA capabilities. A product life cycle is modeled as a plan consisting of processes, material/energy flows, and other plans. Having plans within plans provides a nesting capability similar to the use of assemblies and subassemblies in SimaPro. Gabi can provide access to multiple commercial databases of predefined LCA data, though they have to be merged into a single database to be used at the same time. GaBi provides access to multiple LCA impact assessment methods. Flexibility and visibility in doing LCA calculations in GaBi is on par with SimaPro. All impact characterization factors are visible and contributions to an impact category are traceable down to a substance level.

Like SimaPro, Gabi is significantly more complex to use than streamlined LCA software offerings. GaBi version 5 was used for this paper.

6.3 openLCA

openLCA (openLCA 2011) is an attempt at providing a free open source software package for doing LCA. The intent is a software package with LCA capabilities similar to SimaPro and GaBi. Unfortunately it was found that openLCA was very much a work in progress at the time it was reviewed. Documentation was poor and several problems with using the program were encountered. One significant issue found was that the sequential calculation method could not be made to work properly. Some analysis was done using the alternative matrix calculation method. The ability to trace contributions to an impact category down to a substance level was missing. Open LCA version 1.2 was used for this paper.

6.4 COMPASS

COMPASS (SPC 2011) is a web-based streamlined LCA software program designed for packaging applications. COMPASS does not provide true LCI capabilities; instead a limited dataset of impact indicators previously agreed upon by the members of the Sustainable Packaging Coalition (SPC) has been generated and made available to users of COMPASS. No other datasets can be accessed through the user software, and the methodology for generating the dataset is fixed. Thus multiple assessment methods are not permitted. COMPASS is easier to use than either SimaPro or GaBi, but is also far less flexible. It is not possible to trace contributions to an impact category down to a substance level. COMPASS 2.0 was used for this paper.

6.5 Package Modeling

Package Modeling is the underlying software on which the WalMart Scorecard is based. Like COMPASS, it is intended for packaging applications, does not provide true LCI capabilities, and allows for only a single proprietary assessment method. It generates a single weighted score based on 9 categories of information. The categories include generalized indicators such as cube utilization and energy innovation, but provide little or no information on most environmental emissions other than greenhouse gases. There is little flexibility in application, and no traceability of impact contributions back to substance level emissions. Package Modeling 3.0 was used for this paper.

7. RESEARCH SUBJECT

Every LCA is based on a combination of assumptions and data, so there is always some room for variability in results. Examples available in literature confirm LCAs using different sets of assumptions and data for a common topic can have disparate conclusions (Villanueva and Wenzel 2007). What has not been well studied is whether or not the selection of an LCA software program can contribute significantly to differences in the conclusions that are reached.

To get an idea of the extent software specific to LCA has been used, a review of three LCA and packaging industry related journals was conducted to identify the software used for LCIA. Included in the review were all issues published in 2010 through 2012 of *International Journal of Life Cycle Assessment*, *Journal of Industrial Ecology*, and *Packaging Technology and Science*. Figure 4 shows the number of articles each year that were found to use software specific to LCA for impact assessment. A total of 73 articles over the 3 year period used SimaPro for LCIA, 21 articles used GaBi, and 5 articles use other LCA software. No articles were found to use more than one program for LCIA. In addition, no articles were found that used COMPASS, Package Modeling, or openLCA. When commercial LCA software was used, SimaPro and GaBi were the preferred choices for LCA practitioners submitting articles to these journals. It is also clear that it is common for LCA practitioners to use only one software package when doing an LCA, likely selecting the one they are most versed in.

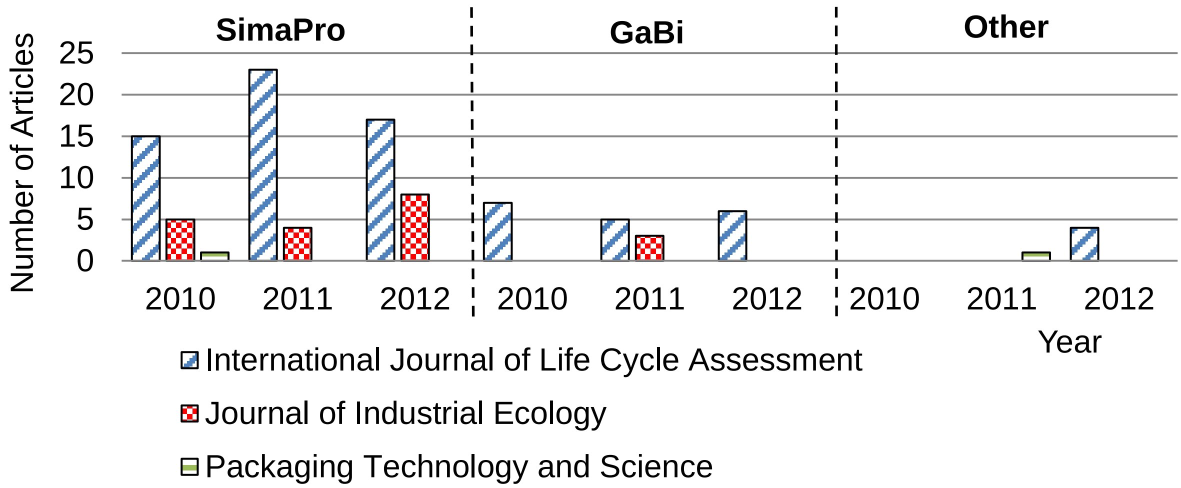


Figure 4: Journal articles using LCA specific software for LCIA.

By using only a single LCA software package in a study, an implicit assumption is being made that the choice of software does not affect the outcome of the study. This assumption is further compounded if, as is often the case, only one impact assessment method is being used as well. There has been only limited investigation into whether LCA software and associated impact methodology implementations significantly influence results. Aissani et al. (2009) presented a comparison of SimaPro and GaBi that was basically a discussion of the features available in the two software packages. Lee and Shan (2000) compared SimaPro and GaBi to EcoPro, using corrugated paperboard and different impact assessment methods, finding that EcoPro reported 50 times the greenhouse gas emissions and 80 times the eutrophication values of the other programs.

The studies mentioned so far cover only SimaPro and GaBi; no good source of comparison has been found for streamlined LCA software. There is no information available as to how consistent results are between streamlined and fully ISO compliant LCA software, nor is there information comparing just streamlined LCA software. As the use of LCA software becomes increasingly common place, there is a need for reliable information as to whether or not LCA software choices affect the results obtained, and how conclusions drawn from those results may be affected. In addition, it would be useful to develop guidelines as to when it is reasonable to employ streamlined LCA software versus using fully ISO compliant software.

The research proposed for this paper is intended to help fill the gap in knowledge that currently exists concerning comparability of LCA software. The basic presumption made by companies using LCA software to guide decisions is that environmental impact estimates will be sufficiently consistent between LCA software as long as assumptions, system boundaries, and other conditions affecting the study remain consistent. To test this presumption, a common set of packages and distribution systems was defined and used as the basis for comparison of multiple LCA software programs.

8. RESEARCH METHODS

The main interest when considering the comparability of LCA software is whether or not the conclusions reached about environmental preference of possible alternatives in a product design will be consistent across the different software. Every software program has the potential to influence the way environmental impacts are assessed. The most obvious factors affecting impact assessments of product systems are differences in data quality and impact assessment methodologies; however, other less obvious factors can come into play, too. It may be that limits in available datasets dictate substitutions, deletions, simplifications, or detailed expansions be made to a product model in one software that would not be done in another. A more subtle possibility is having the functionality of available modeling tools influence the implementation of a model by making some things easier to do in one software than in another. Another aspect is that streamlined LCA software gets that way by limiting available choices, meaning that some decisions are pre-made in the attempt to simplify operation, and details of those decisions may not be readily visible to the user.

To study the different LCA software programs, three sets of common packaging systems were chosen as the basis for comparison. Each set consisted of two or more containers that could be used for a similar purpose. Table 2 presents a summary of these packaging systems. Beverage containers were selected for one set as they have been widely studied and allow for a variety of materials to be considered (Romero-Hernández et al. 2009; Mourad et al. 2008). This set included aluminum cans, glass bottles, polyethylene terephthalate (PET) bottles, aseptic cartons, and polylactic acid (PLA) bottles. The functional unit for comparison of this set is one liter of fluid (beverage). The second set of containers explores flexible versus rigid packaging options by comparing multilayer pouches and steel cans used in packaging tuna. This sets utilizes one kilogram of tuna as the functional unit. The third set of containers is aimed at studying the effect of reuse by comparing reusable polypropylene (PP) crates to single-use corrugated boxes for distribution of cut flowers. Each PP crate and corrugated box can carry an amount of flowers equivalent to ½ flower box, a standard unit of measure in the cut flower industry and the functional unit for this comparison.

Table 2: Packaging systems compared

Container Type	Functional Unit	Containers Per Functional Unit
Aluminum Carbonated Beverage Can, 12 fluid ounces (354.9mL)	1.00 lt fluid	2.82
Glass Beer Bottle, 12 fluid ounces (354.9mL)	1.00 lt fluid	2.82
Polyethylene Terephthalate (PET) Carbonated Beverage Bottle, 12 fluid ounces (354.9mL)	1.00 lt fluid	2.82
Aseptic Carton, 200mL	1.00 lt fluid	5.00
Polylactic Acid (PLA) Water Bottle, 500mL	1.00 lt fluid	2.00
Multilayer Pouch, 74g net weight	1.00 kg tuna	13.51
Steel Can, 142g net weight	1.00 kg tuna	7.04
Corrugated Box, 1/2 flower box	1/2 flower box	1.00
Polypropylene Crate (PP), 1/2 flower box	1/2 flower box	1.00

Flow diagrams representing simplified product life cycles were created for the nine packaging systems selected as a basis of comparison for this study. Simplified life cycles were used to facilitate comparison of the software systems; consequently the information presented in this paper should <u>not</u> be construed as providing valid comparisons of the actual packaging systems themselves. The assumptions made to simplify these systems are listed in Appendix B. Data on the physical characteristics needed to model the nine containers in the LCA software programs are given in Appendix C. Some of this data has been taken from previous studies; the rest was obtained by measuring samples of the different containers. The simplified flow diagrams are presented in Appendix D. To keep the number of tests that needed to be conducted down to a manageable level, it was decided to study the effects of varying transport distances, recycling rates, recycled content, and number of reuses only in selected comparisons. Appendix E provides details on how test parameters were varied to obtain the comparison data of interest. U.S. datasets were used wherever possible in creating software models of packaging systems.

Using the flow diagrams and associated data as common references, models of the packaging systems were created in SimaPro 7.2.4, GaBi 5, COMPASS 2.0, and Packaging Modeling 3.0. Problems encountered with using the version of openLCA that was available when these tests were conducted led to it being dropped from this portion of the testing.

It quickly became apparent that some software offered choices that could significantly reduce the amount of work involved, while other software did not. For example, SimaPro had available data files from Franklin Associates for aluminum, glass, and PET containers that rolled the entire set of processes for the container, from getting raw material in the ground to producing a finished container, into a single cradle-to-gate file. Thus an LCA practitioner using SimaPro could do either a detailed model for producing one of these containers where each required process is represented individually, or they could use a single cradle-to-gate file. GaBi did not have these cradle-to-gate files available, necessitating more detailed and time consuming models be implemented. COMPASS was the opposite of GaBi, generally providing only one appropriate conversion (manufacturing) process for each container, with no means for the LCA practitioner to do their own detailed model. Package Modeling did not provide a means of adding conversion processes. Faced with this inconsistency in the way product system models could be implemented across the different LCA software, it was decided to allow the models to be implemented in the manner that provided the simplest approach for each software. Clearly this can cause differences in inventory data that may affect the results, but it does create valid models for each software. Furthermore, it is believed that the simplest method of implementing a model reflects the most likely approach users will take in using a software program.

The lack of comparable impact categories is an obvious difficulty when evaluating LCA software. The impact assessment methodology used for SimaPro and GaBi in this part of the study was Impact 2002+ version 2.1, supplemented by ReCiPe Midpoint (H) version 1.04 in SimaPro and version 1.05 in GaBi for water consumption. SimaPro and GaBi have 15 midpoint categories using Impact 2002+, and 18 with ReCiPe, but only global warming, non-renewable energy, aquatic eutrophication, and water depletion can be matched to output indicators in COMPASS. Once Package Modeling is added, global warming becomes the only category of impact information common to these 4 software programs. Things are further complicated when trying to include openLCA. Its implementation of Impact 2002+ reports only 2 of the standard 15 midpoint categories, neither of which is global warming. The other impacts are translated directly to damage (endpoint) categories and reported in “points”. Among the other software being studied, only SimaPro and GaBi have the option of viewing impact categories in units of “points”, a technique for normalizing results in terms of the average impact to one person in one year for a specified region (Humbert 2005). Thus openLCA results using Impact 2002+ could not be compared directly to COMPASS or Package Modeling. Both COMPASS and Package Modeling report impact categories that have no comparable counterpart in the other software, examples are a “Material Health” score reported in COMPASS and the “Innovation Different from Energy Standard” metric used in Package Modeling. With the wide variation in the type and presentation of impact information available, the potential exists for software to influence decision making not only by the impact category results presented, but by which categories are included. Evaluations of this type of influence would be subjective and are not within the scope of this paper. However, the lack of common impact categories does create limitations for this study that must be addressed. All comparisons in this paper will be based on the values of an impact category indicator common to the software being included, meaning that some evaluations will involve only a subset of the software programs being studied, the others being eliminated from specific comparisons due to the absence of the impact category under consideration.

Using packaging system flow diagrams as the starting point, while allowing for a useful broad comparison, does not provide the means to easily track down the cause of differences that may occur. Any variation in impact assessment can be the result of an amalgamation of the different data, assumptions, and modeling choices dictated by, or at least influenced by, the functionality of the software being compared. For example, SimaPro and GaBi can use commercially available datasets of LCA information while streamlined LCA software such as COMPASS does not. What COMPASS makes available to users is a web based set of impact indicators that were previously compiled using a proprietary assessment method and SimaPro. An attempt to duplicate the process outlined for COMPASS, using the input datasets identified for COMPASS along with information about the proprietary assessment method, resulted in significant differences in impact values compared to those reported by COMPASS. Without access to the actual inventory database used to produce the impact indicator dataset for COMPASS, it was not possible to definitively determine the causes of any differences involving COMPASS. Attempts to trace differences in impact results between SimaPro and GaBi for the packaging systems also proved difficult.

As a means of providing a base line of comparison, one that would aid the effort in exploring causes of any impact differences that might be encountered, it was decided to do another series of comparisons using more minimalistic systems to cut down on the number of variables involved. Each system would consist of obtaining and disposing of 1 kg of a single basic packaging material. Four materials were selected: aluminum, corrugated board, glass, and PET. Table 3 shows the parameters used with these basic material test scenarios. SimaPro 7.2.4, GaBi 5, openLCA 1.2, and COMPASS 2.0 were used for the basic material comparisons. Packaging Modeling was not included as it is designed specifically for packages, not for obtaining and disposing of materials.

Values for recycling rate, landfill, and waste-to-energy at end-of-life (EOL) for the base materials were chosen to match those used in COMPASS, as COMPASS did not allow modification of these parameters. Input data for openLCA, SimaPro and GaBi was limited to files from the Ecoinvent 2.2 database, with efforts made to identify and use the same data files called out in reference documentation as being used in creating the COMPASS dataset (Mistry 2010). Because many U.S. datasets are adapted from European datasets by adjusting energy inputs to match U.S. energy production averages, European datasets originating in the EcoInvent 2.2 database were chosen for the base materials to eliminate potential variations that might have occurred in doing the energy conversions. The impact assessment methodology used with SimaPro and GaBi for the basic material tests was Impact 2002+ version 2.1, supplemented by ReCiPe Midpoint (H) version 1.04 in SimaPro and version 1.05 in GaBi for water consumption. The methodologies used with openLCA were Impact 2002+ and ReCiPe; however, no information was found that identified the versions being used.

Table 3: Parameters for basic material test scenarios

Basic Material	Functional Unit (kg)	Recycled Content (%)	Recycled At End of Life (%)	Landfill At End of Life (%)	Waste To Energy At End of Life (%)
Aluminum	1	50	67.9	32.1	0
Corrugated Board	1	12	76.4	10.7	12.9
Corrugated Board	1	50	76.4	10.7	12.9
Corrugated Board	1	87	76.4	10.7	12.9
Packaging Glass	1	55.5	63.8	36.2	0
Polyethylene Terephthalate (PET)	1	0	26.1	45.1	28.8

The final part of this study involved tracing any discrepancies in results between software to their root causes. SimaPro and GaBi lend themselves well to examining differences in impact assessment values coming from the basic material tests. Both software programs provide complete transparency in all calculations, and in the characterization factors used to implement impact assessment methodologies. COMPASS and openLCA were less transparent, which can make tracing impact contributions back to input sources difficult, if not impossible. For SimaPro and GaBi, built-in functions allow all the substances contributing to an impact assessment category indicator value to be viewed, as well as the characterization factors used to implement the assessment method.

To trace how differences in impact assessment values occur, the approach used was to start with the LCIA output and work backward to the inputs. While there can potentially be hundreds, or even thousands, of substances contributing to an impact category, generally only a small number are significant. By sorting on total contribution to an impact category, it is easy to see which substances contribute the most to the category. To minimize time, it was originally decided to look at the substances that combined for the first 90% of an impact indicator value, but it was often found that the number of significant contributors was small enough to make it practical to look at substances responsible for 95% or more of the total contributions. Once the significant contributors were identified, the amount of each input substance could be found, as well as the characterization factor used to convert the input substance to the common reference substance of the impact category. With the significant inputs, input amounts, characterization factors, and impact category contributions known, all the pertinent information was available for pointing to the cause of any important discrepancy in impact category indicator values between software programs.

Due to an upgrade, SimaPro 7.3.3 was used for this last part of the study, with the impact assessment methodologies for SimaPro and GaBi being Impact 2002+ version 2.1, ReCiPe Midpoint (H) version 1.06 in SimaPro and version 1.05 in GaBi, plus TRACI 2. TRACI 2 methodology was added for both SimaPro and GaBi as a third point of reference when looking for inconsistencies in results.

9. PACKAGE SYSTEM COMPARISONS

The stated goal of the packaging system comparisons was to evaluate whether the choice of LCA software was likely to influence decisions based on the LCA results. Since some variation in magnitude of impact indicators was likely due to differences in datasets and modeling, tests were created that looked at the relative order each software would rank a group of similar containers, as well as provide a comparison of impact indicator magnitudes across software. While the life cycle scenarios of containers were varied between tests to study different facets of how impact assessment was affected, the key point for data presented in this paper is that every software program was presented the same set of container scenarios for a given comparison.

A note of caution is in order regarding impact category results presented here; no representation is being made as to what constitutes an environmentally significant amount of emissions or energy use for any impact category. Determining if the value of an impact category indicator represents a significant environmental impact for a given situation is beyond the scope of this paper. What is being investigated here is the consistency of results between LCA software programs.

The data for all graphs presented in this section can be found in Appendix G.

9.1 Beverage Containers

The parameters used in the beverage container comparison presented here are given in Table 4. This represents a small subset of the comparisons conducted for this study; a more complete listing of test parameter combinations explored is given in

Appendix E. All beverage container comparison data is based on a functional unit of 1 liter of fluid (beverage).

Table 4: Parameters for beverage container comparison

Container Type	Recycled Content (%)	Recycled At EOL[1] (%)	Composted At EOL[1] (%)	Truck (km)	Rail (km)	Air (km)	Ship (km)
Aluminum can	70	50	0	100	0	0	0
PET bottle	10	30	0	100	0	0	0
Glass bottle	25	40	0	100	500	0	0
Aseptic carton	0	0	0	100	0	0	0
PLA Bottle	0	0	0	100	0	0	0

[1] EOL = End of Life.

The results obtained for the global warming impact category are shown in Figure 5. While the relative ranking order (lowest to highest) of the beverage containers was the same in COMPASS and SimaPro, the rankings of the aluminum can versus PLA bottle differed in GaBi. Further, the results for the beverage containers did not maintain the same ratios to each other when moving from COMPASS to SimaPro, indicating that changes in weights of the containers being compared could affect the relative rankings differently in each software. Package Modeling differed substantially from the other software. While COMPASS, SimaPro, and GaBi all ranked the aluminum can, glass bottle, and PET bottle in that order relative to each other for lowest to highest emissions, Package Modeling had the aluminum can and glass bottle approximately equal, with both at twice the emissions of the PET bottle. Package Modeling had the emissions for the aluminum can being greater than any of the other software, and the emissions for the PET and glass bottles significantly less than the other software.

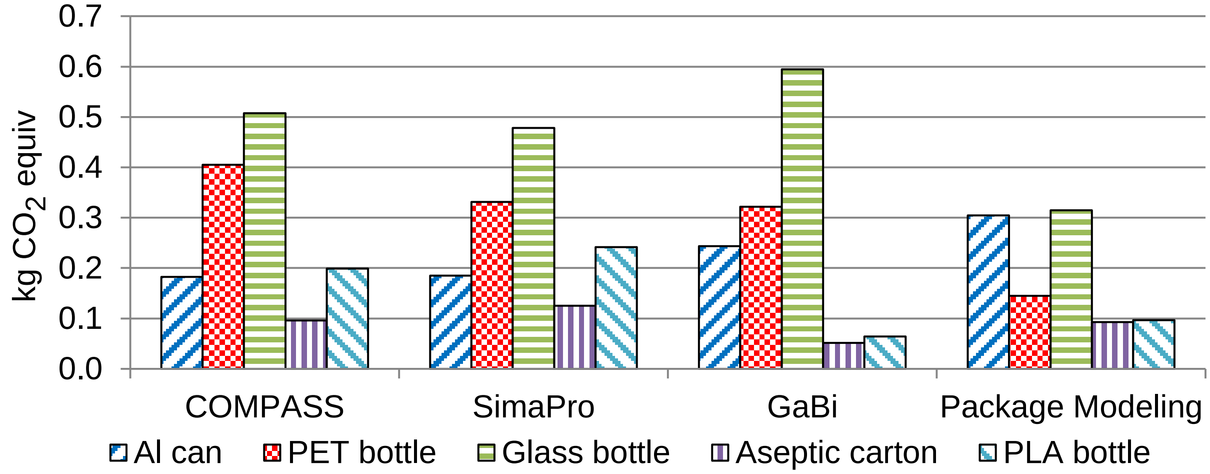


Figure 5: Greenhouse gas emissions for selected beverage containers.

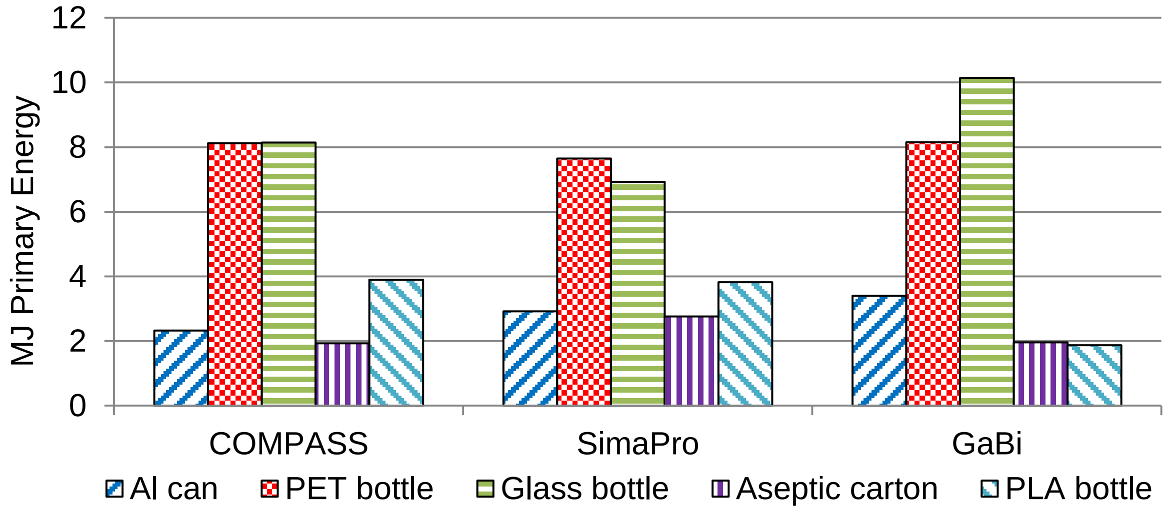


Figure 6: Fossil fuel/non-renewable energy for selected beverage containers.

Figure 6 shows the comparison results for fossil fuel/non-renewable energy use. The COMPASS fossil fuel category did not include electricity generated from nuclear energy, part of the standard U.S energy mix, while the Impact 2002+ non-renewable energy category used in SimaPro and Gabi did include it. Despite this, COMPASS fossil fuel results were 6% higher for PET bottles and 18% higher for glass bottles than the corresponding non-renewable energy values from SimaPro. The relative rankings of the containers also differed. While glass and PET bottles in this comparison required roughly the same amount of energy in COMPASS, glass required less energy than PET in SimaPro and more energy than PET in GaBi. PLA bottles required approximately the same energy in COMPASS and SimaPro, yet GaBi reported less than half as much energy required.

Distinctly different results arose from the three software programs used to look at eutrophication in the beverage container comparison, as shown in Figure 7. COMPASS and GaBi reported significantly higher impact values than SimaPro, with ratios ranging from 1.39 to 140. There was little agreement between software on how the containers should be ranked relative to each other for this impact category. COMPASS and SimaPro ranked the PLA bottle as the highest impact, but disagreed on the order for the remaining containers. COMPASS and GaBi only agreed that PET had the second highest impact; there was no agreement between them for the remaining containers.

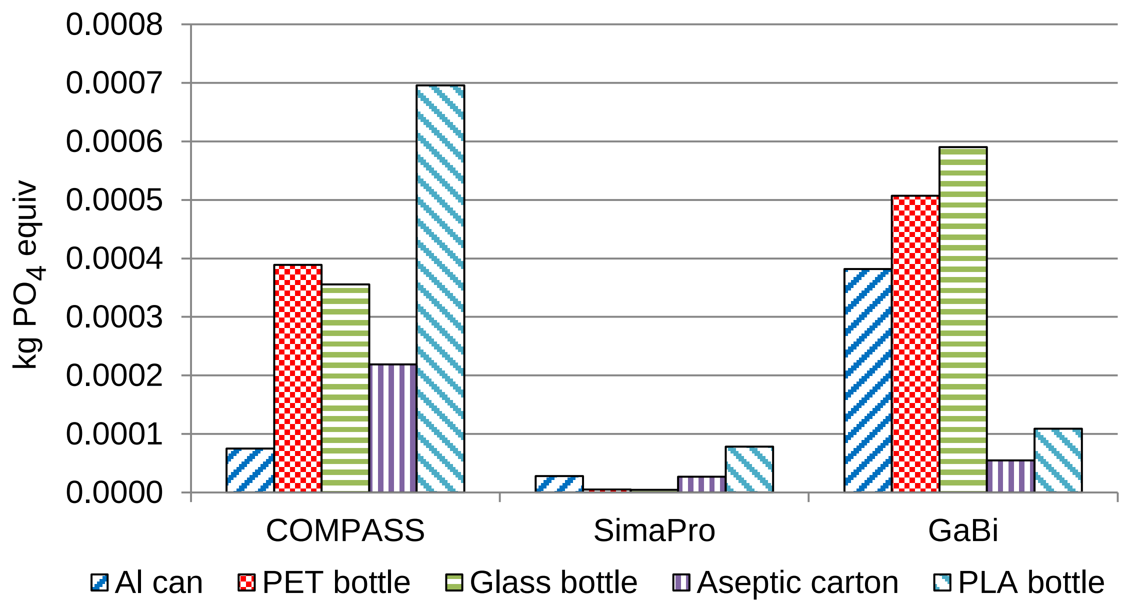


Figure 7: Eutrophication for selected beverage containers.

Results of the beverage container comparison for water depletion, or water consumption as it is referred to in COMPASS, are shown in Figure 8. Notice that the vertical scale for this graph is logarithmic; this is necessitated by GaBi reporting water depletion that was several orders of magnitude greater than COMPASS or SimaPro. The greatest difference occurred for the aluminum can; COMPASS and SimaPro reported less than 1.0 liter of water depletion while GaBi reported over 4,200 liters. Even the smallest relative difference was sizable, occurring for the aseptic carton with COMPASS reporting 3.6 liters, SimaPro 2.3 liters, and GaBi 376 liters. In addition, the relative ranking of the containers for water depletion varied with software; COMPASS had the glass bottle requiring the most water, in SimaPro it was the aseptic carton, and there was a tie in GaBi between the aluminum can and the glass bottle

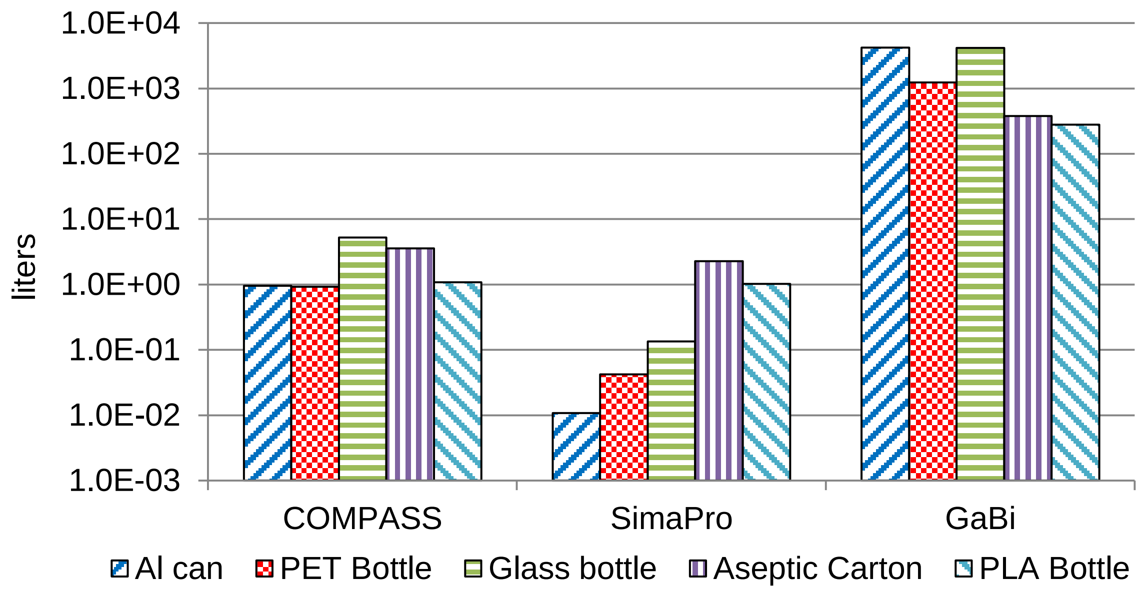


Figure 8: Water depletion/consumption for selected beverage containers.

The effect of truck and rail transport on impact indicators was looked at using beverage container scenarios as the basis of comparison. Package Modeling was removed from consideration in these tests after it was discovered that the available transport distance selections had no effect on the greenhouse gas emissions reported by this software. Table 5 lists parameters for the truck and rail comparisons for the glass bottle.

Table 5: Parameters for truck and rail transport comparison

Container Type	Recycled Content (%)	Recycled At EOL[1] (%)	Composted At EOL[1] (%)	Truck (km)	Rail (km)	Air (km)	Ship (km)
Truck Tests							
Glass bottle	25	40	0	100	500	0	0
Glass bottle	25	40	0	1000	500	0	0
Rail Tests							
Glass bottle	25	40	0	100	0	0	0
Glass bottle	25	40	0	100	500	0	0
Glass bottle	25	40	0	100	4000	0	0

[1] EOL = End of Life.

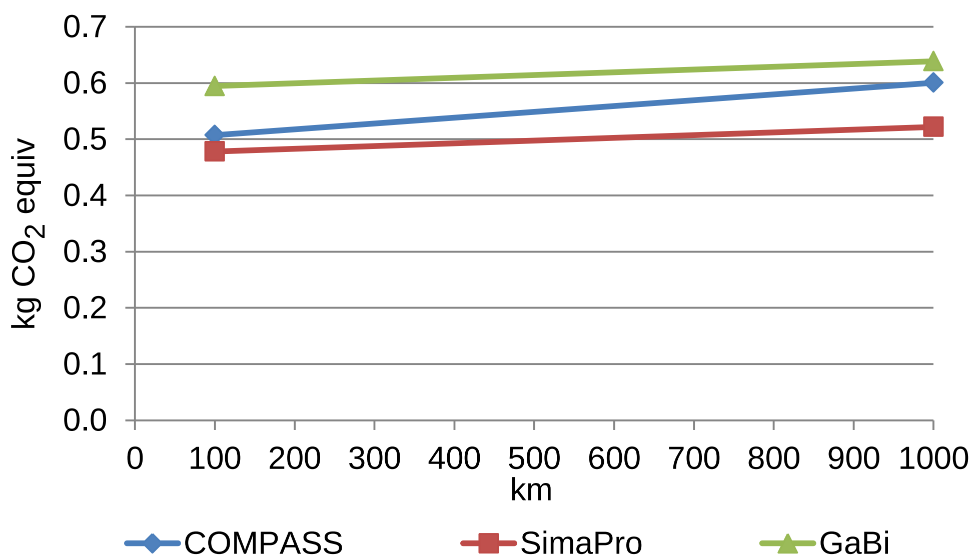


Figure 9: Greenhouse gas emissions for glass bottle using truck transport.

Figure 9 shows the plot of greenhouse gas emissions versus truck transport distance for the glass bottle; all other parameters were held constant. SimaPro and GaBi produced basically identical slopes, 4.87×10^{-5} kg CO_2/km and 4.88×10^{-5} kg CO_2/km respectively, while the slope from COMPASS was 1.04×10^{-4} kg CO_2/km, more than double the others. Given the initial starting points at 100 km, COMPASS results grew increasing larger than those of SimaPro from the start, but it would take approximately 1,600 km of truck transport distance before COMPASS would report higher greenhouse gas emissions than GaBi. The change in emissions from 100 km to 1,000 km represented a 15.5% increase in COMPASS, an 8.4% increase in SimaPro, and a 6.9% increase in GaBi.

Figure 10 shows how greenhouse gas emissions varied with rail transport distance for the glass bottle. Rail transport distance was the only variable; all other parameters were held constant. The slope produced by SimaPro, 2.81 $x10^{-5}$ kg CO_2/km, was similar to that from GaBi at 2.63 $x10^{-5}$ kg CO_2/km, while the 1.15 $x10^{-5}$ kg CO_2/km slope from COMPASS was less than half the others. Given the initial offset points, GaBi results grew increasing larger than COMPASS from the start, but it took approximately 2,250 km of rail transport distance before SimaPro reported higher greenhouse gas emissions than COMPASS. The change in emissions from 0 km to 4,000 km represented a 9.2% increase in COMPASS, a 24.2% increase in SimaPro, and an 18.1% increase in GaBi.

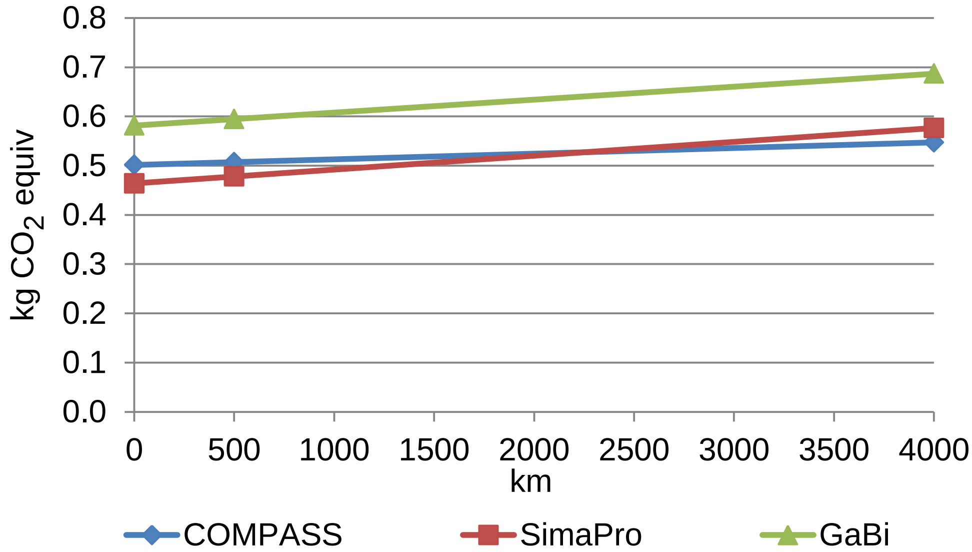


Figure 10: Greenhouse gas emissions for glass bottle using rail transport.

9.2 Flexible Versus Rigid Containers

The parameters used in the flexible versus rigid container comparison presented here are given in Table 6. All data are based on a functional unit of 1 kilogram of tuna. A difficulty arose in trying to account for recycled content of steel when comparing results from different software. The database used with GaBi fixed the recycled content of steel at 25%, Package Modeling fixed it at 28%, COMPASS fixed it at 37%, and the database used with SimaPro allowed 0% to 100%. Since it was not possible to compare results from all the software with the same amount of recycled content for steel, it was decided to compare GaBi to SimaPro at 25%, and COMPASS to SimaPro at 37%. With Package Modeling only able to provide a comparison to the other software for global warming, it was further decided to group it with the GaBi and SimaPro comparison for this single impact category.

Table 6: Parameters for flexible versus rigid container comparison

Container Type	Recycled Content (%)	Recycled At EOL[1] (%)	Composted At EOL[1] (%)	Truck (km)	Rail (km)	Air (km)	Ship (km)
Flexible Pouch	0	0	0	100	0	0	0
Steel Can	25	70	0	100	0	0	0
Steel Can	37	70	0	100	0	0	0

[1] EOL = End of Life.

The comparison of greenhouse gas emissions for the global warming impact category is given in Figure 11. It can be seen in Figure 11A that while the relative ranking of the 37% recycled content steel can versus the flexible pouch was the same in SimaPro and COMPASS, SimaPro reported significantly higher greenhouse gas emissions for the steel can than COMPASS did, 62% higher. Emissions for the flexible pouch had better agreement, with SimaPro 5% lower than COMPASS. Figure 11B shows the 25% to 28% recycled content steel can was consistently ranked by all three software programs as having higher greenhouse gas emissions than the flexible pouch. The variation of greenhouse gas emissions reported for the steel can was less, as shown Figure 11B, with SimaPro results 26% higher than Package Modeling. On the other hand, variation of greenhouse gas emissions for the flexible pouch was higher, as shown in Figure 11B, with SimaPro results 73% higher than Package Modeling. For both containers, GaBi results fell between those of SimaPro and Package Modeling.

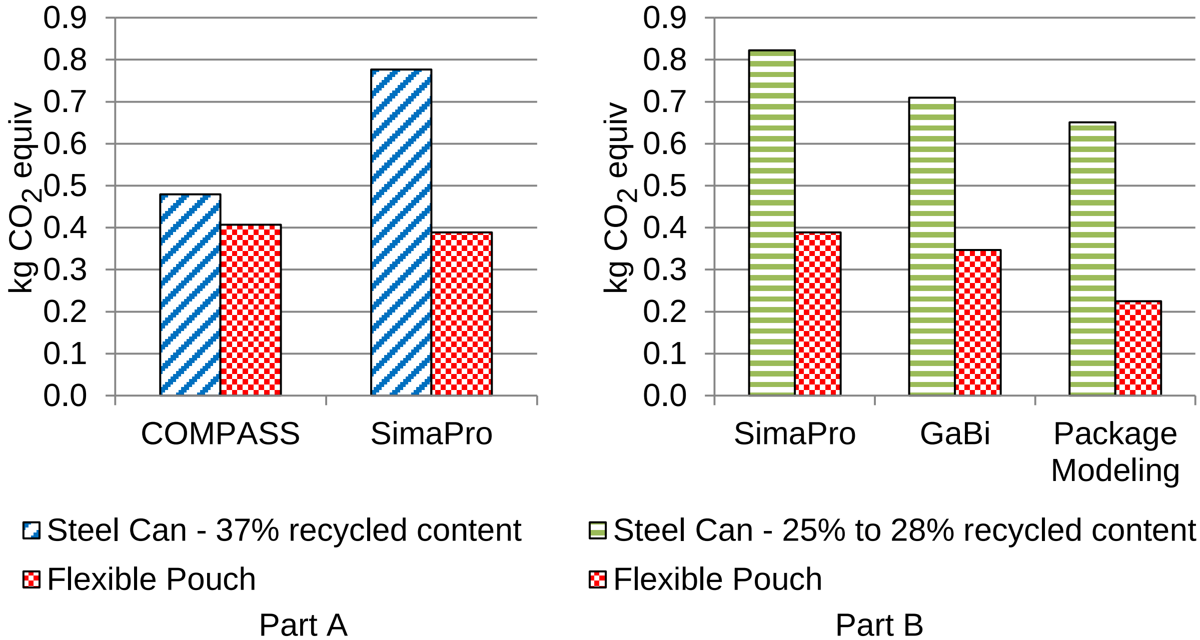


Figure 11: Greenhouse gas emissions for steel cans and flexible pouch.

Figure 12 presents results for the fossil fuel/non-renewable energy impact category. COMPASS and SimaPro reversed rankings for the 37% recycled content steel can versus the flexible pouch, as can be seen in Figure 12A. COMPASS reported the steel can 20% lower than the pouch while SimaPro placed the can 8% higher. SimaPro was 58% higher in reported equivalent energy for the steel can when compared to COMPASS, and 17% higher for the flexible pouch. Figure 12B shows the results for the 25% recycled content steel can versus flexible pouch in SimaPro and GaBi. There was a reversal in ranking between the software; SimaPro reported the steel can 13% higher than the pouch while GaBi placed the can 5% lower. SimaPro reported higher equivalent energy requirements compared to GaBi, 43% higher for the steel can and 20% higher for the flexible pouch.

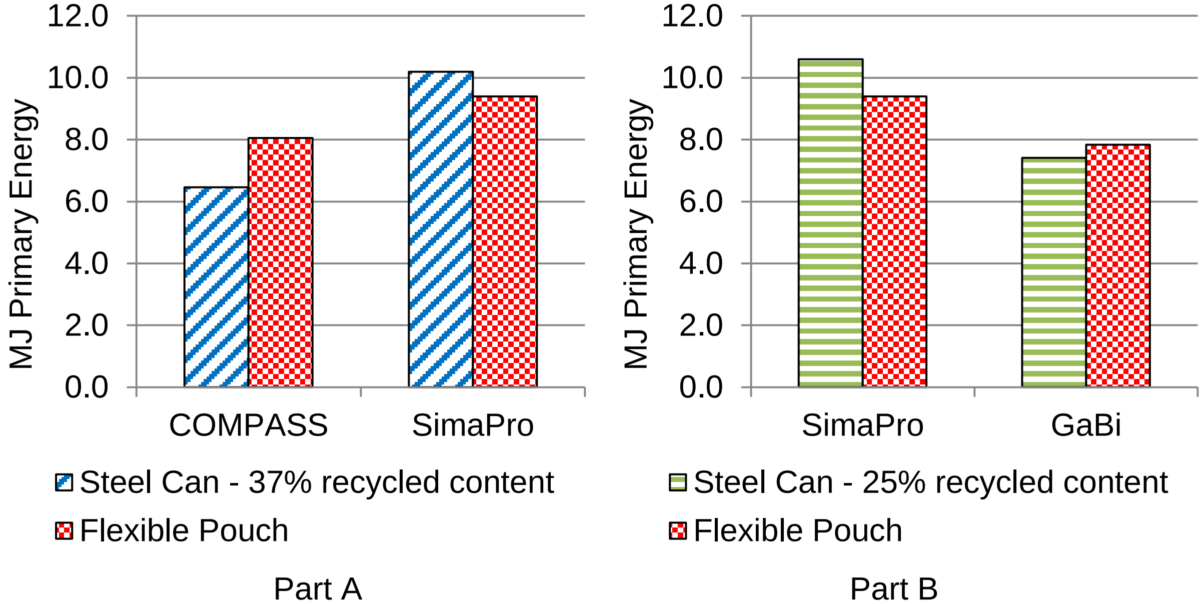
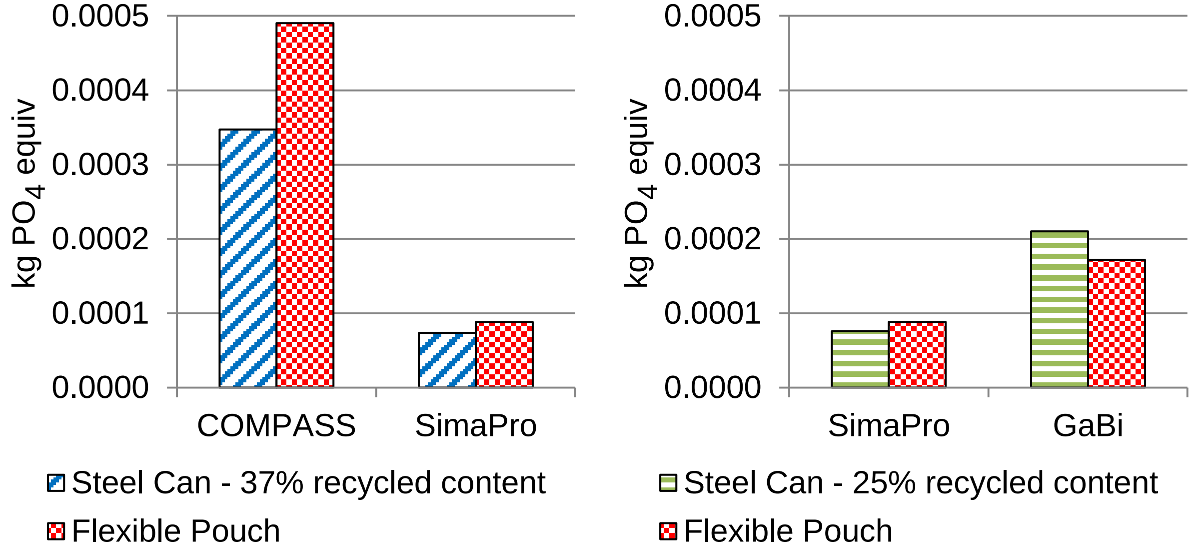


Figure 12: Fossil fuel/non-renewable energy for steel cans and flexible pouch.

Eutrophication results are shown in Figure 13. It can be seen in Figure 13A that COMPASS and SimaPro agreed on the ranking order of the 37% recycled content steel can versus the flexible pouch; however, COMPASS results were considerably larger in magnitude, by a multiplication factor of 4.7 for the steel can and 5.6 for the pouch. SimaPro and GaBi reversed the ranking order for the 25% recycled content steel can versus the flexible pouch, as shown in Figure 13B. SimaPro reported emissions for the steel can were 14% lower than the pouch, while GaBi had the can 22% higher. GaBi reported eutrophication results that were 2.8 times those of SimaPro for the steel can, and 2.0 for the flexible pouch.



Part A Part B

Figure 13: Eutrophication for steel cans and flexible pouch.

Water depletion/consumption results for the steel cans and flexible pouch are shown in Figure 14. The results reported by GaBi greatly exceed those from SimaPro and COMPASS, forcing the use of a logarithmic scale for the comparison graphs, just as happened in the beverage container comparison for water depletion. GaBi reported 502 liters of water required for the 25% recycled content steel can, compared to 6.4 liters reported by SimaPro. GaBi had the flexible pouch requiring 1,460 liters of water, SimaPro estimated 0.69 liters, and COMPASS 1.0 liter. GaBi also reversed the ranking order compared to the other software, with lower water usage reported for the steel can instead of the flexible pouch.

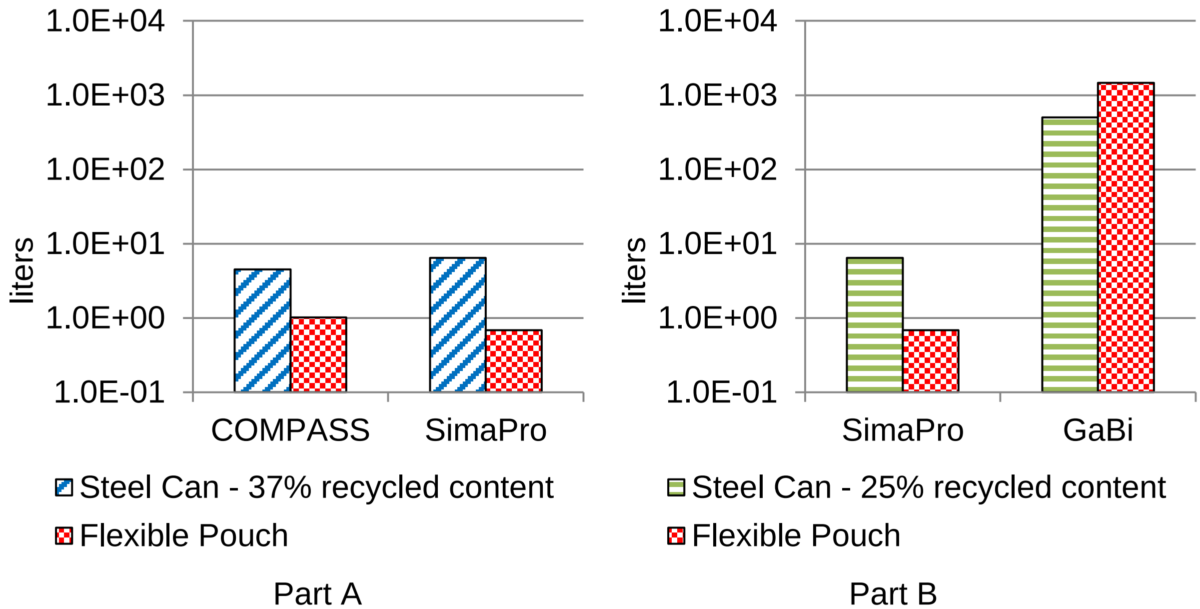


Figure 14: Water depletion/consumption for steel cans and flexible pouch.

9.3 Single Use Box Versus Reusable Crate

Test parameters for exploring how the software handled comparison of a single use corrugated box to a reusable plastic (PP) crate are given in Table 7. All data is based on a functional unit of ½ flower box, a standard unit of measure for the cut flower industry. For this comparison all containers were subject to 200 km of truck transport and 2,500 km of air transport on the out going journey, with the return trip involving 2,100 km by ship (ocean) transport and 1,200 km additional truck transport. This loop is based on a model for shipment of cut flowers which required air shipment for quick delivery, but the return of the empty reusable PP crate was done by more cost effective means. Please note that there is no return of the PP crate from its last use, meaning that a single use crate did not go through a return cycle.

Table 7: Parameters for reuse comparison

Container Type	Recycled Content (%)	Recycled At EOL[1] (%)	Composted At EOL[1] (%)	Truck[2] (km)	Rail[2] (km)	Air[2] (km)	Ship[2] (km)
PP Crate, 1 use	0	10	0	200	0	2,500	0
PP Crate, 10 uses	0	10	0	1,400	0	2,500	2,100
PP Crate, 100 uses	0	10	0	1,400	0	2,500	2,100
Corrugated Box, 1 use	50	80	0	200	0	2,500	0

[1] EOL = End of Life.

[2] Transport distances are on per use basis, except no return transport on last use.

Results of the reuse comparison for the global warming impact category are presented in Figure 15 in terms of average emissions per use, where each use constitutes one trip through the distribution cycle. As previously stated, it was found that Package Modeling did not vary reported greenhouse gas emissions with changes in shipping distance; thus it did not provide a means to account for the contribution to emissions made by each pass through the distribution cycle. For this reason, the results from Package Modeling are shown only for reference as single use values. Looking at results from the other software, it can be seen that each software produced a different result. GaBi had the single use corrugated box having 19% lower greenhouse gas emissions than the 100-use PP crate, SimaPro reversed the order with the corrugated box having 73% more emissions, and COMPASS rated them approximately equal with only a 2% difference.

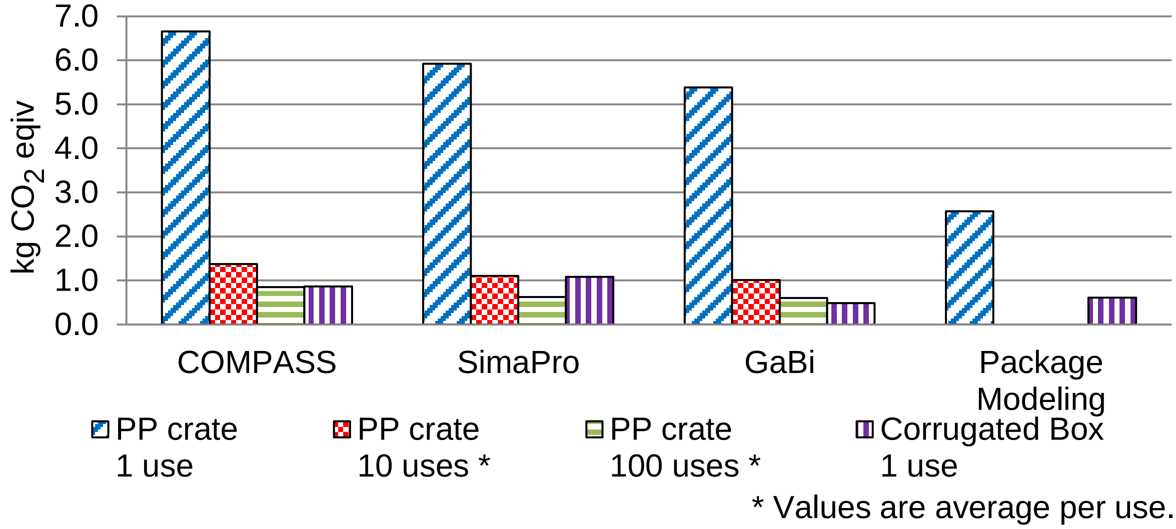


Figure 15: Greenhouse gas emissions for reuse comparison.

Figure 16 shows the reuse comparison for the fossil fuel/non-renewable energy impact category, again in terms of average per use values. Here SimaPro and GaBi agreed on the ranking order of the results, though not on magnitudes. GaBi had the corrugated box taking 30% more energy than the 100-use PP crate, while SimaPro had the corrugated box taking 62% more energy. COMPASS ranked the corrugated box and 100-use PP crate about equal, with only a 6% difference in energy between them.

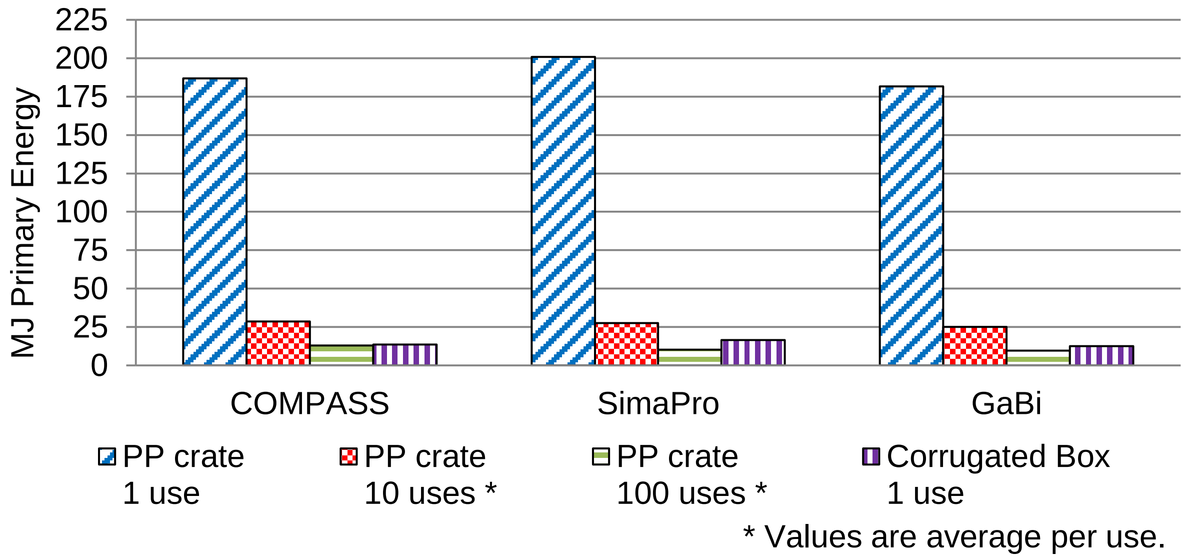


Figure 16: Fossil fuel/non-renewable energy for reuse comparison.

The eutrophication results for the reuse comparison are given in Figure 17. Notice that the vertical scale of the graph is logarithmic; this is due to the results reported by SimaPro being substantially smaller in magnitude than results from COMPASS or GaBi. COMPASS values are 7 to 136 times those of SimaPro, and GaBi values are 5 to 24 times those of SimaPro. The three software programs differed on where they ranked the corrugated box relative to the PP crate options; SimaPro ranked the corrugated box as having the highest emissions, GaBi ranked it as second highest, and COMPASS ranked it as third highest.

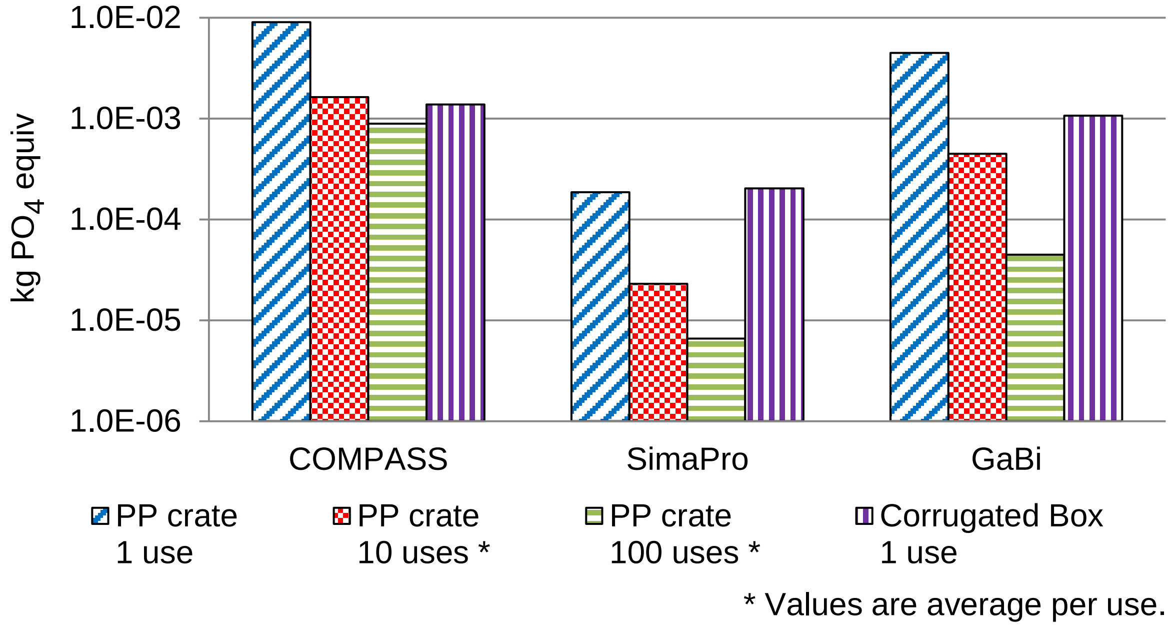


Figure 17: Eutrophication for reuse comparison.

Water depletion/consumption results for the reuse comparison are given in Figure 18. Note the vertical scale of the graph is logarithmic, a consequence of GaBi producing numbers several orders of magnitude greater than the other software. As an example, GaBi reported approximately 11,200 liters of water depletion associated with the single use PP crate, COMPASS put the number at 12.6 liters, and SimaPro at 8.6

liters. These water depletion/consumption magnitude differences are consistent with those obtained for the other packaging systems considered in this paper; GaBi always reported significantly higher water depletion than the other software. In addition to differences in magnitudes, GaBi also differed from the other programs by reporting the single use PP crate required more water than the corrugated box.

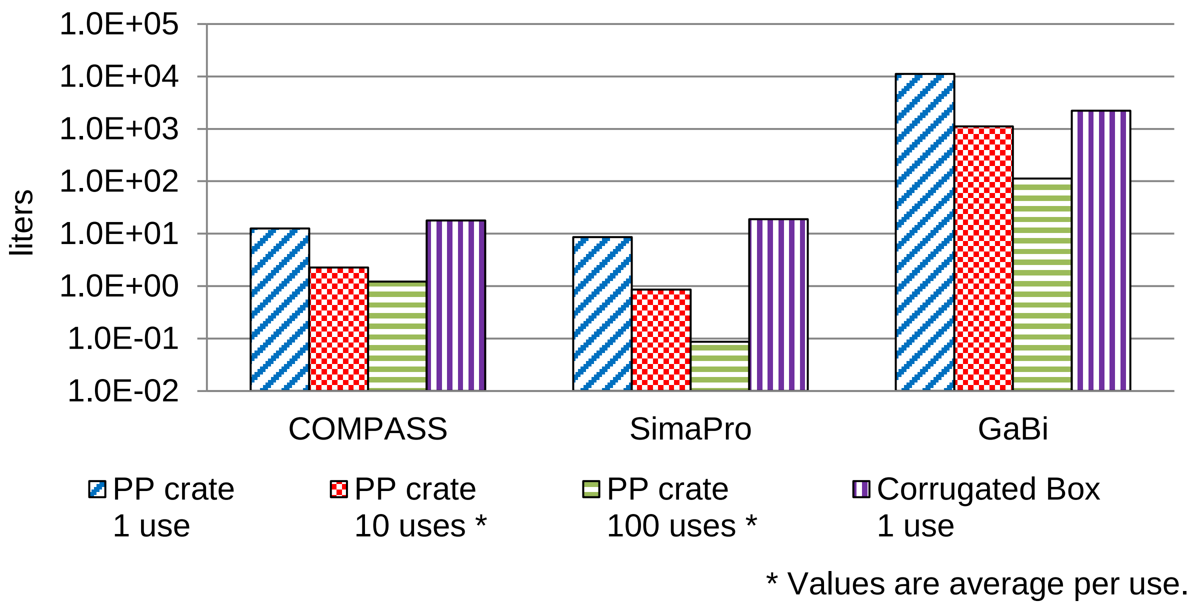


Figure 18: Water depletion/consumption for reuse comparison.

The corrugated box package system was also used to explore how the software compared when dealing with varying amounts of recycled content in a package. Table 8 lists the parameters associated with this series of tests. The only parameter being varied is the recycled content; all other parameters remained constant. As originally conceived, the tests called for recycled content of 0%, 25%, 50%, and 100%. However, it was discovered that COMPASS only allowed recycled content of corrugated board to be 12% to 87%. Rather than alter the basis of comparison in the middle of collecting data, it was decided to look at this as an LCA practitioner trying to model a package as closely as possible to a set of requirements s/he has been given. Under this premise, 12% and 87% are substituted in the COMPASS model as the closest match possible to the desired values of 0% and 100%.

Table 8: Parameters for corrugated box recycled content comparison

Container Type	Recycled Content (%)	Recycled At EOL[1] (%)	Composted At EOL[1] (%)	Truck (km)	Rail (km)	Air (km)	Ship (km)
Corrugated Box - 1 use	0 (12) [2]	80	0	200	0	2,500	0
Corrugated Box - 1 use	25	80	0	200	0	2,500	0
Corrugated Box - 1 use	50	80	0	200	0	2,500	0
Corrugated Box - 1 use	100 (87) [2]	80	0	200	0	2,500	0

[1] EOL = End of Life.
[2] Values in parentheses are for COMPASS.

Greenhouse gas emissions reported by COMPASS, SimaPro, and GaBi for corrugated boxes with varying amounts of recycled fiber content are shown in Figure 19. Package Modeling had no means of varying recycled content of corrugated board, so it could not be included in this comparison. While there are differences in magnitudes of the emissions reported by the remaining three programs, the most striking result of the comparison is the complete reversal of ranking order between software. COMPASS and GaBi reported the lowest greenhouse gas emissions occurred when recycled content was small, meaning large virgin fiber content, and the highest emissions occurred when recycled content was large. SimaPro reported the exact opposite order, with highest emissions coinciding with the smallest recycled content. The implication of this discrepancy is that COMPASS and GaBi would drive a design toward using less recycled fiber content to reduce greenhouse gas emissions, while SimaPro would direct designs toward using more recycled fiber content to accomplish the same goal.

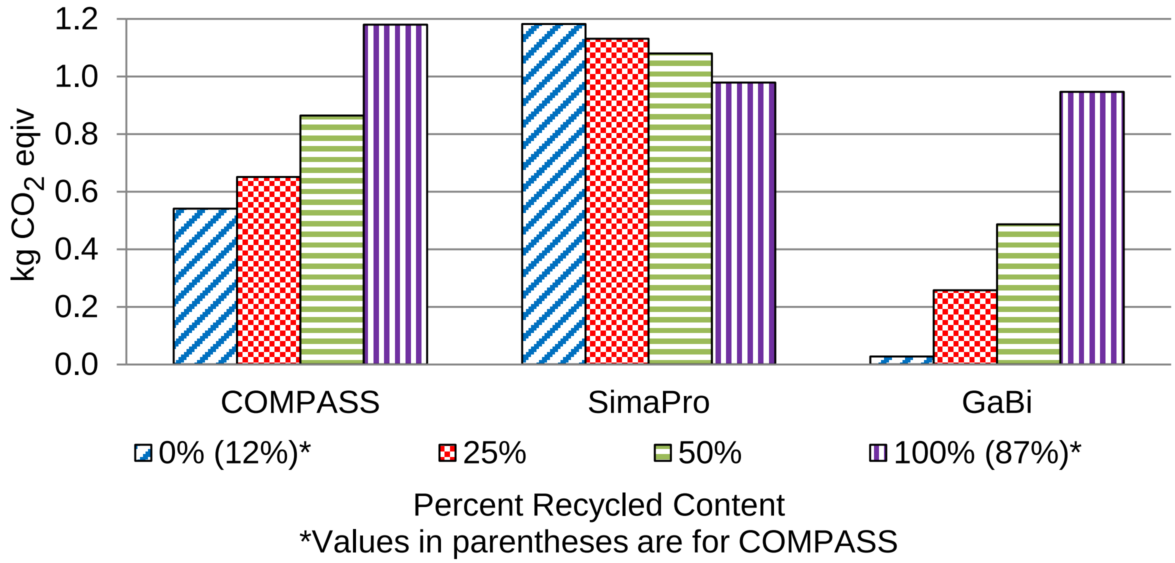


Figure 19: Greenhouse gas emissions for corrugated box comparison.

Fossil fuel/non-renewable energy results for the corrugated box recycled content comparison are given in Figure 20. All the software were in agreement regarding ranking order; there was no reversal for this impact category. There was some variation in the magnitudes of the reported emissions, with SimaPro ranging from 15% to 27% higher than COMPASS, and 28% to 35% higher than GaBi.

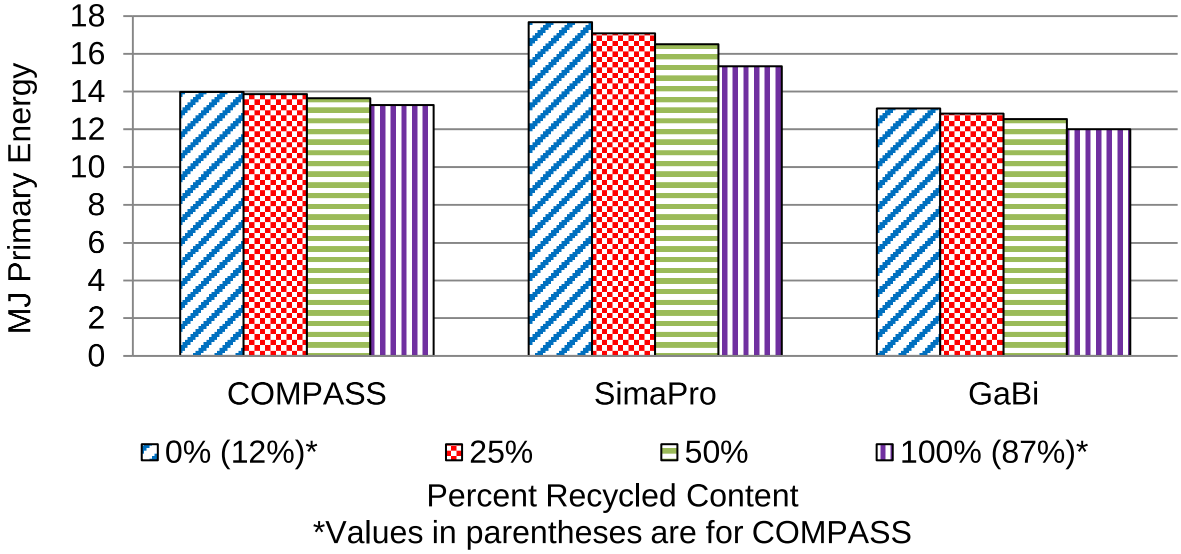


Figure 20: Fossil fuel/non-renewable energy for corrugated box comparison.

Figure 21 shows the results of the corrugated box recycled content comparison for eutrophication. The software agreed on the ranking order, however, there was noticeable disagreement in the reported magnitudes of emissions. SimaPro emission numbers ranged from 6% to 21% of those from COMPASS, and from 11% to 23% of the values from GaBi.

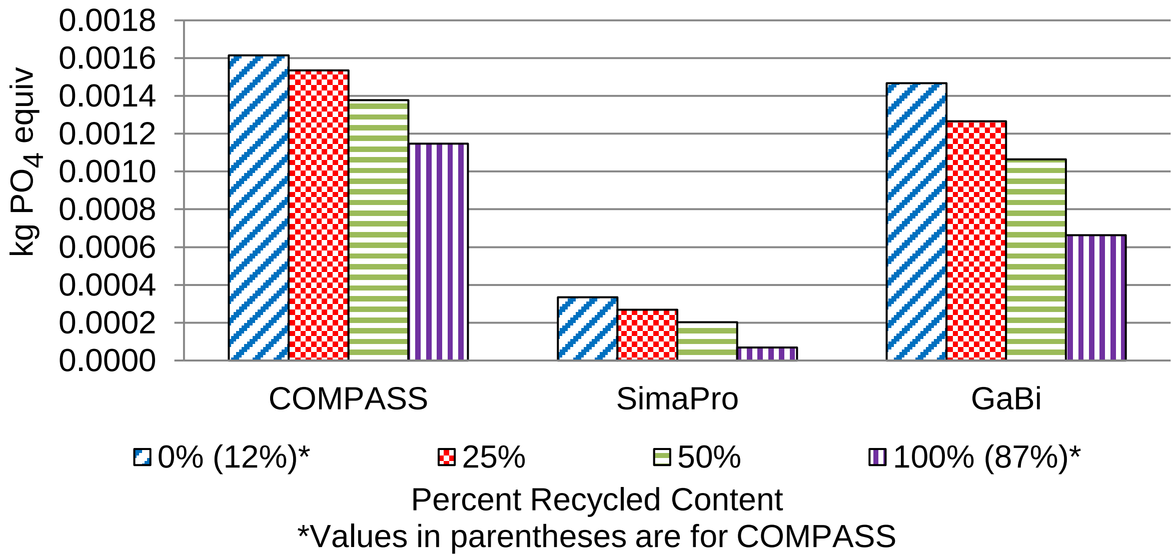
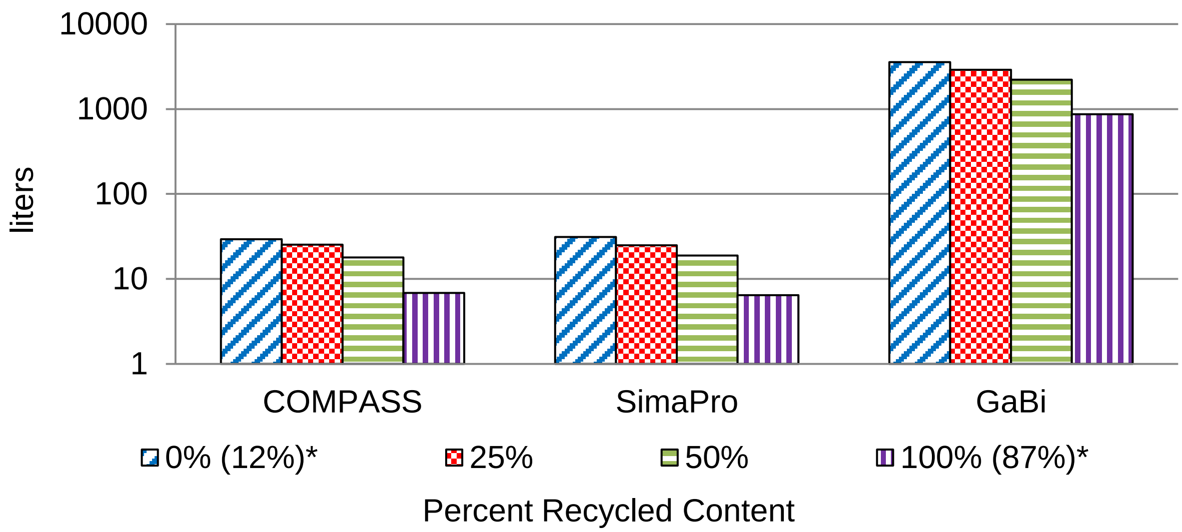


Figure 21: Eutrophication for corrugated box comparison.

Water depletion/consumption for the corrugated box recycled content comparison is given in Figure 22. Once again the vertical scale of the graph is logarithmic to accommodate GaBi consistently reporting water depletion more than two orders of magnitude greater than either COMPASS or SimaPro. All the software agreed on the ranking order for this impact category.



*Values in parentheses are for COMPASS

Figure 22: Water depletion/consumption for corrugated box comparison.

The effect of air and ship (ocean) transport on impact indicators was looked at using the corrugated box and PP crate reuse scenarios as the basis of comparison. As with the truck and rail comparisons earlier, Package Modeling was removed from consideration in these tests after it was discovered that the available transport distance selections had no effect on the greenhouse gas emissions reported by this software. Table 9 lists parameters for the air and ship transport comparisons. The only parameters varied in these tests were the transport distances, and only one mode of transport was varied at a time for a given packaging system.

Table 9: Parameters for air and ship transport comparisons

Container Type	Recycled Content (%)	Recycled At EOL[1] (%)	Composted At EOL[1] (%)	Truck [2] (km)	Rail [2] (km)	Air [2] (km)	Ship [2] (km)
Air							
Corrugated Box - 1 use	50	80	0	200	0	500	0
Corrugated Box - 1 use	50	80	0	200	0	2500	0
PP Crate - 10 uses	0	10	0	1,400	0	500	2,100
PP Crate - 10 uses	0	10	0	1,400	0	2,500	2,100
Ship							
PP Crate - 10 uses	0	10	0	1,400	0	2,500	500
PP Crate - 10 uses	0	10	0	1,400	0	2,500	2,100

[1] EOL = End of Life.

[2] Transport distances are on per use basis, except no return transport on last use.

Figure 23 gives the greenhouse gas emissions reported for the air transport comparisons. It can be seen in Figure 23A that the slopes of the plots for the corrugated box were all similar, ranging from 4.18×10^{-5} kg CO_2/km to 4.42×10^{-5} kg CO_2/km. Figure 23B shows the slopes of the plots for the PP crate had good agreement, ranging from 1.07×10^{-4} kg CO_2/km to 1.09×10^{-4} kg CO_2/km. The difference in slopes between the corrugated box versus the PP crate was due primarily to the difference in weight, the corrugated box was 0.7kg and the PP crate was 1.8kg. Figure 24 gives the greenhouse gas emissions reported for the ship (ocean) transport comparisons. The slopes of these plots were also very similar, ranging from 2.89×10^{-5} kg CO_2/km to 2.92×10^{-5} kg CO_2/km.

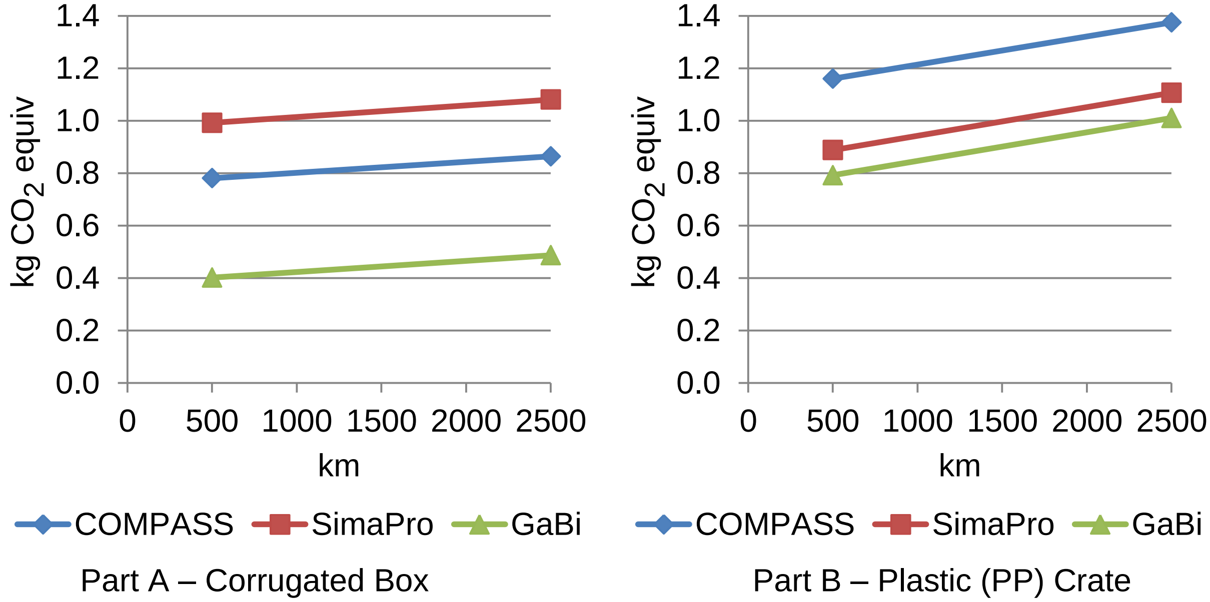


Figure 23: Greenhouse gas emissions versus air transport distance.

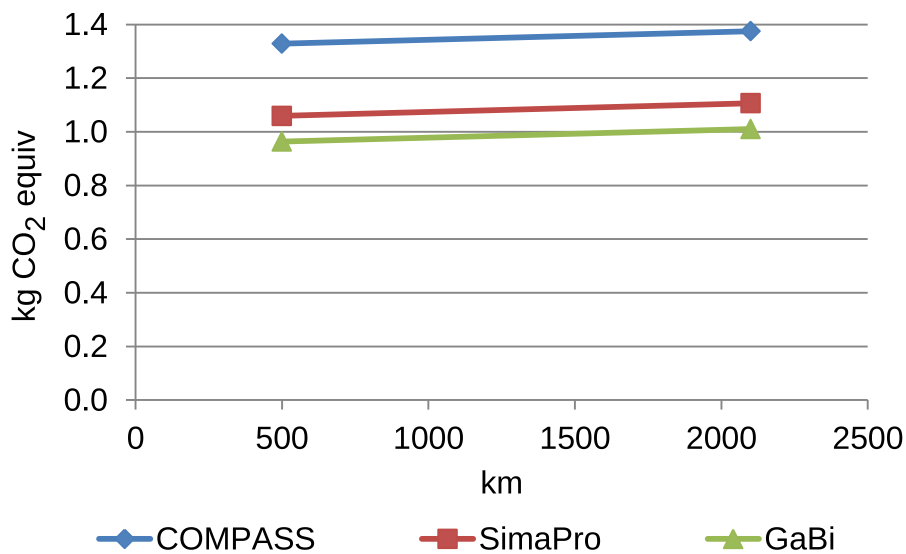


Figure 24: Greenhouse gas emissions for ship transport of plastic (PP) crate.

9.4 Comparison Summary for Package Systems

Significant discrepancies were found in the results reported by the various LCA software programs for the packaging system comparisons. Notable among them were the large magnitudes of water depletion/consumption reported by GaBi relative to COMPASS and SimaPro for every package system comparison, and the complete reversal of ranking order that COMPASS and GaBi had relative to SimaPro when looking at how greenhouse gas emissions varied with recycled content of a corrugated box. All four impact categories studied had variations in magnitudes and ranking order of results at some point in the comparisons, and all packaging systems studied had multiple inconsistencies in results between software programs.

In work contemporary to what was done here for package system comparisons, researchers from the Laboratory for Manufacture and Sustainability at the University of California, Berkeley, performed a study comparing various LCA software (Simon et al. 2012). Their approach involved doing detailed LCAs on 19 products in each of 5 LCA software programs: GaBi, SimaPro, COMPASS, Wal-Mart Sustainable Packaging Scorecard (Package Modeling), and Sustainable Minds. They came across many discrepancies in results, concluding “that each tool has advantages and opportunities for improvement” and recommending “users select the tool that best suits their needs.” While providing guidance in what could be expected in using the various LCA software, their published research ends at this point. In contrast, the package system comparisons in this paper represent the start of the research. With the presence of significant discrepancies in using the various software established, work then turned to finding an effective and efficient way to isolate and identify the causes of the discrepancies.

10. BASIC MATERIAL COMPARISONS

The package system comparisons, while providing a high level look at the consistency of results across several LCA software programs, do not directly address the question of where discrepancies in the results come from. Differences could be due to several things, including choices made when implementing system models. To reduce the human factor in the comparisons, and to provide a more consistent basis for further exploration of inconsistencies, another series of tests was performed using simple systems, ones that minimized the number of variables even more than the package system comparisons. To accomplish this, four basic packaging materials were selected: aluminum, corrugated board, glass, and PET. Each basic system studied consisted of obtaining and disposing of a single material. No additional materials, converting, distribution, or other processes were included. The functional unit for each system was 1 kilogram of the selected material.

It was decided to limit SimaPro and GaBi to using only files from the Ecoinvent 2.2 database, with every effort made to use the same database components for both software programs. The intent was to create a set of results that could be used to identify likely areas for further research in tracing any discrepancies down to the level of how specific input files from the database were handled. COMPASS was included in the basic material comparisons to see how a streamlined LCA program would stack up against the fully ISO 14040/14044 compliant programs, though the proprietary nature of the COMPASS dataset precluded it from being part of the effort to determine the causes of any differences. Package Modeling is designed for complete packages, not materials, so it was not included in these tests.

Consideration of using openLCA in the basic material comparisons faced a set of pros and cons. Pros included that openLCA could use the Ecoinvent database, as well as the Impact 2002+ and ReCiPe impact assessment methods. Cons included that openLCA was found to be a work in progress, documentation was poor, several operational problems were encountered, and the implementation of Impact 2002+ for openLCA would only produce endpoint values for many impact categories, not the desired midpoint values. Another issue was that no reference could be found to identify the versions of Impact 2002+ and ReCiPe that were available to use with openLCA. In the end, it was decided that some openLCA results would be compared with SimaPro separately for reference purposes, but openLCA was not included in the analysis of causes of differences in results.

The data for all graphs presented in this section can be found in Appendix H.

10.1 COMPASS, SimaPro, and GaBi Comparisons

The parameters used for the comparisons of the four basic materials are listed in Table 10. The greenhouse gas emissions reported for 1 kg of each of these materials are shown in Figure 25. All three software programs reported aluminum as having the highest emissions, and PET as the second highest. There was some variation in the magnitude of emissions reported for aluminum, with GaBi numbers being 19% greater than SimaPro and 21% greater than COMPASS. The magnitudes of emissions for PET varied less than 4% across the three software programs. The ranking order of corrugated board and glass did vary between the software. COMPASS had emissions for corrugated board 13% lower than the emissions for glass, while SimaPro reported corrugated board 9% higher than glass, and GaBi reported corrugated board 28% higher.

Table 10: Parameters for comparison of four basic materials

Basic Material	Functional Unit (kg)	Recycled Content (%)	Recycled At End of Life (%)	Landfill At End of Life (%)	Waste To Energy At End of Life (%)
Aluminum	1	50	67.9	32.1	0
Corrugated Board	1	50	76.4	12.9	10.7
Packaging Glass	1	55.5	63.8	36.2	0
Polyethylene Terephthalate (PET)	1	0	26.1	45.1	28.8

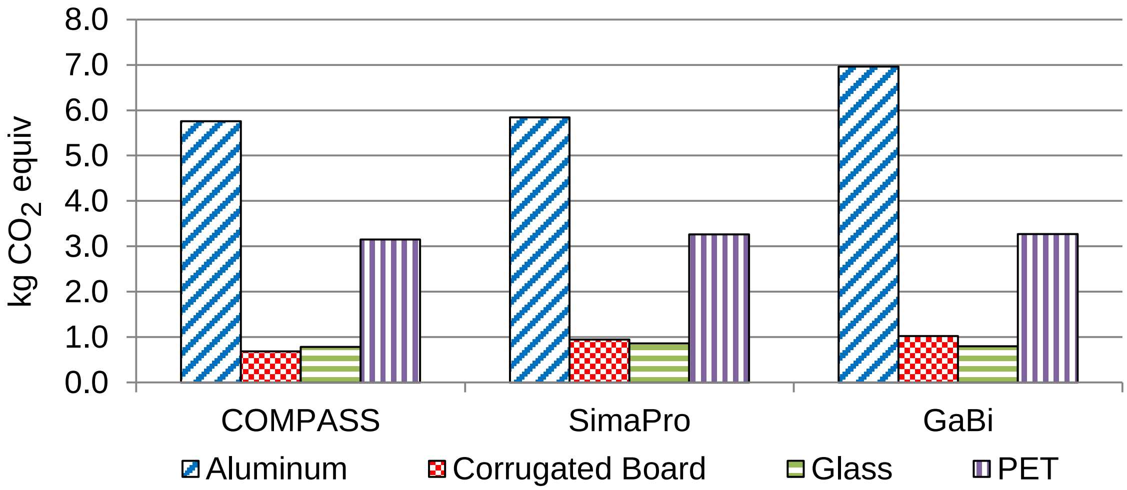


Figure 25: Greenhouse gas emissions for basic material comparison.

The comparison of fossil fuel/non-renewable energy requirements for the four basic materials is given in Figure 26. All software reported the same ranking order, with aluminum having the greatest energy requirements and corrugated board the lowest. There was some variation in reported magnitudes across the software, most notably that COMPASS reported lower magnitudes than either SimaPro or GaBi. COMPASS only reported fossil fuel use; it did not include nuclear energy, which may be a factor here.

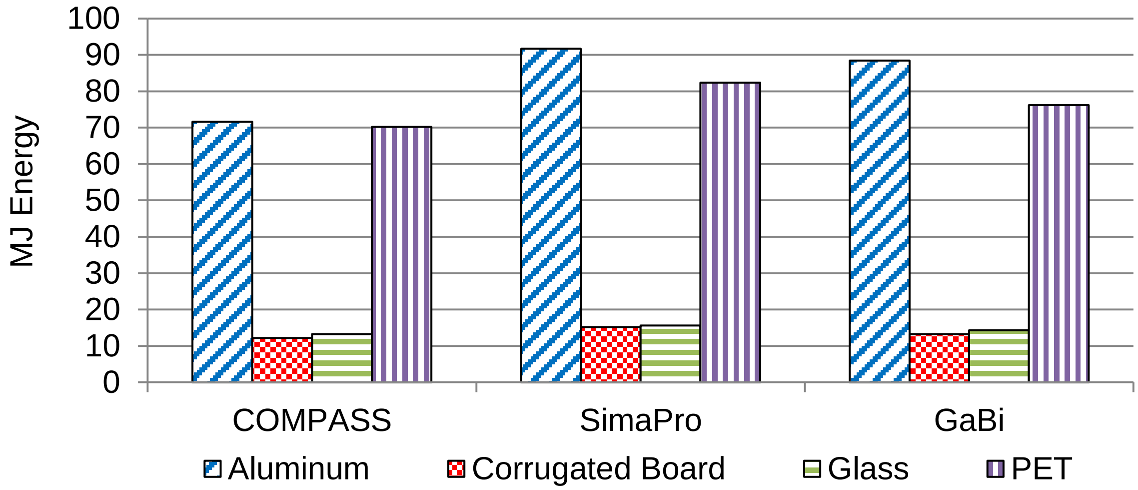


Figure 26: Fossil fuel/non-renewable energy for basic material comparison.

Eutrophication emissions for the basic materials are presented in Figure 27. SimaPro and GaBi had the same ranking order for the materials, placing aluminum as having the highest emissions and PET as second highest. COMPASS reversed the order of the first two, placing PET higher in emissions than aluminum. There were differences in magnitudes of emissions, with GaBi reporting emissions for aluminum that were a multiplication factor of 3.6 of those reported by COMPASS, and 6.1 of those reported by SimaPro. At the same time, GaBi reported emissions for the other materials that were only 52% to 67% of what COMPASS reported. Emissions reported by SimaPro were consistently lower than the other software, 10% to 27% of what COMPASS reported and 19% to 40% of what GaBi reported.

Water depletion/consumption results for the basic material comparisons are given in Figure 28. Note the use of a logarithmic vertical scale; this is due to GaBi reporting water use that was orders of magnitude greater than what was reported by either COMPASS or SimaPro. As an example, GaBi reported 165,000 liters of water associated with producing and disposing of 1kg of aluminum, compared to 32 liters reported by both COMPASS and SimaPro. This is similar to results for water depletion/consumption found in the comparisons of packaging systems; estimates from GaBi were consistently orders of magnitude higher than estimates from other software.

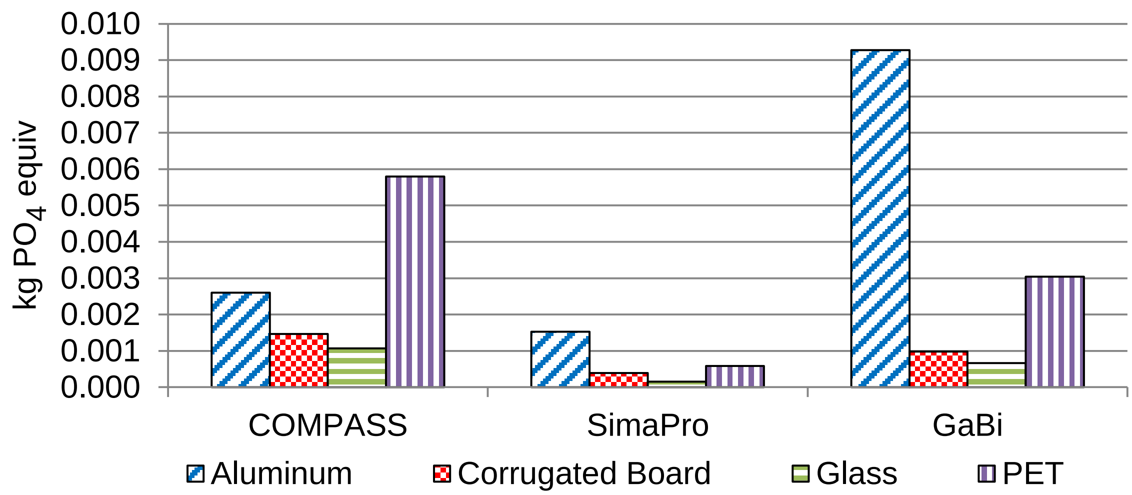


Figure 27: Eutrophication for basic material comparison.

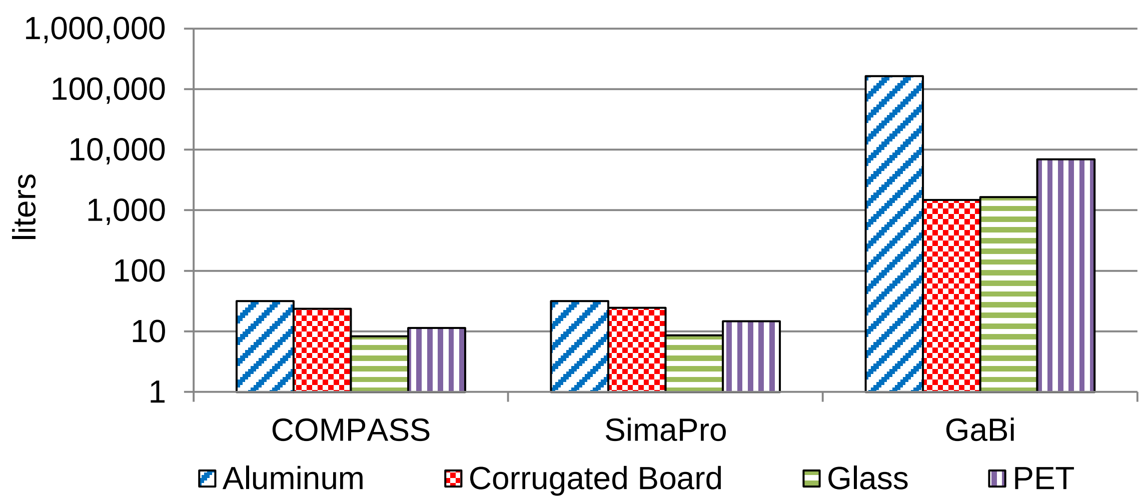


Figure 28: Water depletion/consumption for basic material comparison.

The effect recycled content can have on impact category indicators was explored for the basic materials using corrugated board. The parameters used for the recycled content comparison are listed in Table 11. The estimates of greenhouse gas emissions for varying recycled fiber content of corrugated board are given in Figure 29. COMPASS and GaBi had emissions increasing as recycled content increased, similar to what was found for the corrugated box in the packaging systems comparisons. Results from SimaPro had a nearly flat response to varying recycled content, clearly disagreeing with COMPASS and GaBi, but somewhat different than what was found for the corrugated box in the packaging systems comparison. The flat response effect was traced to energy usage data coming from European datasets for the basic materials, while energy data for comparisons of packaging systems came from U.S. datasets.

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Table 11: Parameters for recycled content comparison of basic corrugated board.

Basic Material	Functional Unit (kg)	Recycled Content (%)	Recycled At End of Life (%)	Landfill At End of Life (%)	Waste To Energy At End of Life (%)
Corrugated Board	1	12	76.4	12.9	10.7
Corrugated Board	1	50	76.4	12.9	10.7
Corrugated Board	1	87	76.4	12.9	10.7

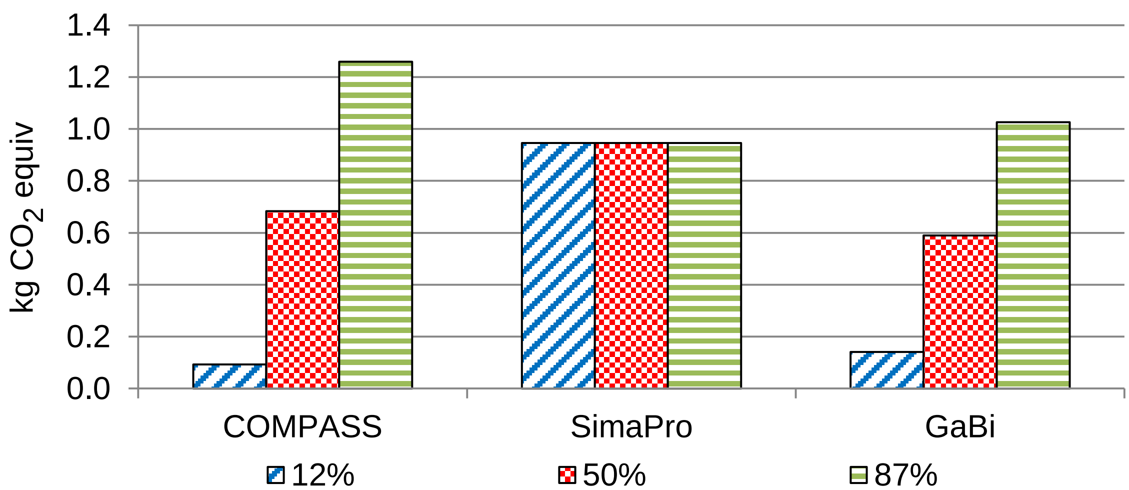

Figure 29: Greenhouse gas emissions for basic corrugated board.

Results for fossil fuel/non-renewable energy requirements when varying recycled content of corrugated board are given in Figure 30. COMPASS and GaBi reversed ranking order, with COMPASS having energy requirements increasing as recycled content increased, and GaBi having energy requirements decreasing. SimaPro had a flat response, keeping energy use nearly constant as recycled fiber content varied. SimaPro reported magnitudes of energy usage that were 6% to 14% higher than GaBi, and 15% to 36% higher than COMPASS.

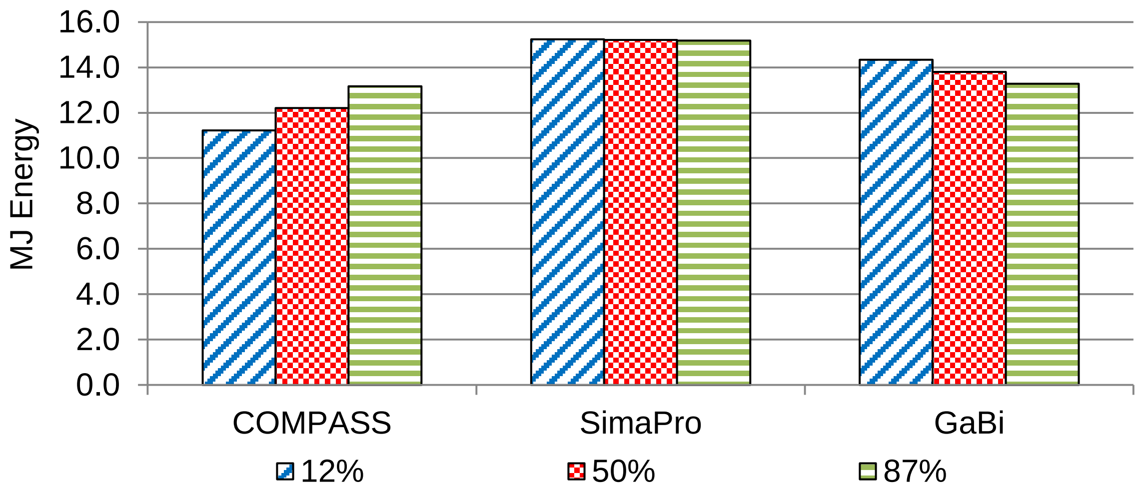

Figure 30: Fossil fuel/non-renewable energy for basic corrugated board.

Figure 31 covers the effect of varying recycled fiber content on eutrophication emissions for corrugated board. While all three software programs had the same ranking order, with emissions decreasing as recycled content increased, there are noticeable differences in the magnitudes of emissions reported by SimaPro versus the other software. The values from SimaPro are 20% to 32% of those from COMPASS, and 24% to 32% of the values obtained from GaBi.

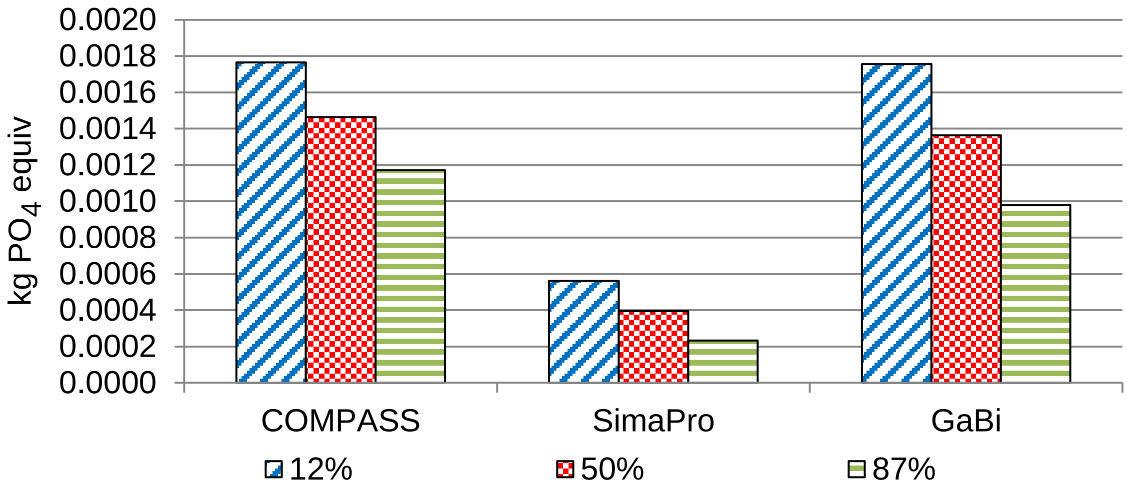

Figure 31: Eutrophication for basic corrugated board.

Water depletion/consumption results versus recycled fiber content for corrugated board are shown in Figure 32. Note that the vertical scale of the graph is logarithmic, as once again GaBi reported significantly higher water depletion than COMPASS and SimaPro. GaBi had water consumption ranging from 1,480 liters to 4,080 liters, while COMPASS ranged from 7.7 liters to 40.2 liters and SimaPro ranged from 12.5 liters to 37.0 liters. All three software programs reported the same ranking order, with water depletion decreasing as recycled fiber content increased.

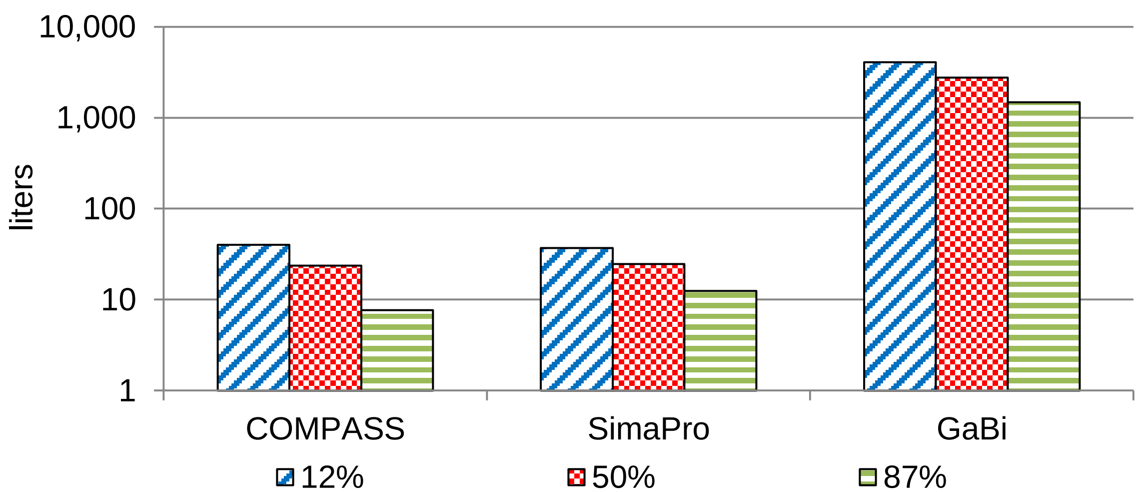

Figure 32: Water depletion/consumption for basic corrugated board.

10.2 SimaPro and openLCA Comparisons

The SimaPro and openLCA basic material comparisons used the same test parameters listed in Table 10 of section 10.1 for the COMPASS, SimaPro, and GaBi comparisons. The difference is that some of the impact categories are expressed in points rather than equivalent amounts of reference substances. Figure 33 shows the comparisons for greenhouse gas emissions. The ranking orders from the programs were the same, but SimaPro did have corrugated board and glass more evenly matched than openLCA. SimaPro results were consistently higher in points than openLCA. Similar results for non-renewable energy can be seen in Figure 34.

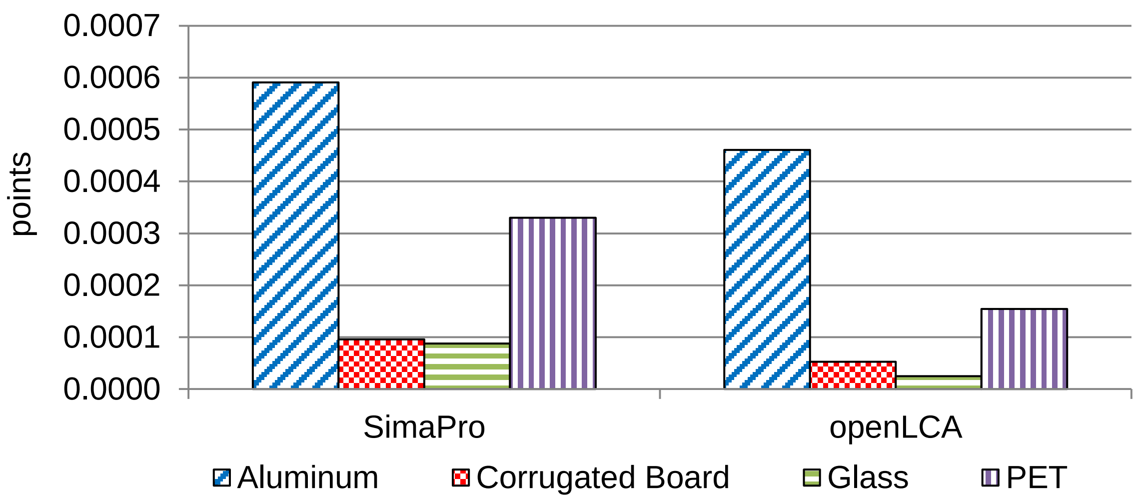

Figure 33: openLCA greenhouse gas emissions for basic materials.

Eutrophication results are shown in Figure 35. SimaPro again had higher magnitudes, with openLCA values only 17% to 39% those of SimaPro. There was a slight change in ranking order of aluminum and corrugated board between the two software programs, with SimaPro placing emissions for aluminum 4% higher than emissions for corrugated board, while openLCA reversed the order with corrugated board 15% higher than aluminum.

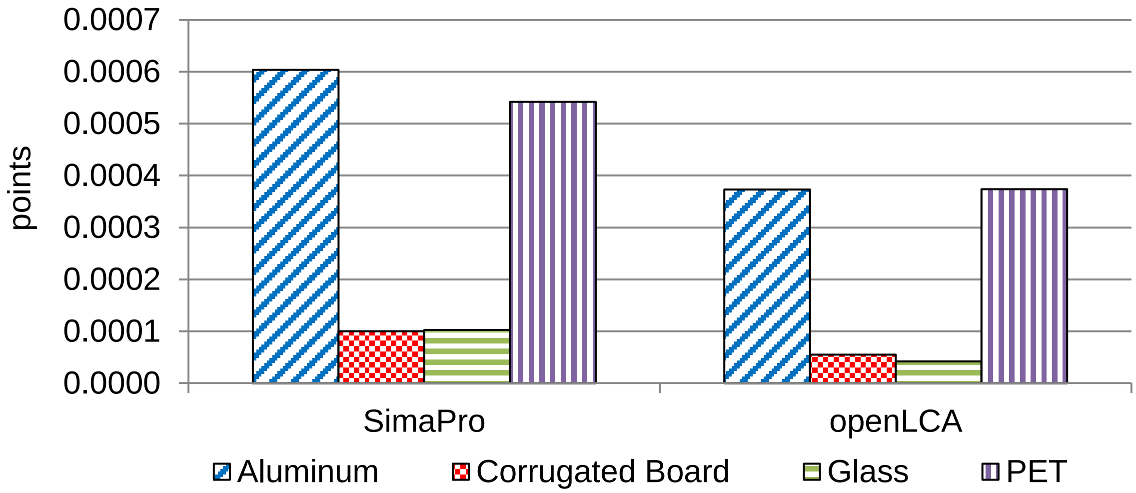

Figure 34: openLCA non-renewable energy for basic materials.

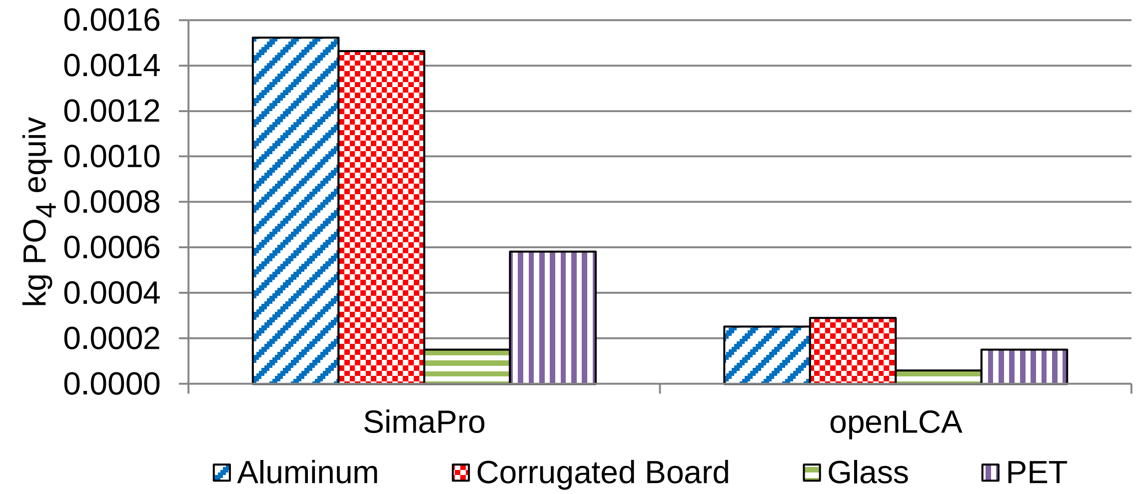

Figure 35: openLCA eutrophication for basic materials.

Water depletion results are given in Figure 36. The vertical scale is logarithmic, this time due to the significantly smaller amount of water depletion reported by openLCA for glass. SimaPro had 9.0 liters of water being depleted for 1 kg of glass, while openLCA placed the amount at 0.08 liters. There was a reversal of ranking order for aluminum and corrugated board; SimaPro reported aluminum needed 34% more water than corrugated board, while openLCA indicated aluminum used 25% less water.

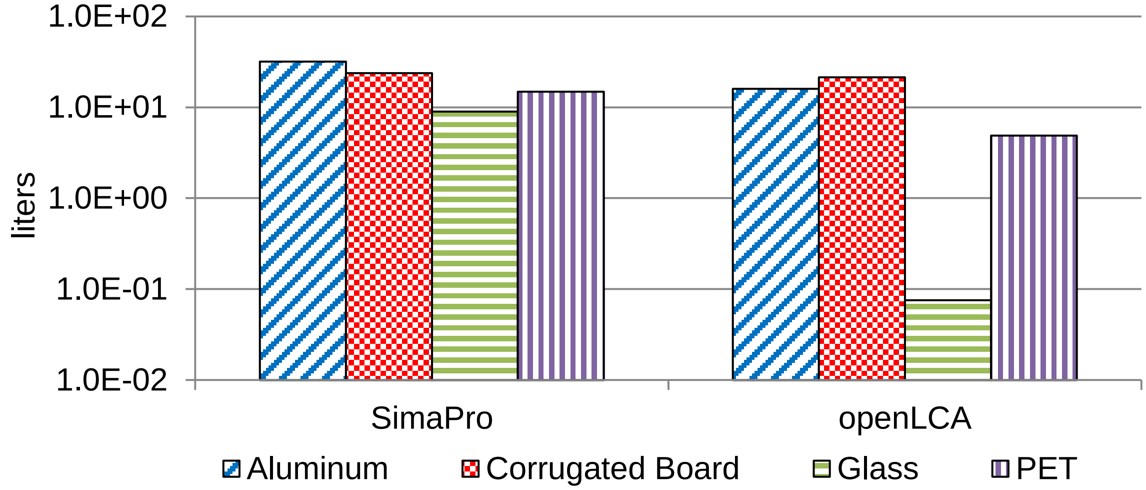

Figure 36: openLCA water depletion for basic materials.

Tests looking at the effects varying recycled content had on impact assessment indicators were done with openLCA, similar to the comparisons for COMPASS, SimaPro, and GaBi reported in section 10.1. The same set of parameters listed in Table 11 for the earlier tests were also used with openLCA. Greenhouse gas emissions for these openLCA tests are shown in Figure 37, along with results from SimaPro for comparison. The emissions estimates from openLCA increased slightly as the recycled fiber content increased, while SimaPro estimates remain flat. The magnitudes of openLCA estimates were 50% to 60% of the estimates from SimaPro. Similar results were obtained for non-renewable energy, shown in Figure 38.

Eutrophication estimates, shown in Figure 39, have values reported by openLCA that are 11% to 26% of those reported by SimaPro. The two programs did provide the same ranking order, with emissions going down as recycled content increased. Ranking order for water depletion was also the same between the two programs, as can be seen in Figure 40.

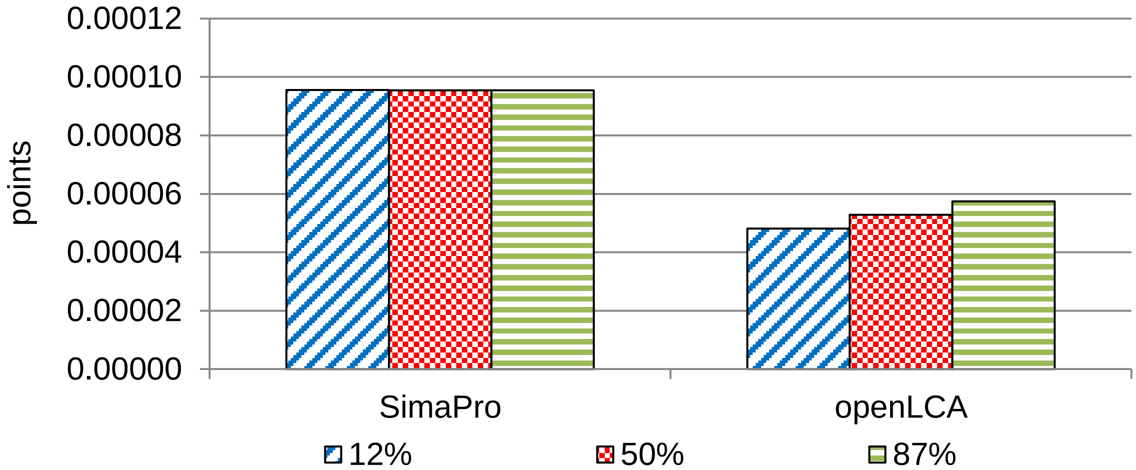

Figure 37: openLCA greenhouse gas emissions for corrugated board.

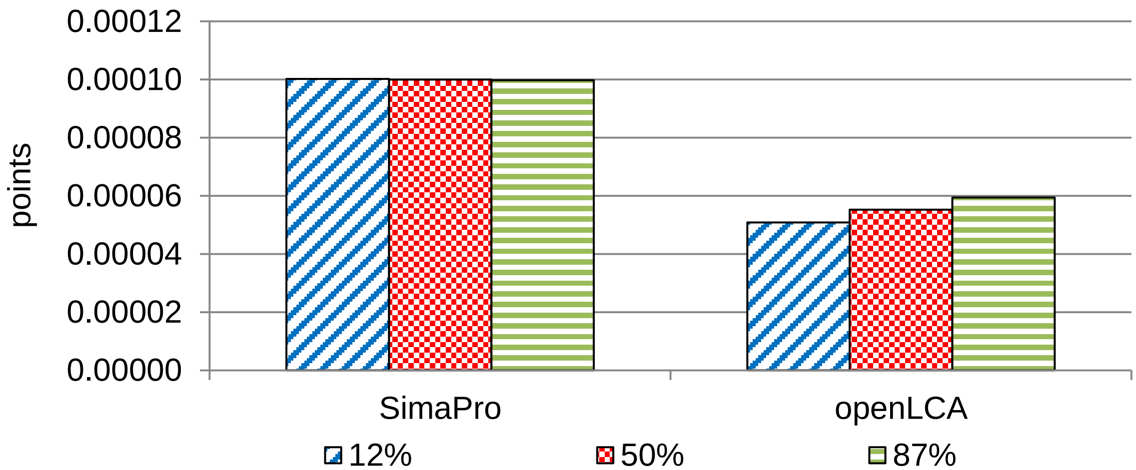

Figure 38: openLCA non-renewable energy for corrugated board.

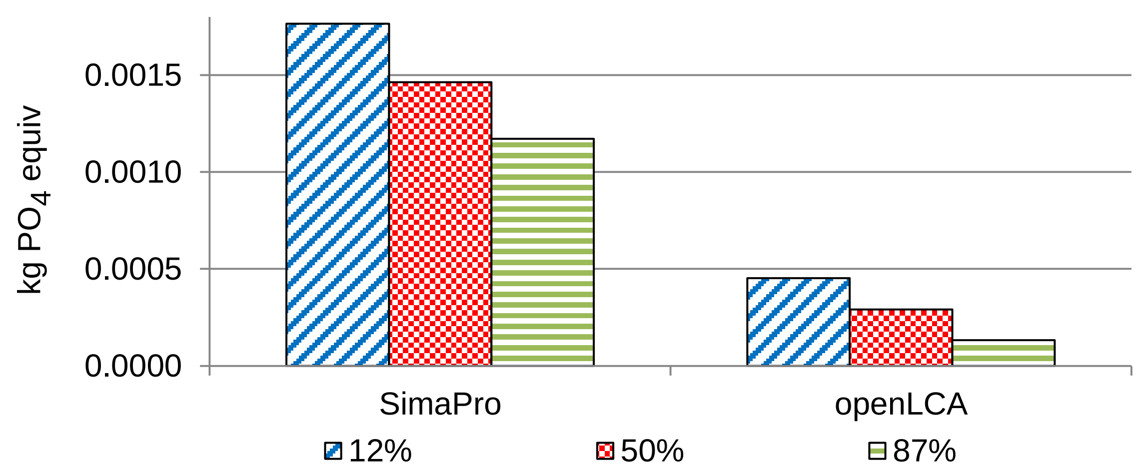

Figure 39: openLCA eutrophication for corrugated board.

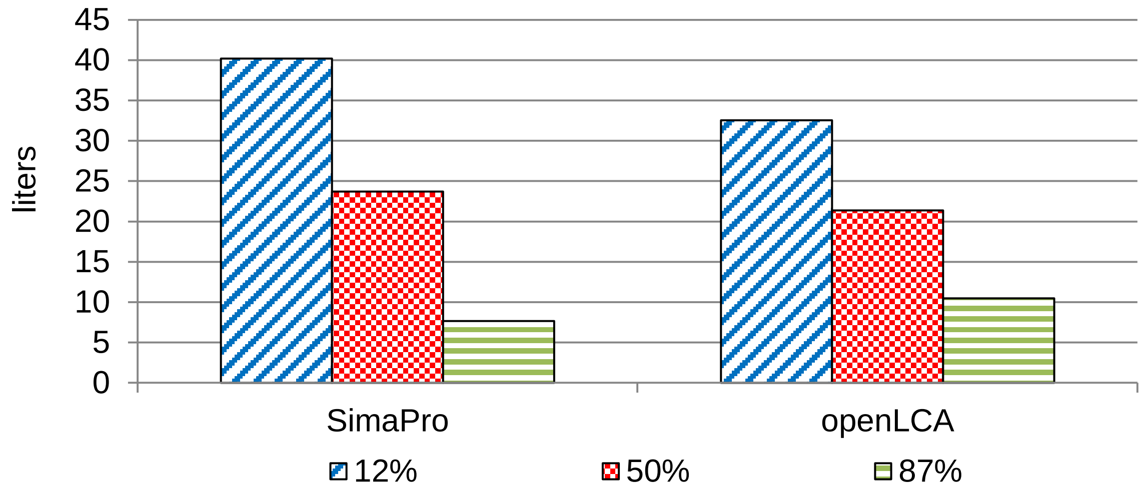

Figure 40: openLCA water depletion for corrugated board.

10.3 Other Impact Categories

Up to this point the comparisons between software were limited to four impact categories due to the inclusion of COMPASS. However, additional comparisons can be made between SimaPro and GaBi. Impact 2002+ and ReCiPe impact assessment methods have been used with SimaPro and GaBi throughout this paper. Impact 2002+ has 15 different midpoint impact categories, and ReCiPe has 18. Therefore, the question of how many of these impact categories might show significant differences for the basic materials being considered was examined.

Table 12 shows all Impact 2002+ and ReCiPe impact category results for aluminum as used in the earlier basic material comparisons. Rows that are highlighted in **bold text** indicate impact categories where the result from one software program is at least twice the result from the other. This factor of 2 equates to a difference value in Table 12 of either less than or equal to -50%, or greater than or equal to 100%, where % Difference = 100% x (GaBi - SimaPro) / SimaPro. It can be seen that 7 of the Impact 2002+ categories fit this criteria for aluminum, and 5 categories from ReCiPe also fit.

Table 13 shows that 9 Impact 2002+ categories fit the factor of 2 criteria for corrugated board, while 4 categories fit for ReCiPe, with marine eutrophication falling out of the group. The same 9 categories for Impact 2002+ fit the factor of 2 criteria for glass as shown in Table 14; however, marine eutrophication replaced terrestrial ecotoxicity for the ReCiPe group. For PET, as shown in Table 15, the same 9 Impact 2002+ categories fit the criteria, and the number of categories that fit the criteria for ReCiPe stays at 4, though terrestrial ecotoxicity replaced marine eutrophication.

Table 12: Aluminum impact assessment data, 50% recycled content

Impact Category	Unit	SimaPro	GaBi	% Difference[1]
Impact 2002+				
Aquatic acidification	kg SO2 eq	3.013E-02	2.225E-02	-26
Aquatic ecotoxicity	**kg TEG water**	**1.217E+03**	**1.230E+06**	**100,960**
Aquatic eutrophication	**kg PO4 P-lim**	**1.523E-03**	**9.270E-03**	**509**
Carcinogens	**kg C2H3Cl eq**	**3.040E-01**	**9.620E-02**	**-68**
Global warming	kg CO2 eq	5.845E+00	6.959E+00	19
Ionizing radiation	Bq C-14 eq	1.790E+02	1.708E+02	-5
Land occupation	**m2org.arable**	**2.701E-02**	**3.216E-06**	**-100**
Mineral extraction	MJ surplus	1.416E+00	1.779E+00	26
Non-carcinogens	**kg C2H3Cl eq**	**3.645E-02**	**1.290E+00**	**3,439**
Non-renewable energy	MJ primary	9.169E+01	8.839E+01	-4
Ozone layer depletion	**kg CFC-11 eq**	**3.181E-08**	**4.430E-07**	**1,293**
Photochemical oxidation - Respiratory organics	**kg C2H4 eq**	**1.477E-04**	**1.126E-03**	**662**
Respiratory effects - Respiratory inorganics	kg PM2.5 eq	5.735E-03	7.821E-03	36
Terrestrial acid/nutrification	kg SO2 eq	8.596E-02	8.598E-02	0
Terrestrial ecotoxicity	kg TEG soil	7.669E+01	1.451E+02	89
ReCiPe				
Agricultural land occupation	m^2a	8.306E-02	8.306E-02	0
Climate change	kg CO2 eq	6.812E+00	6.812E+00	0
Fossil depletion	kg oil eq	1.752E+00	1.752E+00	0
Freshwater ecotoxicity	kg 1,4-DB eq	7.355E-02	6.239E-02	-15
Freshwater eutrophication	kg P eq	3.059E-03	3.059E-03	0
Human toxicity	**kg 1,4-DB eq**	**3.218E+00**	**1.111E+00**	**-65**

Table 12 (cont'd)

Ionizing radiation	**kg U235 eq**	**1.705E+00**	**5.637E-01**	**-67**
Marine ecotoxicity	kg 1,4-DB eq	7.843E-02	6.096E-02	-22
Marine eutrophication	**kg N eq**	**1.056E-03**	**4.979E-03**	**371**
Metal depletion	kg Fe eq	3.964E-01	3.925E-01	-1
Natural land transformation	m^2	1.243E-03	1.243E-03	0
Ozone depletion	kg CFC-11 eq	5.988E-07	5.988E-07	0
Particulate matter formation	kg PM10 eq	1.319E-02	1.319E-02	0
Photochemical oxidant formation	kg NMVOC	1.703E-02	1.703E-02	0
Terrestrial acidification	kg SO2 eq	2.787E-02	2.787E-02	0
Terrestrial ecotoxicity	**kg 1,4-DB eq**	**7.209E-04**	**1.917E-04**	**-73**
Urban land occupation	m^2a	3.806E-02	3.806E-02	0
Water depletion	$\mathbf{m^3}$	**3.174E-02**	**1.651E+02**	**520,108**

[1] % Difference = 100% x (GaBi - SimaPro) / SimaPro

[2] Rows in **bold text** have at least a factor of 2 difference between SimaPro and GaBi.

Table 13: Corrugated board impact assessment data, 50% recycled content

Impact Category	Unit	SimaPro	GaBi	% Difference[1]
Impact 2002+				
Aquatic acidification	kg SO2 eq	4.244E-03	2.341E-03	-45
Aquatic ecotoxicity	**kg TEG water**	**1.701E+02**	**3.938E+03**	**2,215**
Aquatic eutrophication	**kg PO4 P-lim**	**3.955E-04**	**1.363E-03**	**245**
Carcinogens	**kg C2H3Cl eq**	**2.288E-02**	**5.583E-03**	**-76**
Global warming	kg CO2 eq	9.455E-01	5.892E-01	-38
Ionizing radiation	Bq C-14 eq	1.927E+01	1.838E+01	-5
Land occupation	**m2org.arable**	**4.154E-01**	**3.336E-05**	**-100**
Mineral extraction	**MJ surplus**	**1.546E-02**	**1.341E-01**	**768**
Non-carcinogens	**kg C2H3Cl eq**	**6.085E-03**	**6.505E-02**	**969**
Non-renewable energy	MJ primary	1.520E+01	1.380E+01	-9
Ozone layer depletion	**kg CFC-11 eq**	**5.042E-09**	**8.844E-08**	**1,654**
Photochemical oxidation - Respiratory organics	**kg C2H4 eq**	**5.769E-05**	**3.726E-04**	**546**
Respiratory effects - Respiratory inorganics	kg PM2.5 eq	8.385E-04	9.012E-04	7
Terrestrial acid/nutrification	kg SO2 eq	1.881E-02	1.886E-02	0
Terrestrial ecotoxicity	**kg TEG soil**	**4.826E+00**	**2.970E+01**	**515**

Table 13 (cont'd)

ReCiPe				
Agricultural land occupation	m^2a	3.133E+00	3.133E+00	0
Climate change	kg CO2 eq	1.142E+00	1.116E+00	-2
Fossil depletion	kg oil eq	3.091E-01	3.090E-01	0
Freshwater ecotoxicity	kg 1,4-DB eq	1.021E-02	8.118E-03	-21
Freshwater eutrophication	kg P eq	4.500E-04	4.491E-04	0
Human toxicity	**kg 1,4-DB eq**	**4.561E-01**	**8.425E-02**	**-82**
Ionizing radiation	**kg U235 eq**	**1.837E-01**	**6.179E-02**	**-66**
Marine ecotoxicity	kg 1,4-DB eq	8.375E-03	5.806E-03	-31
Marine eutrophication	kg N eq	1.300E-03	2.153E-03	66
Metal depletion	kg Fe eq	3.946E-02	3.907E-02	-1
Natural land transformation	m^2	5.513E-04	5.523E-04	0
Ozone depletion	kg CFC-11 eq	8.860E-08	8.857E-08	0
Particulate matter formation	kg PM10 eq	1.458E-03	1.460E-03	0
Photochemical oxidant formation	kg NMVOC	3.660E-03	3.656E-03	0
Terrestrial acidification	kg SO2 eq	3.758E-03	3.761E-03	0
Terrestrial ecotoxicity	**kg 1,4-DB eq**	**2.899E-04**	**1.041E-04**	**-64**
Urban land occupation	m^2a	5.432E-02	5.424E-02	0
Water depletion	**m^3**	**2.462E-02**	**2.763E+00**	**11,123**

[1] % Difference = 100% x (GaBi - SimaPro) / SimaPro

[2] Rows in **bold text** have at least a factor of 2 difference between SimaPro and GaBi.

Table 14: Glass impact assessment data, 55.5% recycled content

Impact Category	Unit	SimaPro	GaBi	% Difference[1]
Impact 2002+				
Aquatic acidification	kg SO2 eq	7.771E-03	5.470E-03	-30
Aquatic ecotoxicity	**kg TEG water**	**1.309E+02**	**1.963E+04**	**14,896**
Aquatic eutrophication	**kg PO4 P-lim**	**1.494E-04**	**6.620E-04**	**343**
Carcinogens	**kg C2H3Cl eq**	**1.514E-02**	**5.632E-03**	**-63**
Global warming	kg CO2 eq	8.655E-01	8.020E-01	-7
Ionizing radiation	Bq C-14 eq	1.554E+01	1.482E+01	-5
Land occupation	**m2org.arable**	**3.126E-02**	**2.640E-06**	**-100**
Mineral extraction	**MJ surplus**	**6.366E-03**	**5.229E-02**	**721**
Non-carcinogens	**kg C2H3Cl eq**	**9.931E-03**	**8.118E-02**	**717**
Non-renewable energy	MJ primary	1.558E+01	1.434E+01	-8

Table 14 (cont'd)

Ozone layer depletion	**kg CFC-11 eq**	**6.444E-09**	**1.005E-07**	**1,460**
Photochemical oxidation - Respiratory organics	**kg C2H4 eq**	**2.435E-05**	**2.379E-04**	**877**
Respiratory effects - Respiratory inorganics	kg PM2.5 eq	1.181E-03	1.227E-03	4
Terrestrial acid/nutrification	kg SO2 eq	2.433E-02	2.434E-02	0
Terrestrial ecotoxicity	**kg TEG soil**	**3.898E+00**	**8.731E+00**	**124**
ReCiPe				
Agricultural land occupation	m^2a	2.516E-01	2.516E-01	0
Climate change	kg CO2 eq	8.985E-01	8.985E-01	0
Fossil depletion	kg oil eq	3.267E-01	3.267E-01	0
Freshwater ecotoxicity	kg 1,4-DB eq	5.612E-03	4.462E-03	-21
Freshwater eutrophication	kg P eq	2.236E-04	2.183E-04	-2
Human toxicity	**kg 1,4-DB eq**	**3.637E-01**	**1.438E-01**	**-60**
Ionizing radiation	**kg U235 eq**	**1.480E-01**	**5.050E-02**	**-66**
Marine ecotoxicity	kg 1,4-DB eq	5.724E-03	4.362E-03	-24
Marine eutrophication	**kg N eq**	**2.267E-04**	**1.372E-03**	**505**
Metal depletion	kg Fe eq	2.602E-02	2.567E-02	-1
Natural land transformation	m^2	2.833E-04	2.833E-04	0
Ozone depletion	kg CFC-11 eq	1.006E-07	1.006E-07	0
Particulate matter formation	kg PM10 eq	2.191E-03	2.191E-03	0
Photochemical oxidant formation	kg NMVOC	4.121E-03	4.120E-03	0
Terrestrial acidification	kg SO_2 eq	7.004E-03	7.004E-03	0
Terrestrial ecotoxicity	kg 1,4-DB eq	2.627E-04	2.374E-04	-10
Urban land occupation	m^2a	9.111E-03	9.111E-03	0
Water depletion	**m^3**	**8.641E-03**	**1.652E+00**	**19,021**

[1] % Difference = 100% x (GaBi - SimaPro) / SimaPro

[2] Rows in **bold text** have at least a factor of 2 difference between SimaPro and GaBi.

Table 15: PET impact assessment data, 0% recycled content

Impact Category	Unit	SimaPro	GaBi	% Difference[1]
Impact 2002+				
Aquatic acidification	kg SO2 eq	1.054E-02	7.063E-03	-33
Aquatic ecotoxicity	**kg TEG water**	**5.689E+02**	**1.003E+04**	**1,663**
Aquatic eutrophication	**kg PO4 P-lim**	**5.818E-04**	**3.040E-03**	**423**

Table 15 (cont'd)

Carcinogens	**kg C2H3Cl eq**	**1.307E+00**	**1.616E-02**	**-99**
Global warming	kg CO2 eq	3.266E+00	3.270E+00	0
Ionizing radiation	Bq C-14 eq	6.499E+01	6.195E+01	-5
Land occupation	**m2org.arable**	**1.232E-02**	**1.297E-06**	**-100**
Mineral extraction	**MJ surplus**	**6.255E-02**	**5.740E-01**	**818**
Non-carcinogens	**kg C2H3Cl eq**	**2.665E-02**	**2.321E-01**	**771**
Non-renewable energy	MJ primary	8.238E+01	7.618E+01	-8
Ozone layer depletion	**kg CFC-11 eq**	**1.134E-08**	**1.448E-07**	**1,177**
Photochemical oxidation - Respiratory organics	**kg C2H4 eq**	**1.527E-04**	**1.922E-03**	**1,158**
Respiratory effects - Respiratory inorganics	kg PM2.5 eq	1.702E-03	1.922E-03	13
Terrestrial acid/nutrification	kg SO2 eq	3.472E-02	3.473E-02	0
Terrestrial ecotoxicity	**kg TEG soil**	**8.800E+00**	**1.944E+01**	**121**
ReCiPe				
Agricultural land occupation	m^2a	5.022E-02	5.022E-02	0
Climate change	kg CO2 eq	3.514E+00	3.514E+00	0
Fossil depletion	kg oil eq	1.745E+00	1.745E+00	0
Freshwater ecotoxicity	kg 1,4-DB eq	4.449E-02	4.047E-02	-9
Freshwater eutrophication	kg P eq	1.003E-03	1.003E-03	0
Human toxicity	**kg 1,4-DB eq**	**1.133E+00**	**3.869E-01**	**-66**
Ionizing radiation	**kg U235 eq**	**6.185E-01**	**2.115E-01**	**-66**
Marine ecotoxicity	kg 1,4-DB eq	4.416E-02	3.803E-02	-14
Marine eutrophication	kg N eq	3.317E-03	3.133E-03	-6
Metal depletion	kg Fe eq	2.025E-01	2.007E-01	-1
Natural land transformation	m^2	3.649E-04	3.649E-04	0
Ozone depletion	kg CFC-11 eq	1.450E-07	1.450E-07	0
Particulate matter formation	kg PM10 eq	3.409E-03	3.409E-03	0
Photochemical oxidant formation	kg NMVOC	8.445E-03	8.299E-03	-2
Terrestrial acidification	kg SO_2 eq	9.719E-03	9.719E-03	0
Terrestrial ecotoxicity	**kg 1,4-DB eq**	**2.725E-04**	**1.308E-04**	**-52**
Urban land occupation	m^2a	1.347E-02	1.347E-02	0
Water depletion	**m^3**	**1.476E-02**	**6.990E+00**	**47,257**

[1] % Difference = 100% x (GaBi - SimaPro) / SimaPro

[2] Rows in **bold text** have at least a factor of 2 difference between SimaPro and GaBi.

10.4 Comparison Summary For Basic Materials

Even with the test scenarios reduced to nothing more than the creation and disposal of a basic packaging material, significant differences were found in the results provided by the LCA programs being studied. Notable among these differences were the large magnitudes of water depletion/consumption reported by GaBi, and the ranking orders reported by the various software for greenhouse gas emissions when varying recycled fiber content of corrugated board. These results were similar to what was found in the higher level packaging systems comparisons, indicating that at least some of the issues causing differences in the higher level comparisons are likely rooted in how the basic materials are handled. Combined with the sheer number of discrepancies found in the limited testing done so far, there was reason for concern that the choice of LCA software may affect the results obtained. This raised the question of why are these discrepancies happening? Could it be firmly established that the issues encountered were truly with the software, and not how the systems were implemented in the software? This was the next challenge to be addressed.

11. UNDERLYING CAUSES OF DISSIMILAR RESULTS

Having established that using the same impact assessment methods in SimaPro and GaBi can produce dissimilar results in several impact assessment categories, attention now turned to establishing why this was happening. The information presented so far was not sufficient to rule out any cause. Human error in modeling, software errors in calculations, implementation differences for the assessment methods, or some issue not yet thought of were all possibilities. The task at hand was to isolate the causes in order to ascertain why the differences were occurring.

SimaPro and GaBi both allow users to view life cycle inventories (LCI) down to a basic substance level, covering all the inputs and emissions that are associated with a system. Both software programs also provide a means to see the contribution each substance makes to an impact category indicator, and the characterization factors used to convert inputs and emissions to impact indicators. These capabilities, when used in conjunction with the Ecoinvent database and basic material models of the earlier tests, allow common inputs to be traced through to impact indicators, providing a basis for comparing what is happening in the software. In practice, things are made difficult by SimaPro and GaBi categorizing inputs in different manners. SimaPro appears to map Ecoinvent data on a one-to-one basis, while GaBi may combine items. For example, in one test it was found that SimaPro had 4 varieties of copper ore as input, while GaBi combined the mass of these 4 ores into a single entry for copper. Other differences in the way inputs are handled between the two software programs also exist.

SimaPro maps information from the Ecoinvent database into compartments such as air, raw, soil, and water. Air, soil, and water generally contain emissions, while the “raw” compartment covers raw materials used in production, including things like ore mined from the ground. Each of these compartments can be divided into sub-compartments. For example; groundwater, groundwater long-term, lake, ocean, and river are all sub-compartments of water. A given emission to water can be assigned to a sub-compartment, or it can be allocated to the general compartment, in which case it is referred to as unassigned. A substance or emission can have a unique characterization factor assigned to it for each compartment and sub-compartment. If a substance does not have a characterization factor assigned to a sub-compartment, then the software defaults to using the characterization factor of the substance assigned for the general compartment. Zero is considered a valid characterization factor for a substance in a SimaPro sub-compartment, and in this case there is no defaulting to the compartment value. If a substance has no characterization factors assigned at all, either in the general compartment or the sub-compartments, then zero is used.

GaBi often combines one or more of the inputs for a substance into a single entry in the LCI, whereas SimaPro typically places them in separate sub-compartments. There does not appear to be a great deal of consistency in how this is done; in some cases all the mass of a substance is combined together, and in other cases it may be split between two or more categories. For example; an amount of a substance SimaPro places in the groundwater long-term sub-compartment may end up in GaBi under the category “ecoinvent long-term to fresh water”, or it may be combined with other amounts of the same substance and place in a category such as “Heavy metals to fresh water” or “Inorganic emissions to fresh water”. The only way to accurately compare inputs and emissions between SimaPro and GaBi is to trace out and match the total amount of a substance for each type of input and emission, and then examine what characterization factors are used in converting the mass to an impact assessment indicator. In this way it can be established whether both programs are dealing with the same amount of input for a given substance, what characterization factors are used with the substance, and what contribution the substance makes to the impact indicator in question. This can be time consuming to do, but is a viable method of ensuring a consistent comparison of the software programs.

A total of 14 impact assessment categories were examined covering 3 different impact assessment methodologies: Impact 2002+, ReCiPe, and TRACI 2. All comparisons were done using SimaPro 7.3.3 and GaBi 5. Comparisons between software were made using pairs of tables, each pair consisting of a table for SimaPro (Table xxA) and a table for GaBi (Table xxB). Even with the simple basic material systems being used as the basis for comparison, there can be hundreds, possibly thousands, of substances included in a life cycle inventory. However, generally only a small subset are significant to the final impact indicator value, and it is these subsets that are included in the tables. Item numbers in tables have been arranged so there is a one-to-one correspondence between tables within a pair; meaning that item 5 in the SimaPro table corresponds to item 5 in the GaBi table. Any differences in characterization factors between SimaPro and GaBi are highlighted in **bold text** in the tables.

11.1 IMPACT 2002+

Up to this point, the implementation of Impact 2002+ version 2.1 being used for SimaPro was one downloaded via an internet link contained in the methods library manual for SimaPro (Goedkoop et al. 2008). When SimaPro was upgraded to version 7.3.3, another copy of Impact 2002+ version 2.1 was included. While both files indicated they were the same version, a check of the comments included in the files found the one from the software upgrade was last modified in 2010, while the one from the download link had no changes listed since 2005. After downloading the methods manual again, a follow up check found that the original file is still the one accessed via the internet link. Faced with two potentially different variants of Impact 2002+ version 2.1 being available, it was decided to do the tests in this section using both for completeness. Unless otherwise noted, all SimaPro Impact 2002+ data presented in comparison tables in this section came from the software upgrade variant, or “new” Impact 2002+ version 2.1. Any differences found with the original variant, or “old” Impact 2002+ version 2.1, are noted in the discussion of the results accompanying each pair of tables. All GaBi Impact 2002+ data comes from the Impact 2002+ version 2.1 method included with GaBi 5.

One issue that does exist for the old variant of Impact 2002+, but not the new one, is an error in the downloaded installation file. The file contained an inadvertent blank line in the middle of the data for the terrestrial ecotoxicity impact category. A blank line represents the end of a impact category in the installation file, so SimaPro stopped loading impact characterization factors for terrestrial ecotoxicity when it encountered the blank line. No warning was issued because SimaPro saw this as a proper indication of the end of the category. It was not until investigating differences in results between software packages that it was discovered that 671 (48.3%) of the 1389 impact characterization factors for terrestrial ecotoxicity never got installed. The blank line was removed from the installation file and the old variant of Impact 2002+ was reinstalled to fix the problem. This problem was still present in the file posted on the download website at the time this paper was being written.

11.1.1 Aquatic Ecotoxicity

Impact 2002+ data for the aquatic ecotoxicity impact category when obtaining and disposing of 1 kg of aluminum with 50% recycled content is given in Table 16A for SimaPro, and Table 16B for GaBi. The first thing to note at the bottom of the tables is that SimaPro reported 2,385 kg TEG (Tri Ethylene Glycol) to water versus 1,229,700 kg TEG to water reported by GaBi, meaning the two software programs differed by a multiplication factor of 516. The next thing to note at the bottom of the tables is that the 19 items in each table account for 2,357 kg TEG to water for SimaPro and 1,229,643 kg TEG to water for GaBi, or in simpler terms 98.8% of the total impact reported by SimaPro and effectively 100% for GaBi. This establishes that SimaPro and GaBi differed significantly from each other for this impact category, and that the 19 items contained in each table were the significant contributors to the impact category results.

Looking at the far right column in the two tables, the total contribution each item made to the impact indicator value can be seen. Item 1, aluminum (U.S. spelling) or “aluminium” (English spelling), clearly had a significant difference in impact contribution between SimaPro and GaBi. This was caused by the Impact 2002+ implementation in

SimaPro setting the characterization factor for aluminum in the “groundwater, long term” sub-compartment (item 1A) to zero, effectively removing it from making any contribution. The Impact 2002+ implementation in SimaPro did have a characterization factor for aluminum in the “river” sub-compartment (item 1B), the same factor that GaBi used for “aluminum (+III)”. The total mass of aluminum for items 1A and 1B in SimaPro (Table 16A) matched the mass GaBi had for item 1 (Table 16B), showing that total aluminum emissions to water were identical for the two programs. It should also be noted that GaBi assigned all the aluminum mass to the category “Inorganic emissions to fresh water”, even though GaBi did use the category “ecoinvent long-term to fresh water” for other substances.

While item 1 was clearly the dominant issue in this comparison of SimaPro and GaBi, it was not the only problem. Items 2 through 11A had characterization factors of zero in SimaPro and non zero in GaBi. Examination of the method file in SimaPro found that all the characterization factors for substances assigned to the “groundwater” and “groundwater, long-term” sub-compartments were set to zero. When the characterization factor for an impact category is set to zero, a substance makes no contribution to the reported impact indicator value. While these items were not significant in this comparison due to their limited mass, they could easily be significant in other comparisons where one or more of them has greater emissions to water.

The roles were reversed for items 12, 13, 16, 17, and 18. These items had non-zero characterization factors in SimaPro, but did not contribute to the impact reported by GaBi, even though the mass was accounted for. A check of the Impact 2002+ implementation in GaBi showed no characterization factors for these substances in the stated categories, which for GaBi means an effective characterization factor of zero. Again this is a case where any of these items could be significant in other comparisons where they have greater emissions to water.

The Impact 2002+ method file in SimaPro did include a comment that while characterization factors for “groundwater” and “groundwater, long-term” were set to zero for aquatic ecotoxicity and some other impact categories, it did not mean there were no impacts, just that such characterization factors were not currently available. The GaBi version of Impact 2002+ referred those seeking information on Impact 2002+ to an internet link that returned an error when accessed.

There were two significant differences between the new Impact 2002+ variant for SimaPro, used in Table 16A, and the old Impact 2002+ variant. In the old variant, shown in Table 16C, the name “aluminium” (English spelling) was used as the substance name, while “aluminum” (U.S. spelling) was used for the characterization factor. Because the names differed by a single character, SimaPro could not match the characterization factor to the input substance, resulting in an effective value of zero for the characterization factor of items 1B, 13, 16, and 17. In addition, items 2, 3, 6, 7, 9, 10, and 11A had characterization factors in the old SimaPro Impact 2002+ variant that matched those of GaBi, allowing them to contribute to the reported impact indicator value, while the new SimaPro Impact 2002+ variant had characterization factors of zero.

Table 16A: SimaPro / Impact 2002+ aquatic ecotoxicity for aluminum

50% Recycled Content						
Item	Substance			Amount (kg)	Characterization Factor (kg TEG water)	Impact (kg TEG water)
	Name	Compartment	Sub-compartment			
1A	Aluminium	Water	groundwater, long-term	0.34044	**0**	**0**
1B	Aluminium	Water	river	0.00052	3.60E+06	1879
	Total Aluminum In Water: 0.34096 kg					
2	Antimony	Water	groundwater, long-term	4.68E-06	**0**	**0**
3	Barium	Water	groundwater, long-term	8.74E-05	**0**	**0**
4	Cobalt	Water	groundwater, long-term	6.44E-05	**0**	**0**
5	Copper, ion	Water	groundwater, long-term	8.73E-05	**0**	**0**
6	Lead	Water	groundwater, long-term	1.82E-05	**0**	**0**
7	Mercury	Water	groundwater, long-term	6.05E-07	**0**	**0**
8	Nickel	Water	groundwater, long-term	2.10E-04	**0**	**0**
9	Selenium	Water	groundwater, long-term	1.37E-05	**0**	**0**
10	Zinc, ion	Water	groundwater, long-term	5.76E-04	**0**	**0**
11A	Arsenic, ion	Water	groundwater; groundwater, long-term	1.98E-05	**0**	**0**
11B	Arsenic, ion	Water	river	2.13E-05	3.88E+05	8.25
	Total Arsenic, Ion In Water: 4.10E-5 kg					
12	Chromium VI	Water	river	3.31E-05	**4.53E+05**	**15.00**
13	Aluminium	air	(combined)	4.36E-04	**4.93E+05**	**215**
14	Copper	air	(combined)	9.78E-06	2.94E+06	28.76
15	Zinc	air	(combined)	7.92E-05	2.04E+05	16.15
16	Aluminium	soil	agricultural	6.21E-07	**3.50E+06**	**2.17**
17	Aluminium	soil	industrial	1.89E-05	**3.50E+06**	**66.20**
18	Chromium VI	soil	(combined)	9.60E-06	**4.49E+05**	**4.31**
19	Copper	soil	(combined)	6.00E-06	2.04E+07	123
Total kg TEG Water For Items In Table						2357
Reported kg TEG Water						2385

[1] Items in **bold text** differ in characterization factors between SimaPro and GaBi.

Table 16B: GaBi / Impact 2002+ aquatic ecotoxicity for aluminum

50% Recycled Content					
Item	Substance		Amount (kg)	Characterization Factor (kg TEG to water per kg)	Impact (kg TEG to water)
	Category	Name			
1	Inorganic emissions to fresh water	Aluminum (+III)	0.34096	**3.60E+06**	**1,226,263**
2	ecoinvent long-term to fresh water	Antimony	4.68E-06	**2.10E+06**	**9.84**
3	ecoinvent long-term to fresh water	Barium	8.74E-05	**8.05E+04**	**7.04**
4	ecoinvent long-term to fresh water	Cobalt	6.44E-05	**3.86E+06**	**249**
5	ecoinvent long-term to fresh water	Copper (+II)	8.73E-05	**2.06E+07**	**1,794**
6	ecoinvent long-term to fresh water	Lead (+II)	1.82E-05	**2.64E+05**	**4.79**
7	Heavy metals to fresh water	Mercury (+II)	6.22E-07	**1.58E+07**	**9.82**
8	Heavy metals to fresh water	Nickel	2.11E-04	**1.27E+06**	**268**
9	ecoinvent long-term to fresh water	Selenium	1.37E-05	**3.40E+06**	**46.52**
10	ecoinvent long-term to fresh water	Zinc (+II)	5.76E-04	**1.40E+06**	**808**
11	Heavy metals to fresh water	Arsenic (+V)	4.10E-05	3.88E+05	15.93
12	Heavy metals to fresh water	Chromium (+VI)	3.37E-05	**0**	**0**
13	Particles to air	Aluminum	4.36E-04	**0**	**0**
14	Heavy metals to air	Copper (+II)	9.78E-06	2.94E+06	28.76
15	Heavy metals to air	Zinc (+II)	7.92E-05	2.04E+05	16.15
16	Inorganic emissions to agricultural soil	Aluminum	6.21E-07	**0**	**0**
17	Inorganic emissions to industrial soil	Aluminum	1.89E-05	**0**	**0**
18	Heavy metals to industrial soil	Chromium (VI)	9.60E-06	**0**	**0**
19	Heavy metals to industrial soil	Copper (+II)	6.00E-06	2.04E+07	123
Total kg TEG To Water For Items In Table					1,229,643
Reported kg TEG To Water					1,229,700

[1] Items in **bold text** differ in characterization factors between SimaPro and GaBi.

Table 16C: SimaPro / Old Impact 2002+ variant aquatic ecotoxicity for aluminum

Item	Substance			Amount (kg)	Characterization Factor (kg TEG water)	Impact (kg TEG water)
50% Recycled Content						
	Name	Compartment	Sub-compartment			
1A	Aluminium	Water	groundwater, long-term	0.34044	0	0
1B	Aluminium	Water	river	0.00052	**3.60E+06**	**0** [2]
	Total Aluminium In Water: 0.34096 kg					
2	Antimony	Water	groundwater, long-term	4.68E-06	**2.10E+06**	**9.84**
3	Barium	Water	groundwater, long-term	8.74E-05	**8.05E+04**	**7.04**
4	Cobalt	Water	groundwater, long-term	6.44E-05	0	0
5	Copper, ion	Water	groundwater, long-term	8.73E-05	0	0
6	Lead	Water	groundwater, long-term	1.82E-05	**2.64E+05**	**4.79**
7	Mercury	Water	groundwater, long-term	6.05E-07	**1.58E+07**	**9.56**
8	Nickel	Water	groundwater, long-term	2.10E-04	0	0
9	Selenium	Water	groundwater, long-term	1.37E-05	**3.40E+06**	**46.52**
10	Zinc, ion	Water	groundwater, long-term	5.76E-04	**1.40E+06**	**808**
11A	Arsenic, ion	Water	groundwater; groundwater, long-term	1.98E-05	3.88E+05	7.67
11B	Arsenic, ion	Water	river	2.13E-05	3.88E+05	8.25
	Total Arsenic, Ion In Water: 4.10E-5 kg					
12	Chromium VI	Water	river	3.31E-05	4.53E+05	15.00
13	Aluminium	air	(combined)	4.36E-04	4.93E+05	**0** [2]
14	Copper	air	(combined)	9.78E-06	2.94E+06	28.76
15	Zinc	air	(combined)	7.92E-05	2.04E+05	16.15
16	Aluminium	soil	agricultural	6.21E-07	3.50E+06	**0** [2]
17	Aluminium	soil	industrial	1.89E-05	3.50E+06	**0** [2]
18	Chromium VI	soil	(combined)	9.60E-06	4.49E+05	4.31
19	Copper	soil	(combined)	6.00E-06	2.04E+07	123
Total kg TEG Water For Items In Table						1089
Reported kg TEG Water						1217

Table 16C (cont'd)

[1] Items in **bold text** differ in characterization factors between old and new variants of SimaPro.
[2] Difference between substance and characterization factor names caused a zero.

11.1.2 Global Warming

Impact 2002+ data for the global warming impact category when obtaining and disposing of 1 kg of corrugated board with 12% recycled content is shown in Table 17A for SimaPro, and Table 17B for GaBi. The tables show that SimaPro reported 1.008 kg CO_2 equivalent while GaBi reported only 0.140 kg CO_2 equivalent, meaning the two software programs differ by a factor of 7.20. The 9 items in the table account for 1.006 kg CO_2 equivalent of the impact reported by SimaPro, or 99.8%, and 0.137 kg CO_2 equivalent of what GaBi reported, or 97.7%, again giving good coverage of the significant contributors to the impact category.

The most significant difference occurred with item 3 in the tables. GaBi effectively gave a credit for the sequestration of carbon in the biomass used to produce the corrugated board, and SimaPro did not. The second difference between the programs is item 1, where GaBi included biotic carbon dioxide while SimaPro did not. GaBi also included biotic carbon monoxide in item 5 while SimaPro did not. GaBi and SimaPro both included variants of methane in items 8 and 9, but with different characterization factors.

The old variant of SimaPro Impact 2002+ had different characterization factors for items 4, 8, and 9. “Carbon dioxide, land transformation” (item 4) and “methane, biogenic” (item 8) both had zero as characterization factors in the old variant. “Methane, fossil” (item 9) had a characterization factor in the old variant of 7.00, the same as used by GaBi. Checking comments in the new variant SimaPro Impact 2002+ method file, a statement was found that characterization factors for “methane, biogenic” and “methane, fossil” were changed to their current values in 2010. There was also a comment that "carbon dioxide, land transformation" was included in 2008. There were no comments available with the GaBi implementation of Impact 2002+.

Table 17A: SimaPro / Impact 2002+ global warming for corrugated board, part 1

12% Recycled Content					
Item	Substance: Name	Substance: Compartment	Amount (kg)	Characterization Factor (kg CO_2 per kg)	Impact (kg CO_2 Equiv.)
1	Carbon dioxide, biogenic	air	1.48E+00	**0**	**0**
2	Carbon dioxide, fossil	air	9.15E-01	1.00	0.91490
3	Carbon dioxide, in air	raw	2.35E+00	**0**	**0**
4	Carbon dioxide, land transformation	air	4.13E-04	1.00	0.00041
5	Carbon monoxide, biogenic	air	8.06E-05	**0**	**0**
6	Carbon monoxide, fossil	air	4.41E-03	1.57	0.00693
7	Dinitrogen monoxide	air	5.70E-05	156	0.00890
8	Methane, biogenic	air	7.19E-03	**7.60**	**0.05465**
9	Methane, fossil	air	1.92E-03	**10.35**	**0.01984**
Total kg CO_2 For Items In Table					1.006
Reported kg CO_2					1.008

[1] Items in **bold text** differ in characterization factors between SimaPro and GaBi.

Table 17B: GaBi / Impact 2002+ global warming for corrugated board, part 1

12% Recycled Content					
Item	Substance: Category	Substance: Name	Amount (kg)	Characterization Factor (kg CO_2 per kg)	Impact (kg CO_2 Equiv.)
1	Inorganic emissions to air	Carbon dioxide (biotic)	1.50E+00	**1.00**	**1.50000**
2	Inorganic emissions to air	Carbon dioxide	9.15E-01	1.00	0.91500
3	Renewable resources	Carbon dioxide	2.35E+00	**-1.00**	**-2.35000**
4	Inorganic emissions to air	Carbon dioxide, land transformation	4.13E-04	1.00	0.00041
5	Inorganic emissions to air	Carbon monoxide (biotic)	8.49E-05	**1.57**	**0.00013**
6	Inorganic emissions to air	Carbon monoxide	4.41E-03	1.57	0.00692
7	Inorganic emissions to air	Nitrous oxides (laughing gas)	5.72E-05	156	0.00892
8	Organic emissions to air (group VOC)	Methane (biotic)	6.00E-03	**7.00**	**0.04200**
9	Organic emissions to air (group VOC)	Methane	1.92E-03	**7.00**	**0.01344**
Total kg CO_2 For Items In Table					0.137
Reported kg CO_2					0.140

[1] Items in **bold text** differ in characterization factors between SimaPro and GaBi.

In order to look at how the differences between SimaPro and GaBi influence reported impacts when recycled content is varied, the Impact 2002+ global warming data for creating and disposing of 1 kg of corrugated board with 87% recycled content is given in Table 18A for SimaPro, and Table 18B for GaBi. SimaPro and GaBi came close to reporting the same impact value, 1.007 kg CO_2 equivalent for SimaPro and

1.026 kg CO_2 equivalent for GaBi. This was due primarily to items 1 and 3 in GaBi, where the amount of biotic carbon dioxide and the amount of sequestered carbon from carbon dioxide in the air both decreased with the increase in recycled content. At 12% recycled content these two items combined for 1.50 - 2.35 = -0.85 kg CO_2 equivalent, but at 87% recycled content the combined value decreased to 0.468 – 0.429 = -0.039 kg CO_2 equivalent, so the net carbon credit given by GaBi for using virgin fiber was reduced, bring the results reported by the two programs into better agreement.

Table 18A: SimaPro / Impact 2002+ global warming for corrugated board, part 2

87% Recycled Content					
Item	Substance		Amount (kg)	Characterization Factor (kg CO_2 per kg)	Impact (kg CO_2 Equiv.)
	Name	Compartment			
1	Carbon dioxide, biogenic	air	4.41E-01	**0**	**0**
2	Carbon dioxide, fossil	air	9.17E-01	1.00	0.91664
3	Carbon dixoide, in air	raw	4.29E-01	**0**	**0**
4	Carbon dioxide, land transformation	air	4.27E-04	1.00	0.00043
5	Carbon monoxide, biogenic	air	4.14E-05	**0**	**0**
6	Carbon monoxide, fossil	air	2.47E-03	1.57	0.00388
7	Dinitrogen monoxide	air	6.46E-05	156	0.01007
8	Methane, biogenic	air	7.07E-03	**7.60**	**0.05373**
9	Methane, fossil	air	1.98E-03	**10.35**	**0.02050**
Total kg CO_2 For Items In Table					1.005
Reported kg CO_2					1.007

[1] Items in **bold text** differ in characterization factors between SimaPro and GaBi.

Table 18B: GaBi / Impact 2002+ global warming for corrugated board, part 2

87% Recycled Content					
Item	Substance		Amount (kg)	Characterization Factor ($kg CO_2$ per kg)	Impact ($kg CO_2$ Equiv.)
	Category	Name			
1	Inorganic emissions to air	Carbon dioxide (biotic)	4.68E-01	**1.00**	**0.46800**
2	Inorganic emissions to air	Carbon dioxide	9.17E-01	1.00	0.91700
3	Renewable resources	Carbon dioxide	4.29E-01	**-1.00**	**-0.42900**
4	Inorganic emissions to air	Carbon dioxide, land transformation	4.27E-04	1.00	0.00043
5	Inorganic emissions to air	Carbon monoxide (biotic)	4.57E-05	**1.57**	**0.00007**
6	Inorganic emissions to air	Carbon monoxide	2.47E-03	1.57	0.00388
7	Inorganic emissions to air	Nitrous oxides (laughing gas)	6.47E-05	156	0.01009
8	Organic emissions to air (group VOC)	Methane (biotic)	5.88E-03	**7.00**	**0.04116**
9	Organic emissions to air (group VOC)	Methane	1.98E-03	**7.00**	**0.01386**
Total kg CO_2 For Items In Table					1.025
Reported kg CO_2					1.026

[1] Items in **bold text** differ in characterization factors between SimaPro and GaBi.

11.1.3 Mineral Extraction

Impact 2002+ data for the mineral extraction impact category when obtaining and disposing of 1 kg of glass with 55.5% recycled content is given in Table 19A for SimaPro, and Table 19B for GaBi. SimaPro reported 0.00645 MJ equivalent while GaBi reported 0.0523 MJ equivalent, differing by a factor of 8.11. The 11 items in each table combine for effectively the entire impact. There are several issues causing the difference between reported values from the software; each has the potential of being significant in comparisons that include larger amounts of the substances involved.

The most significant contribution to the difference in this comparison came from item 9. The characterization factor for nickel ore in SimaPro was 16.32 MJ per kg, but GaBi used 163 MJ per kg, a factor of 10 greater. According to literature, mineral extraction characterization factors for Impact 2002+ were taken from the Eco-indicator 99 assessment method (Jolliet et al. 2003). A check of Eco-indicator 99 in GaBi revealed a characterization factor for nickel ore of 16.32 MJ per kg, matching the factor SimaPro had for Impact 2002+, making it appear the factor used for Impact 2002+ in GaBi may have been entered incorrectly. Interestingly, a check of Eco-indicator 99 in SimaPro found the characterization factor for nickel ore to be 23.75 MJ per kg, which matched the factor found in Eco-indicator 99 literature (Goedkoop and Spriensma 2001), but not anything else.

Another problem dealing with nickel ore in SimaPro occurred in item 9A of Table 19A. Here the substance name differed somewhat from the closest name assigned a non zero characterization factor, resulting in a factor of zero being used. See Table 20 for the difference in names.

Item 4 in the Table 19 A and B was the next problem. SimaPro distributed copper ore among 4 types, but had a characterization factor assigned only to the type in item 4A; the remaining 3 types of copper ore did not contribute to the reported impact. GaBi combined all the copper under a single entry and applied a characterization factor that matched what SimaPro had for the more general “copper, in ground” substance name.

A similar problem occurred with molybdenum ore in item 8. Here SimaPro distributed the ore among 5 types, but had no effective characterization factor. The closest SimaPro came was for the ore type in item 8E, but again a mismatch of characterization and substance names caused a factor of zero to be used. Table 20 shows the difference in names. GaBi combined all the molybdenum into one entry and applied a characterization factor that matches what SimaPro had for the more general “molybdenum, in ground” substance name.

Item 11 of Tables 19 A and B was another case of SimaPro not matching substance names to characterization factor names, this time for zinc ore, with the result that a factor of zero was used (see Table 20). The characterization factor that GaBi applied did not match any for zinc in the new variant of SimaPro Impact 2002+, but did match what the old variant had for “zinc (in ore)”.

Item 6 in Tables 19 A and B was a case of SimaPro not having a characterization factor for any specific type of lead ore that came close to matching the substance name. The closest SimaPro came was the more general “lead, in ground” which had a factor of 7.35, matching what GaBi used.

Item 3 in Tables 19A and B shows SimaPro had a characterization factor for cinnabar while GaBi did not. A check of a spreadsheet version of Impact 2002+ obtained from the same internet link that the old variant came from did not have an entry for cinnabar, yet the old variant of Impact 2002+ had the same entry as the new variant.

One additional naming difference was found between the old and new variants of SimaPro Impact 2002+ version 2.1. When dealing with chromium ore, item 2 in Table 19A, the old variant left out a percent sign in the characterization factor name, causing another mismatch that resulted in a factor of zero being used. See Table 20 for the difference in names.

Table 19A: SimaPro / Impact 2002+ mineral extraction for glass

55.5% Recycled Content				
Item	Substance Name [2]	Amount (kg)	Characterization Factor (MJ per kg)	Impact (MJ Equiv.)
1	Aluminium, 24% in bauxite, 11% in crude ore, in ground	4.63E-04	2.38	0.001102
2	Chromium, 25.5% in chromite, 11.6% in crude ore, in ground	9.39E-05	0.9165	0.000086
3	Cinnabar, in ground	1.00E-08	**165.5**	**0.000002**
4A	Copper, 0.99% in sulfide, Cu 0.36% and Mo 8.2E-3% in crude ore, in ground	1.61E-05	36.80	0.000593
4B	Copper, 1.18% in sulfide, Cu 0.39% and Mo 8.2E-3% in crude ore, in ground	8.88E-05	**0**	**0**
4C	Copper, 1.42% in sulfide, Cu 0.81% and Mo 8.2E-3% in crude ore, in ground	2.36E-05	**0**	**0**
4D	Copper, 2.19% in sulfide, Cu 1.83% and Mo 8.2E-3% in crude ore, in ground	1.17E-04	**0**	**0**
	Total Copper Ore: 2.46E-04 kg			

Table 19A (cont'd)

5	Iron, 46% in ore, 25% in crude ore, in ground	5.76E-03	0.051	0.000294
6	Lead, 5.0% in sulfide, Pb 3.0%, Zn, Ag, Cd, In, in ground	6.41E-06	**0**	**0**
7	Manganese, 35.7% in sedimentary deposit, 14.2% in crude ore, in ground	1.91E-05	0.313	0.000006
8A	Molybdenum, 0.010% in sulfide, Mo 8.2E-3% and Cu 1.83% in crude ore, in ground	2.18E-06	**0**	**0**
8B	Molybdenum, 0.014% in sulfide, Mo 8.2E-3% and Cu 0.81% in crude ore, in ground	3.09E-07	**0**	**0**
8C	Molybdenum, 0.022% in sulfide, Mo 8.2E-3% and Cu 0.36% in crude ore, in ground	2.11E-07	**0**	**0**
8D	Molybdenum, 0.025% in sulfide, Mo 8.2E-3% and Cu 0.39% in crude ore, in ground	1.13E-06	**0**	**0**
8E	Molybdenum, 0.11% in sulfide, Mo 4.1E-2% and Cu 0.36% in crude ore, in ground	4.22E-07	**37.14**	**0** [3]
	Total Molybdenum Ore: 4.26E-06			
9A	Nickel, 1.13% in sulfide, Ni 0.76% and Cu 0.76% in crude ore, in ground	1.28E-06	**16.32**	**0** [3]
9B	Nickel, 1.98% in silicates, 1.04% in crude ore, in ground	2.50E-04	**16.32**	**0.004086**
	Total Nickel Ore: 2.52E-04 kg			
10	Tin, 79% in cassiterite, 0.1% in crude ore, in ground	4.73E-07	600.00	0.000284
11	Zinc, 9.0% in sulfide, Zn 5.3%, Pb, Ag, Cd, In, in ground	1.39E-04	**3.8367**	**0** [3]
Total MJ Equivalent For Items In Table				0.00645
Reported MJ Equivalent				0.00645

[1] Items in **bold text** differ in characterization factors between SimaPro and GaBi.

[2] Substances are from the SimaPro compartment "Raw".

[3] Difference between substance and characterization factor names caused a zero.

Table 19B: GaBi / Impact 2002+ mineral extraction for glass

55.5% Recycled Content				
Item	Substance Name [2]	Amount (kg)	Characterization Factor (MJ per kg)	Impact MJ Equiv.)
1	Aluminum	4.63E-04	2.38	0.001102
2	Chromium	9.39E-05	0.917	0.000086
3	Cinnabar	1.00E-08	**0**	**0**
4	Copper	2.46E-04	**36.7**	**0.009023**
5	Iron	5.76E-03	0.051	0.000294
6	Lead	6.41E-06	**7.35**	**0.000047**
7	Manganese	1.91E-05	0.313	0.000006
8	Molybdenum	4.26E-06	**41.0**	**0.000175**
9	Nickel	2.52E-04	**163**	**0.041015**
10	Tin	4.73E-07	600	0.000284
11	Zinc	1.39E-04	**1.89**	**0.000263**
Total MJ Equivalent For Items In Table				0.0523
Reported MJ Equivalent				0.0523

[1] Items in **bold text** differ in characterization factors between SimaPro and GaBi.
[2] Substances are from the GaBi category "Non renewable elements".

Table 20: SimaPro naming differences for mineral extraction

Substance Name	Characterization Factor Name	Impact 2002+ Variant Affected
Chromium, 25.5**%** in chromite, 11.6% in crude ore, in ground	Chromium, 25.5 in chromite, 11.6% in crude ore, in ground	Old
Molybdenum, 0.11% in sulfide, Mo **4.1E-2**% and Cu 0.36% in crude ore, in ground	Molybdenum, 0.11% in sulfide, Mo **0.41%** and Cu 0.36% in crude ore, in ground	Old and New
Nickel, 1.13% in sulfide, **Ni** 0.76% **and Cu 0.76%** in crude ore, in ground	Nickel, 1.13% in sulfide**s**, 0.76% in crude ore, in ground	Old and New
Zinc, 9**.0**% in sulfide, **Zn 5.3%, Pb, Ag, Cd, In,** in ground	Zinc 9%**, Lead 5%,** in sulfide in ground	Old and New

[1] Differences between names are highlighted in **bold text**.

11.1.4 Ozone Layer Depletion

In earlier work for this paper using the old SimaPro Impact 2002+ variant, Table 15 (section 10.3) showed GaBi reported an impact for ozone layer depletion that was different from what SimaPro had by more than a factor of 10 when obtaining and disposing of 1kg of PET with 0% recycled content. Data in Tables 21A and 21B using the new SimaPro Impact 2002+ variant show both software reported 1.448E-07 kg CFC_11 equivalent. This difference between variants was investigated. It was found that for items 4, 5, and 6 in the tables, the old variant of SimaPro Impact 2002+ had a single character difference in the names of characterization factors versus names of substances. In each case a hyphen ("-") was substituted for a space in the characterization factor name between "Halon" and the number at the end of the name. This mismatch led to factors of zero being used, which had the effect of eliminating most of the impact from being reported. Table 22 shows the difference in names.

Table 21A: SimaPro / Impact 2002+ ozone layer depletion for PET

0% Recycled Content				
Item	Substance Name [1]	Amount (kg)	Characterization Factor (kg CFC-11 per kg)	Impact (kg CFC-11 Equiv.)
1	Ethane, 1,1,1-trichloro-, HCFC-140	2.31E-12	0.120	2.773E-13
2	Methane, tetrachloro-, CFC-10	1.01E-09	0.730	7.364E-10
3	Methane, monochloro-, R-40	6.58E-11	0.0200	1.315E-12
4	Methane, bromochlorodifluoro-, Halon 1211	1.23E-08	6.00	7.409E-08
5	Methane, bromotrifluoro-, Halon 1301	4.95E-09	12.00	5.935E-08
6	Methane, bromo-, Halon 1001	2.47E-17	0.380	9.371E-18
7	Methane, trichlorofluoro-, CFC-11	1.01E-12	1.000	1.012E-12
8	Ethane, 1,1,2-trichloro-1,2,2-trifluoro-, CFC-113	9.43E-11	1.000	9.432E-11
9	Ethane, 1,2-dichloro-1,1,2,2-tetrafluoro-, CFC-114	8.17E-09	0.940	7.677E-09
10	Methane, dichlorodifluoro-, CFC-12	2.90E-10	1.000	2.898E-10
11	Methane, dichlorofluoro-, HCFC-21	6.24E-13	0.0400	2.495E-14
12	Methane, chlorodifluoro-, HCFC-22	5.07E-08	0.0500	2.537E-09
Total kg CFC-11 Equivalent For Items In Table				1.448E-07
Reported kg CFC-11 Equivalent				1.448E-07

[1] Substances are from the SimaPro compartment "Air".

Table 21B: GaBi / Impact 2002+ ozone layer depletion for PET

0% Recycled Content				
Item	Substance Name [1]	Amount (kg)	Characterization Factor (kg CFC-11 per kg)	Impact (kg CFC-11 Equiv.)
1	1,1,1-Trichloroethane	2.31E-12	0.120	2.773E-13
2	Carbon tetrachloride (tetrachloromethane)	1.01E-09	0.730	7.364E-10
3	Chloromethane (methyl chloride)	6.58E-11	0.0200	1.315E-12
4	Halon (1211)	1.23E-08	6.00	7.408E-08
5	Halon (1301)	4.95E-09	12.00	5.935E-08
6	Methyl bromide	2.47E-17	0.380	9.371E-18
7	R 11 (trichlorofluoromethane)	1.01E-12	1.000	1.012E-12
8	R 113 (trichlorofluoroethane)	9.43E-11	1.000	9.432E-11
9	R 114 (dichlorotetrafluoroethane)	8.17E-09	0.940	7.677E-09
10	R 12 (dichlorodifluoromethane)	2.90E-10	1.000	2.898E-10
11	R 21 (Dichlorofluoromethane)	6.24E-13	0.0400	2.495E-14
12	R 22 (chlorodifluoromethane)	5.07E-08	0.0500	2.537E-09
Total kg CFC-11 Equivalent For Items In Table				1.448E-07
Reported kg CFC-11 Equivalent				1.448E-07

[1] Substances are from GaBi category "Organic emissions to air (group VOC)".

Table 22: SimaPro naming differences for ozone depletion

Substance Name	Characterization Factor Name	Impact 2002+ Variant Affected
Methane, bromochlorodifluoro-, Halon 1211	Methane, bromochlorodifluoro-, Halon**-**1211	Old
Methane, bromotrifluoro-, Halon 1301	Methane, bromotrifluoro-, Halon**-**1301	Old
Methane, bromo-, Halon 1001	Methane, bromo-, Halon**-**1001	Old

[1]Differences (spaces versus hyphens) between names are highlighted in **bold text**.

11.1.5 Respiratory Organics

Simapro referred to this impact category as “Respiratory Organics”; however, GaBi referred to it as “Photochemical Oxidation”. In earlier work for this paper using the old SimaPro Impact 2002+ variant, Table 15 (section 10.3) showed GaBi reported an impact for photochemical oxidation/respiratory organics that was different from what SimaPro had by more than a factor of 10 when obtaining and disposing of 1 kg of PET with 0% recycled content. The data in Tables 23A and 23B using the new SimaPro Impact 2002+ variant show a much smaller difference, 0.00185 kg C_2H_4 equivalent for SimaPro and 0.00192 kg C_2H_4 equivalent for GaBi. Investigating the difference between the two SimaPro Impact 2002+ variants uncovered two more cases of mismatched names for characterization factors and substances, item 3 for “aldehydes, unspecified” and item 16 for “NMVOC, non-methane volatile organic compounds, unspecified origin”. One additional mismatch of names was discovered that is common between the variants, item 13 for “methane, fossil”. In all 3 cases the mismatch caused a characterization factor of zero to be used, resulting in no contribution to reported impact. Item 16 was the dominant impact contributor, causing most of the difference between Impact 2002+ variants in SimaPro. Item 13 accounted for most of the difference between the new SimaPro Impact 2002+ variant (Table 23A) and GaBi (Table 23B). See Table 24 for the difference in names.

Tables 23A and 23B show that for items 3, 5, and 6 GaBi had zero for the characterization factors while SimaPro had non-zero values. The lack of any contribution from these 3 items to the impact reported by GaBi accounts for the remainder of the difference between SimaPro and GaBi. Item 5 is interesting in that while GaBi assigned the mass to “Butane” which had no characterization factor in GaBi for this impact category, GaBi did have a characterization factor assigned to “Butane (n-butane) [Group NMVOC to air]” which matched the factor SimaPro used.

Table 23A: SimaPro / Impact 2002+ respiratory organics for PET

0% Recycled Content				
Item	Substance Name [2]	Amount (kg)	Characterization Factor (kg C_2H_4 per kg)	Impact (kg C_2H_4 Equiv.)
1	Acetaldehyde	1.12E-06	0.638	0.0000007
2	Acetic acid	2.22E-04	0.100	0.0000222
3	Aldehydes, unspecified	1.40E-08	**0.657**	**9.20E-09**
4	Benzene	9.77E-06	0.220	0.0000021
5	Butane	1.64E-05	**0.355**	**0.0000058**
6	Ethane	5.01E-05	**0.124**	**0.0000062**
7	Ethene	6.41E-05	1.000	0.0000641
8	Ethyl acetate	3.56E-06	0.216	0.0000008
9	Formaldehyde	4.07E-06	0.521	0.0000021
10	Heptane	1.83E-06	0.521	0.0000010
11	Hexane	6.02E-06	0.479	0.0000029
12	Hydrocarbons, aromatic	3.59E-04	0.9859	0.0003535
13	Methane, fossil	1.36E-02	0.00601	0 [3]
14	Methanol	1.24E-04	0.132	0.0000163
15	Methyl ethyl ketone	3.56E-06	0.380	0.0000014
16	NMVOC, non-methane volatile organic compounds, unspecified origin	2.24E-03	0.601	0.0013450
17	Pentane	2.14E-05	0.400	0.0000085
18	Propane	2.42E-05	0.180	0.0000043
19	Propene	2.67E-06	1.117	0.0000030
20	Toluene	4.81E-06	0.638	0.0000031
21	Xylene	6.47E-06	1.038	0.0000067
Total kg C_2H_4 Equivalent For Items In Table				0.001850
Reported C_2H_4 Equivalent				0.001855

[1] Items in **bold text** differ in characterization factors between SimaPro and GaBi.
[2] All substances are from the SimaPro compartment "Air".
[3] Difference in substance and characterization factor names cause a zero.

Table 23B: GaBi / Impact 2002+ photochemical oxidation for PET

0% Recycled Content				
Item	Substance Name [2]	Amount (kg)	Characterization Factor (kg C_2H_4 per kg)	Impact (kg C_2H_4 Equiv.)
1	Acetaldehyde (Ethanal)	1.12E-06	0.638	0.0000007
2	Acetic acid	2.22E-04	0.100	0.0000222
3	Aldehyde (unspecified)	1.40E-08	**0**	**0**
4	Benzene	9.77E-06	0.220	0.0000021
5	Butane	1.64E-05	**0**	**0**
6	Ethane	5.01E-05	**0**	**0**
7	Ethene (ethylene)	6.41E-05	1.000	0.0000641
8	Ethylene acetate (ethyl acetate)	3.56E-06	0.216	0.0000008
9	Formaldehyde (methanal)	4.07E-06	0.521	0.0000021
10	Heptane (isomers)	1.83E-06	0.521	0.0000010
11	Hexane (isomers)	6.02E-06	0.479	0.0000029
12	Hydrocarbons, aromatic	3.59E-04	0.986	0.0003535
13	Methane	1.36E-02	0.00601	0.0000816
14	Methanol	1.24E-04	0.132	0.0000163
15	Butanone (methyl ethyl ketone)	3.56E-06	0.380	0.0000014
16	NMVOC (unspecified)	2.24E-03	0.601	0.0013450
17	Pentane (n-pentane)	2.14E-05	0.400	0.0000085
18	Propane	2.42E-05	0.180	0.0000043
19	Propene (propylene)	2.67E-06	1.117	0.0000030
20	Toluene (methyl benzene)	4.81E-06	0.638	0.0000031
21	Xylene (dimethyl benzene)	6.47E-06	1.038	0.0000067
Total kg C_2H_4 Equivalent For Items In Table				0.001919
Reported C_2H_4 Equivalent				0.001922

[1] Items in **bold text** differ in characterization factors between SimaPro and GaBi.

[2] All substances are from the GaBi category "Organic emissions to air (group VOC)".

Table 24: SimaPro naming differences for respiratory organics

Substance Name	Characterization Factor Name	Impact 2002+ Variant Affected
Aldehydes**, unspecified**	Aldehydes	Old
Methane**, fossil**	Methane	Old and New
NMVOC**, non-methane volatile organic compounds, unspecified origin**	NMVOC	Old

[1] Differences between names are highlighted in **bold text**.

11.2 ReCiPe

All comparisons for this section were done using ReCiPe Midpoint (H) version 1.06 with SimaPro 7.3.3, and ReCiPe Midpoint (H) version 1.05 with GaBi 5. These are the versions of ReCiPe that were supplied with the released versions of SimaPro and GaBi software available at the time of this study.

11.2.1 Human Toxicity

ReCiPe data for the human toxicity category when obtaining and disposing of 1 kg of PET with 0% recycled content is given in Table 25A for SimaPro, and Table 25B for GaBi. Amounts listed at the bottom of the tables show that SimaPro reported 1.133 kg 1,4-DB equivalent while GaBi reported 0.3869 kg 1,4-DB equivalent, differing by a factor of 2.93. Totals for the 20 items in each table show they account for 97.8% of the impact reported by SimaPro, and 95.7% of the impact reported by GaBi.

The majority of the difference between SimaPro and GaBi for human toxicity had to do with manganese emissions to water, items 12 and 19. SimaPro had non zero characterization factors for these items, allowing them to contribute to the reported impact. GaBi had no impact factors assigned, causing zeros to be used and resulting in no contribution to reported impact. The characterization factors used by SimaPro are the same as found in spreadsheet versions of ReCiPe 1.05, used by GaBi, and the more recent ReCiPe 1.08 files that were downloaded from the ReCiPe website (ReCiPe 2013).

Items 1 through 7 in SimaPro had mass split between two different characterization factors, while GaBi had only a single entry for each item that accounted for the same amount of mass. Furthermore, GaBi had a characterization factor for only one of these items, phosphorus (item 6). The remaining 6 emissions to air did not contribute to the impact reported by GaBi, yet they did contribute in SimaPro. All the characterization factors used by SimaPro were found to match the spreadsheets for ReCiPe 1.05 and ReCiPe 1.08.

The last difference comes from item 8, phosphorus emissions to agricultural soil. GaBi did not have a characterization factor for this item, however, this had to do with the version of ReCiPe being used. There is no characterization factor for phosphorus emissions to agricultural soil in the spreadsheet for ReCiPe 1.05, but it is present in the spreadsheet version of ReCiPe 1.08.

Table 25A: SimaPro / ReCiPe human toxicity for PET

0% Recycled Content						
Item	Substance Name			Amount (kg)	Characterization Factor (kg 1,4-DB eq per kg)	Impact (kg 1,4-DB eq)
	Name	Compartment	Sub-compartment(s)			
1A	Arsenic	air	(unspecified), high. pop.	6.23E-08	**51,300**	**3.20E-03**
1B	Arsenic	air	low. pop.; low. pop., long-term	5.51E-07	**72,000**	**3.97E-02**
	Total arsenic in air: 6.14E-07					
2A	Cadmium	air	(unspecified); high. pop.	8.27E-08	**36,000**	**2.98E-03**
2B	Cadmium	air	low. pop.; low. pop., long-term	1.57E-07	**45,200**	**7.08E-03**
	Total cadmium in air: 2.39E-07 kg					
3A	Lead	air	(unspecified); high. pop.	3.36E-07	**15800**	**5.30E-03**
3B	Lead	air	low. pop.; low. pop., long-term	1.57E-06	**16200**	**2.55E-02**
	Total lead in air: 1.91E-06 kg					
4A	Mercury	air	(unspecified); high. pop.	3.02E-08	**518,000**	**1.56E-02**
4B	Mercury	air	low. pop.; low. pop., long-term	2.90E-08	**56,600**	**1.64E-03**
	Total mercury in air: 5.92E-08					
5A	Nickel	air	(unspecified); high. pop.	8.24E-06	**439**	**3.62E-03**
5B	Nickel	air	low. pop.; low. pop., long-term	1.05E-06	**66.9**	**7.02E-05**
	Total nickel in air: 9.26E-06 kg					
6A	Phosphorus	air	(unspecified); high. pop.	1.26E-07	18,800	2.36E-03
6B	Phosphorus	air	low. pop.; low. pop., long-term	1.73E-08	**14,800**	**2.56E-04**
	Total phosphorus in air: 1.43E-07 kg					
7A	Vanadium	air	(unspecified); high. pop.	6.82E-06	**3,490**	**2.38E-02**

Table 25A (cont'd)

7B	Vanadium	air	low. pop.; low. pop., long-term	9.10E-08	**1,070**	**9.74E-05**
	Total vanadium in air: 6.91E-06 kg					
8	Phosphorus	soil	agricultural	2.43E-07	**9,440**	**2.30E-03**
9	Phosphorus	soil	industrial	2.55E-07	9,440	2.40E-03
10	Antimony	water	groundwater, long-term	4.64E-05	574	2.66E-02
11	Barium	water	groundwater, long-term	6.57E-05	412	2.71E-02
12	Manganese	water	groundwater, long-term	8.62E-04	**700**	**6.03E-01**
13	Molybdenum	water	groundwater, long-term	5.42E-06	1,300	7.05E-03
14	Selenium	water	groundwater, long-term	4.85E-06	10,600	5.14E-02
15	Vanadium	water	groundwater, long-term	2.41E-04	372	8.96E-02
16	Zinc, ion	water	groundwater, long-term	2.41E-04	36.2	8.71E-03
17	Antimony	water	(unspecified); groundwater; river	2.05E-05	574	1.18E-02
18	Arsenic, ion	water	(unspecified); groundwater; groundwater, long-term, river	9.31E-06	14,900	1.39E-01
19	Manganese	water	(unspecified); groundwater; river	5.25E-06	**700**	**3.67E-03**
20	Selenium	water	groundwater; river	3.76E-07	10,600	3.98E-03
Total kg 1,4-DB eq For Items In Table						1.108
Reported kg 1,4-DB eq						1.133

[1] Items in **bold text** differ in characterization factors between SimaPro and GaBi.

Table 25B: GaBi / ReCiPe human toxicity for PET

0% Recycled Content					
Item	Substance		Amount (kg)	Characterization Factor (kg 1,4-DB eq per kg)	Impact (kg 1,4-DB eq)
	Category	Name			
1	Heavy metals to air	Arsenic (+V)	6.14E-07	**0**	**0**
2	Heavy metals to air	Cadmium (+II)	2.39E-07	**0**	**0**
3	Heavy metals to air	Lead (+II)	1.91E-06	**0**	**0**
4	Heavy metals to air	Mercury (+II)	5.92E-08	**0**	**0**
5	Heavy metals to air	Nickel (+II)	9.29E-06	**0**	**0**
6	Inorganic emissions to air	Phosphorus	1.43E-07	18,800	2.69E-03
7	Heavy metals to air	Vanadium (+III)	6.91E-06	**0**	**0**
8	Inorganic emissions to agricultural soil	Phosphorus	2.43E-07	**0**	**0**
9	Inorganic emissions to industrial soil	Phosphorus	2.55E-07	9,440	2.41E-03
10	ecoinvent long-term to fresh water	Antimony	4.64E-05	574	2.66E-02
11	ecoinvent long-term to fresh water	Barium	6.57E-05	412	2.71E-02
12	ecoinvent long-term to fresh water	Manganese (+II)	8.62E-04	**0**	**0**
13	ecoinvent long-term to fresh water	Molybdenum	5.42E-06	1,300	7.05E-03
14	ecoinvent long-term to fresh water	Selenium	4.85E-06	10,600	5.14E-02
15	ecoinvent long-term to fresh water	Vanadium (+III)	2.41E-04	372	8.96E-02
16	ecoinvent long-term to fresh water	Zinc (+II)	2.41E-04	36.2	8.72E-03
17	Heavy metals to fresh water	Antimony	2.05E-05	574	1.18E-02
18	Heavy metals to fresh water	Arsenic (+V)	9.31E-06	14,900	1.39E-01
19	Heavy metals to fresh water	Manganese (+II)	5.25E-06	**0**	**0**
20	Heavy metals to fresh water	Selenium	3.76E-07	10,600	3.98E-03
Total kg 1,4-DB eq For Items In Table					0.3701
Reported kg 1,4-DB eq					0.3869

[1] Items in **bold text** differ in characterization factors between SimaPro and GaBi.

11.2.2 Ionizing Radiation

ReCiPe data for the ionizing radiation category when obtaining and disposing of 1 kg of glass with 55.5% recycled content is given in Table 26A for SimaPro, and Table 26B for GaBi. SimaPro reported 0.1480 kg U235 equivalent while GaBi reported 0.0505 kg U235 equivalent, differing by a factor of 2.93. Totals for the 3 items in each table show they account for 99.6% of the impact reported by SimaPro, and 99.4% of the impact reported by GaBi.

The only difference between software for this impact category was item 3, radon-222 long-term emissions to air. SimaPro had a characterization factor that matched the one in the spreadsheets for ReCiPe 1.05 and ReCipe 1.08, GaBi had no characterization factor assigned. It should be noted that GaBi did assign the same factor as SimaPro for item 2, radon-222 emissions to air (short-term).

Table 26A: SimaPro / ReCiPe ionizing radiation for glass

55.5% Recycled Content						
Item	Substance			Amount (kBq)	Characterization Factor (kg U235 Equiv. per kBq)	Impact (kg U235 Equiv.)
	Name	Compartment	Sub-compartment(s)			
1	Carbon-14	air	low. pop.	4.79E-03	1.00E+01	4.79E-02
2	Radon-222	air	low. pop.	2.04E+00	1.14E-03	2.33E-03
3	Radon-222	air	low. pop., long-term	8.53E+01	**1.14E-03**	**9.72E-02**
Total kg U235 Equiv. For Items In Table						0.1474
Reported kg U235 Equiv.						0.1480

[1] Items in **bold text** differ in characterization factors between SimaPro and GaBi.

Table 26B: GaBi / ReCiPe ionizing radiation for glass

55.5% Recycled Content					
Item	Substance		Amount (kBq)	Characterization Factor (kg U235 Equiv. per kBq)	Impact (kg U235 Equiv.)
	Category	Name			
1	Radioactive emissions to air	Carbon (C14)	4.79E-03	1.00E+01	4.79E-02
2	Radioactive emissions to air	Radon (Rn222)	2.04E+00	1.14E-03	2.33E-03
3	ecoinvent long-term to air	Radon (Rn222)	8.53E+01	**0**	**0**
Total kg U235 Equiv. For Items In Table					0.0502
Reported kg U235 Equiv.					0.0505

[1] Items in **bold text** differ in characterization factors between SimaPro and GaBi.

11.2.3 Marine Ecotoxicity

ReCiPe data for the marine ecotoxicity category when obtaining and disposing of 1 kg of corrugated board with 50% recycled content is given in Table 27A for SimaPro, and Table 27B for GaBi. SimaPro reported 0.008375 kg 1,4-DB equivalent while GaBi reported 0.005806 kg 1,4-DB equivalent, differing by a factor of 1.44. The 18 items in each table account for 97.4% of the impact reported by SimaPro, and 97.9% of the impact reported by GaBi.

The majority of the difference between software came from item 9, manganese emissions to long-term groundwater. SimaPro had a non zero characterization factor for this item, allowing it to contribute to the reported impact. GaBi had no characterization factor assigned, causing a zero to be used and resulting in no contribution to reported impact. The 4.14 kg 1,4-DB equivalent per kg characterization factor used by SimaPro matched the factor found in the spreadsheet versions of ReCiPe 1.05 and ReCiPe 1.08.

Another source of difference between software was that GaBi did not have characterization factors for any of the heavy metal emissions to air, items 1 through 4, so these did not contribute to the impact value reported by GaBi. The impact factors used by SimaPro matched those in the spreadsheet versions of ReCiPe 1.05 and ReCiPe 1.08. It should also be noted that SimaPro split the mass of each of these 4 items between two characterization factors; GaBi accounted for the mass of each item in a single entry per item.

GaBi did not have a characterization factor for item 5, Chlorothalonil emissions to agricultural soil, resulting in no contribution to the impact reported by GaBi. The impact factor used by SimaPro matched the one in the spreadsheet versions of ReCiPe 1.05

and ReCiPe 1.08. GaBi did have a characterization factor for Chlorothalonil emissions to industrial soil.

GaBi did not have a characterization factor for item 16, tributyltinoxide emissions to sea water, resulting in no contribution to the impact reported by GaBi. The impact factor used by SimaPro matched the one in the spreadsheet version of ReCiPe 1.05 for tributyltin compounds, and the one in the spreadsheet version of ReCiPe 1.08 for tributyltin-oxide to ocean.

Table 27A: SimaPro / ReCiPe marine ecotoxicity for corrugated board

50% Recycled Content						
Item	Substance Name			Amount (kg)	Characterization Factor (kg 1,4-DB Equiv. per kg)	Impact (kg 1,4-DB Equiv.)
	Name	Compartment	Sub-compartment(s)			
1A	Copper	air	(unspecified); high. pop.	3.43E-07	**270**	**9.27E-05**
1B	Copper	air	low. pop.; low. pop., long-term	2.41E-07	**388**	**9.36E-05**
	Total copper in air: 5.85E-7 kg					
2A	Nickel	air	(unspecified); high. pop.	8.00E-07	**87.8**	**7.02E-05**
2B	Nickel	air	low. pop.; low. pop., long-term	1.63E-07	**125**	**2.04E-05**
	Total nickel in air: 9.63E-07 kg					
3A	Vanadium	air	(unspecified); high. pop.	2.99E-06	**71.8**	**2.15E-04**
3B	Vanadium	air	low. pop.; low. pop., long-term	2.34E-08	**102**	**2.38E-06**
	Total vanadium in air: 3.02E-06 kg					
4A	Zinc	air	(unspecified); high. pop.	5.96E-07	**22.4**	**1.33E-05**
4B	Zinc'	air	low. pop.; low. pop., long-term	5.60E-07	**32.3**	**1.81E-05**
	Total zinc in air: 1.16E-06 kg					
5	Chlorothalonil	soil	agricultural	1.82E-05	**4.20**	**7.64E-05**
6	Barium	water	groundwater, long-term	2.69E-05	2.77	7.45E-05
7	Beryllium	water	groundwater, long-term	7.49E-07	453	3.39E-04
8	Cobalt	water	groundwater, long-term	9.06E-06	33.1	3.00E-04
9	Manganese	water	groundwater, long-term	4.47E-04	**4.14**	**1.85E-03**
10	Selenium	water	groundwater, long-term	1.55E-06	89.3	1.38E-04
11	Vanadium, ion	water	groundwater, long-term	3.49E-06	94.7	3.31E-04
12	Zinc, ion	water	groundwater, long-term	6.63E-05	6.01	3.99E-04

Table 27A (cont'd)

13	Arsenic, ion	water	combined	2.23E-06	15.1	3.36E-05
14	Bromine	water	(unspecified); groundwater; river	3.66E-06	4.65	1.70E-05
15	Nickel, ion	water	combined	3.94E-05	95.9	3.78E-03
16	Tributyltin compounds	water	ocean	8.42E-09	**2060**	**1.74E-05**
17	Zinc, ion	water	ocean	1.99E-06	69.6	1.38E-04
18	Phosphorus	water	river	2.11E-05	6.71	1.42E-04
Total kg 1,4-DB Equiv. For Items In Table						0.008158
Reported kg 1,4-DB Equiv.						0.008375

[1] Items in **bold text** differ in characterization factors between SimaPro and GaBi.

Table 27B: GaBi / ReCiPe marine ecotoxicity for corrugated board

50% Recycled Content					
Item	Substance: Category	Substance: Name	Amount (kg)	Characterization Factor (kg 1,4-DB Equiv. per kg)	Impact (kg 1,4-DB Equiv.)
1	Heavy metals to air	Copper (+II)	5.85E-07	**0**	**0**
2	Heavy metals to air	Nickel (+II)	9.63E-07	**0**	**0**
3	Heavy metals to air	Vanadium (+III)	3.02E-06	**0**	**0**
4	Heavy metals to air	Zinc (+II)	1.16E-06	**0**	**0**
5	Pesticides to agricultural soil	Chlorothalonil	1.82E-05	**0**	**0**
6	ecoinvent long-term to fresh water	Barium	2.68E-05	2.77	7.44E-05
7	ecoinvent long-term to fresh water	Beryllium	7.45E-07	453	3.37E-04
8	ecoinvent long-term to fresh water	Cobalt	9.06E-06	33.1	3.00E-04
9	ecoinvent long-term to fresh water	Manganese (+II)	4.47E-04	**0**	**0**
10	ecoinvent long-term to fresh water	Selenium	1.58E-06	89.3	1.41E-04
11	ecoinvent long-term to fresh water	Vanadium (+III)	3.50E-06	94.7	3.31E-04
12	ecoinvent long-term to fresh water	Zinc (+II)	6.52E-05	6.01	3.92E-04
13	Heavy metals to fresh water	Arsenic (+V)	2.22E-06	15.1	3.35E-05
14	Inorganic emissions to fresh water	Bromine	3.66E-06	4.65	1.70E-05
15	Heavy metals to fresh water	Nickel (+II)	3.94E-05	95.9	3.78E-03
16	Pesticides to sea water	Tributyltinoxide	8.42E-09	**0**	**0**
17	Heavy metals to sea water	Zinc (+II)	1.99E-06	69.6	1.38E-04
18	Inorganic emissions to fresh water	Phosphorus	2.11E-05	6.71	1.42E-04
Total kg 1,4-DB Equiv. For Items In Table					0.005684
Reported kg 1,4-DB Equiv.					0.005806

[1] Items in **bold text** differ in characterization factors between SimaPro and GaBi.

11.2.4 Marine Eutrophication

ReCiPe data for the marine eutrophication category when obtaining and disposing of 1 kg of aluminum with 50% recycled content is given in Table 28A for SimaPro, and Table 28B for GaBi. SimaPro reported 0.001056 kg N equivalent while GaBi reported 0.004979 kg N equivalent, differing by a factor of 4.71. The 12 items in each table account for 99.9% of the impact reported by SimaPro, and effectively 100% of the impact reported by GaBi.

The majority of the difference between software came from the characterization factors for item 2, nitrogen oxide emissions to air. GaBi used a factor of 0.389, 10 times the value of 0.039 that SimaPro used. The characterization factor used by SimaPro matched the one in the spreadsheet versions of ReCiPe 1.05 and ReCiPe 1.08.

The next issue between the software was the characterization factors for items 5 and 11, organic bound nitrogen emissions to long-term groundwater and to ocean water. SimaPro used characterization factors of 1.00, which matched the factors in the spreadsheets for ReCiPe 1.05 and ReCiPe 1.08. GaBi had no characterization factor assigned, so these items did not contribute to the impact reported by GaBi. GaBi did use a characterization factor of 1.00 for organic bound nitrogen emission to fresh water (short-term), item 12.

SimaPro used a characterization factor of 0.23 for item 9, nitrate emissions to ocean (sea) water, which matched the factor in the spreadsheet version of ReCiPe 1.08. The spreadsheet version of ReCiPe 1.05 had a factor of 0.226, making it appear that at some point between the 1.05 and 1.08 versions the factor was rounded off or adjusted upward. GaBi did not have a characterization factor assigned for nitrate emissions to sea water; however, it did use the 0.226 factor for nitrate emissions to fresh water, item 8.

GaBi did not have a characterization factor for item 7, cyanide emissions to fresh water, which is in agreement with the spreadsheet version of ReCiPe 1.05. SimaPro used a factor of 0.54, which agrees with the spreadsheet for ReCiPe 1.08.

Table 28A: SimaPro / ReCiPe marine eutrophication for aluminum

50% Recycled Content						
Item	Substance Name			Amount (kg)	Characterization Factor (kg N Equiv. per kg)	Impact (kg N Equiv.)
	Name	Compartment	Sub-compartment(s)			
1	Ammonia	air	(unspecified); high. pop.; low. pop.	2.08E-04	0.092	1.92E-05
2	Nitrogen oxides	air	(unspecified); high. pop.; low. pop.	1.13E-02	**0.039**	**4.39E-04**
3	Ammonium ion	water	groundwater, long-term	1.61E-06	0.780	1.26E-06
4	Nitrate [2]	water	groundwater, long-term	2.21E-03	0.230	5.08E-04
5	Nitrogen, organic bound	water	groundwater, long-term	2.63E-06	**1.00**	**2.63E-06**
6	Ammonium ion, to water, river	water	(unspecified); groundwater; river	9.59E-06	0.780	7.48E-06
7	Cyanide	water	river	2.18E-06	**0.540**	**1.18E-06**
8	Nitrate [2]	water	groundwater, river	1.10E-04	0.230	2.53E-05
9	Nitrate	water	ocean	8.64E-06	**0.230**	**1.99E-06**
10	Nitrogen	water	river	2.62E-05	1.00	2.62E-05
11	Nitrogen, organic bound	water	ocean	2.15E-06	**1.00**	**2.15E-06**
12	Nitrogen, organic bound	water	river	2.11E-05	1.00	2.11E-05
Total kg N Equiv. For Items In Table						0.001055
Reported kg N Equiv.						0.001056

[1] Items in **bold text** differ in characterization factors between SimaPro and GaBi.

[2] Characterization factor appears rounded to two digit accuracy versus 3 digit in GaBi.

Table 28B: GaBi / ReCiPe marine eutrophication for aluminum

50% Recycled Content					
Item	Substance		Amount (kg)	Characterization Factor (kg N Equiv. per kg)	Impact (kg N Equiv.)
	Category	Name			
1	Inorganic emissions to air	Ammonia	2.08E-04	0.0920	1.92E-05
2	Inorganic emissions to air	Nitrogen oxides	1.13E-02	**0.389**	**4.38E-03**
3	ecoinvent long-term to fresh water	Ammonium / ammonia	1.61E-06	0.778	1.25E-06
4	ecoinvent long-term to fresh water	Nitrate	2.21E-03	0.226	4.99E-04
5	ecoinvent long-term to fresh water	Nitrogen organic bounded	2.63E-06	**0**	**0**
6	Inorganic emissions to fresh water	Ammonium / ammonia	9.59E-06	0.778	7.46E-06
7	Inorganic emissions to fresh water	Cyanide	2.21E-06	**0**	**0**
8	Inorganic emissions to fresh water	Nitrate	1.10E-04	0.226	2.49E-05
9	Inorganic emissions to sea water	Nitrate	8.64E-06	**0**	**0**
10	Inorganic emissions to fresh water	Nitrogen	2.62E-05	1.00	2.62E-05
11	Inorganic emissions to sea water	Nitrogen organic bounded	2.15E-06	**0**	**0**
12	Inorganic emissions to fresh water	Nitrogen organic bounded	2.11E-05	1.00	2.11E-05
Total kg N Equiv. For Items In Table					0.004979
Reported kg N Equiv.					0.004979

[1] Items in **bold text** differ in characterization factors between SimaPro and GaBi.

11.2.5 Water Depletion

ReCiPe data for the water depletion category when obtaining and disposing of 1 kg of aluminum with 50% recycled content is given in Table 29A for SimaPro, and Table 29B for GaBi. SimaPro reported 0.03174 m^3 of water while GaBi reported 165.1 m^3, differing by a factor of 5,200. The 7 items in each table account for 100% of the impact reported by both programs.

The greatest difference between results occurred due to item 6, “water, turbine use, unspecified natural origin/m3”. Tracing this resource backward through SimaPro, it appears to be water flowing through electrical power generation turbines. GaBi had a characterization factor of 1.00 for this item, and as such it is included in the impact reported by GaBi. SimaPro had a characterization factor of zero, so it did not contribute to the impact reported by SimaPro. Water going through a turbine had a zero characterization factor in the spreadsheet for ReCiPe 1.05, the version used with GaBi, but was changed to a factor of 1.00 in the spreadsheet for ReCiPe 1.08.

SimaPro split the volume of item 1 into two parts, one part with a characterization factor of 1.00 and the other with a zero factor, while GaBi combined the volume into a single entry with a characterization facto of 1.00. The spreadsheet for ReCiPe 1.05 agreed with SimaPro; however, the spreadsheet for ReCiPe 1.08 agreed with GaBi. This seems strange since the GaBi version is stated as being ReCiPe 1.05, while the SimaPro version is stated as being ReCiPe 1.06.

Items 4 and 5 in the tables had characterization factors of 1.00 for GaBi, and factors of zero for SimaPro. In both cases the spreadsheets for ReCiPe 1.05 and ReCiPe 1.08 matched SimaPro.

Table 29A: SimaPro / ReCiPe water depletion for aluminum

50% Recycled Content				
Item	Substance Name [2]	Amount (m^3)	Characterization Factor (m^3 per m^3)	Impact (m^3)
1A	Water, cooling, unspecified natural origin/m3	1.22E-01	**0**	**0**
1B	Water, unspecified natural origin/m^3, raw	9.47E-03	1.00	0.009472
	Total Water, unspecified: 1.31E-01 m^3			
2	Water, lake	8.38E-05	1.00	0.000084
3	Water, river	1.80E-02	1.00	0.018023
4	Water, salt, ocean	2.37E-03	**0**	**0**
5	Water, salt, sole	4.78E-04	**0**	**0**
6	Water, turbine use, unspecified natural origin/m3	1.65E+02	**0**	**0**
7	Water, well, in ground, raw	4.16E-03	1.00	0.004157
Total m^3 For Items In Table				0.03174
Reported m^3				0.03174

[1] Items in **bold text** differ in characterization factors between SimaPro and GaBi.

[2] All substances are from the SimaPro compartment "Raw".

Table 29B: GaBi / ReCiPe water depletion for aluminum

50% Recycled Content				
Item	Substance Name [2]	Amount (m^3)	Characterization Factor (m^3 per m^3)	Impact (m^3)
1	Water	1.31E-01	**1.00**	**0.131352**
2	Water (lake water)	8.38E-05	1.00	0.000084
3	Water (lake river)	1.80E-02	1.00	0.018023
4	Water (sea water)	2.37E-03	**1.00**	**0.002371**
5	Water, salt, sole	4.78E-04	**1.00**	**0.000478**
6	Water, turbine use, unspecified natural origin	1.65E+02	**1.00**	**164.9**
7	Water (ground water)	4.16E-03	1.00	0.004157
Total m^3 For Items In Table				165.1
Reported m^3				165.1

[1] Items in **bold text** differ in characterization factors between SimaPro and GaBi.

[2] All substances are from the GaBi category "Renewable resources".

11.3 TRACI 2

All comparisons for TRACI 2 were done using versions of the methodology supplied with the released versions of SimaPro and GaBi software available at the time. Comments in the SimaPro 7.3.3 method file for TRACI 2 state a version number of 4.00, with the last change occurring in 2012. There were no accessible comments or notes for the GaBi 5 implementation of TRACI 2. A spreadsheet containing the characterization factors for TRACI 2.1 was obtained for reference purposes from the EPA, the U.S. governmental agency responsible for the development of the TRACI methodology.

11.3.1 Ecotoxicity

TRACI 2 data for the ecotoxicity category when obtaining and disposing of 1 kg of glass with 55.5% recycled content is given in Table 30A for SimaPro, and Table 30B for GaBi. SimaPro reported 0.850 CTU_e (**C**omparative **T**oxic **U**nits, **e**cotoxicity potential) while GaBi reported 4.811 CTU_e, differing by a factor of 5.66. The 43 items in each table account for 98.5% of the impact reported by SimaPro, and 99.8% of the impact reported by GaBi.

A total of 24 of the 43 items in each table differ significantly in impact contribution between SimaPro and GaBi. The largest contributors to the difference in reported results came from items 31, 25, 30, and 39, in order of largest difference first. These were all metal ion emissions to water: zinc, copper, vanadium, and nickel. In all 4 cases GaBi had a non zero characterization factor assigned, while SimaPro had no factors assigned. The result was that these items contributed to the impact reported by GaBi, but not to the impact reported by SimaPro. For zinc, copper and nickel (items 31, 25, and 39) GaBi matched the characterization factors assigned to the substances in the spreadsheet version of TRACI 2.1. For vanadium, item 30, GaBi used the characterization factor for vanadium (V) from the spreadsheet version of TRACI 2.1. These same relationships between GaBi and the spreadsheet hold true for items 43, 37, and 42, which were smaller emissions of zinc, copper, and vanadium to other classifications of water.

While the aforementioned substances account for the large majority of difference in results between software for this comparison, there are 7 more instances where GaBi had non zero characterization factors while SimaPro used zeros. These could become significant in other comparisons as the mix of substances involved shift. For cobalt emissions to water in item 24, GaBi used the TRACI 2.1 characterization factor for cobalt (II). For silver ion, or silver, emissions to water in items 27 and 40, GaBi used the TRACI 2.1 characterization factor of silver (I). For cadmium ion, or cadmium (+II), emissions to water in item 35, GaBi matched the characterization factor for this substance in TRACI 2.1. For tin ion, or tin (+IV), emissions to water in items 29 and 41, GaBi used the TRACI 2.1 characterization factor of tin (II). For tin emissions to agricultural soil in item 15, GaBi again used the characterization factor of tin (II).

There are 5 instances shown in the tables where SimaPro had non zero characterization factors while GaBi used zeros. Two of these, items 3 and 12, were for chromium emissions to air and agricultural soil. In both cases it appears SimaPro used the average of the TRACI 2.1 spreadsheet characterization factors for chromium (III) and chromium (VI). The remaining 3 cases where GaBi had a zero characterization factor, items 10, 17, and 21, all involved barium. SimaPro used the TRACI 2.1 spreadsheet factor for barium (II).

There are 4 instances where SimaPro and GaBi both have non zero characterization factors that do not match; these all involved antimony. For items 1, 9, 20, and 32 SimaPro used the TRACI 2.1 spreadsheet characterization factors for antimony (V), while GaBi used the factors for antimony (III). The characterization factors for antimony (V) are approximately 155 times those of antimony (III).

Table 30A: SimaPro / TRACI 2 ecotoxicity for glass

55.5% Recycled Content						
Item	Substance			Amount (kg)	Characterization Factor(s) (CTUe per kg)	Impact (CTUe)
	Name	Compartment	Sub-compartment(s)			
1	Antimony [2]	air	high. pop.; low. pop.; low. pop., long-term	7.78E-08	**76,200 to 76,800**	**0.0059**
2	Arsenic [2]	air	high. pop.; low. pop.; low. pop., long-term	1.61E-07	16,900 to 17,100	0.0027
3	Chromium [2]	air	(unspecified); high. pop.; low. pop.	4.11E-07	**21,200 to 21,300**	**0.0087**
4	Copper [2]	air	(unspecified); high. pop.; low. pop.; low. pop., long-term	4.95E-07	23,100 to 23,300	0.0115
5	Nickel [2]	air	(unspecified); high. pop.; low. pop.; low. pop., long-term	4.06E-07	6,080 to 6,140	0.0025
6	Selenium	air	high. pop.; low. pop.	7.36E-06	2,960	0.0218
7	Vanadium [2]	air	high. pop.; low. pop.; low. pop., long-term	5.41E-07	46,200 to 46,700	0.0250
8	Zinc [2]	air	(unspecified); high. pop.; low. pop.; low. pop., long-term	7.73E-07	16,700 to 16,900	0.0130
9	Antimony	soil	agricultural	1.01E-07	**95,800**	**0.0096**
10	Barium	soil	agricultural	1.92E-06	**763**	**0.0015**
11	Chlorothalonil	soil	agricultural	9.82E-08	57800	0.0057
12	Chromium	soil	agricultural	1.70E-07	**26,600**	**0.0045**
13	Copper	soil	agricultural	2.60E-07	29,200	0.0076
14	Nickel	soil	agricultural	1.36E-07	7,660	0.0010
15	Tin	soil	agricultural	1.98E-07	**0**	**0**
16	Zinc	soil	agricultural	2.78E-07	21,100	0.0059
17	Barium	soil	industrial	2.02E-06	**763**	**0.0015**
18	Copper	soil	(unspecified)	5.07E-08	29,200	0.0015
19	Zinc	soil	(unspecified); industrial	2.35E-07	21,100	0.0050
20	Antimony	water	groundwater, long-term	5.47E-07	**190,000**	**0.1039**

Table 30A (cont'd)

21	Barium	water	groundwater, long-term	1.06E-05	**1,530**	**0.0163**
22	Beryllium	water	groundwater, long-term	3.06E-07	3,720	0.0011
23	Chromium VI	water	groundwater, long-term	2.45E-06	105,000	0.2568
24	Cobalt	water	groundwater, long-term	5.26E-06	**0**	**0**
25	Copper, ion	water	groundwater, long-term	1.35E-05	**0**	**0**
26	Lead	water	groundwater, long-term	1.35E-05	375	0.0051
27	Silver, ion	water	groundwater, long-term	2.65E-08	**0**	**0**
28	Thallium	water	groundwater, long-term	1.16E-07	35,400	0.0041
29	Tin, ion	water	groundwater, long-term	1.37E-06	**0**	**0**
30	Vanadium, ion	water	groundwater, long-term	4.75E-06	**0**	**0**
31	Zinc, ion	water	groundwater, long-term	6.34E-05	**0**	**0**
32	Antimony	water	(unspecified); groundwater; river	4.49E-07	**190,000**	**0.0853**
33	Arsenic, ion	water	groundwater; groundwater, long-term; river	3.12E-06	40,400	0.1262
34	Barium	water	river	4.76E-06	**1,530**	**0.0073**
35	Cadmium, ion	water	(unspecified); groundwater; groundwater, long-term; river	7.38E-07	**0**	**0**
36	Chromium VI	water	groundwater; river	9.03E-07	105,000	0.0948
37	Copper, ion	water	(unspecified); groundwater; river	3.17E-07	**0**	**0**
38	Mercury	water	(unspecified); groundwater; groundwater, long-term; river	6.22E-08	22,100	0.0014
39	Nickel, ion	water	(unspecified); groundwater; groundwater, long-term; river	2.49E-05	**0**	**0**
40	Silver, ion	water	(unspecified); groundwater; river	5.22E-09	**0**	**0**
41	Tin, ion	water	groundwater; river	3.70E-07	**0**	**0**
42	Vanadium, ion	water	groundwater; ocean; river	3.30E-08	**0**	**0**
43	Zinc, ion	water	(unspecified); groundwater; river	1.07E-06	**0**	**0**
Total CTU_e For Items In Table						0.837
Reported CTU_e						0.850

Table 30A (cont'd)

[1] Items in **bold text** differ in characterization factors between SimaPro and GaBi.
[2] Characterization factors vary with sub-compartments, maximum variation does not exceed 2%.

Table 30B: GaBi / TRACI 2 ecotoxicity for glass

55.5% Recycled Content					
Item	Substance		Amount (kg)	Characterization Factor (CTUe per kg)	Impact (CTUe)
	Category	Name			
1	Heavy metals to air	Antimony	7.78E-08	**491**	**0.0000**
2	Heavy metals to air	Arsenic (+V)	1.61E-07	17,000	0.0027
3	Heavy metals to air	Chromium (unspecified)	4.11E-07	**0**	**0**
4	Heavy metals to air	Copper (+II)	4.95E-07	23,200	0.0115
5	Heavy metals to air	Nickel (+II)	4.06E-07	6,110	0.0025
6	Heavy metals to air	Selenium	7.36E-06	2,980	0.0219
7	Heavy metals to air	Vanadium (+III)	5.42E-07	46,400	0.0251
8	Heavy metals to air	Zinc (+II)	7.73E-07	16,800	0.0130
9	Heavy metals to agricultural soil	Antimony	1.01E-07	**615**	**0.0001**
10	Inorganic emissions to agricultural soil	Barium	1.92E-06	**0**	**0**
11	Pesticides to agricultural soil	Chlorothalonil	9.82E-08	57,800	0.0057
12	Heavy metals to agricultural soil	Chromium (unspecified)	1.70E-07	**0**	**0**
13	Heavy metals to agricultural soil	Copper (+II)	2.60E-07	29,200	0.0076
14	Heavy metals to agricultural soil	Nickel (+II)	1.36E-07	7,660	0.0010
15	Heavy metals to agricultural soil	Tin (+IV)	1.98E-07	**1,710**	**0.0003**
16	Heavy metals to agricultural soil	Zinc (+II)	2.78E-07	21,100	0.0059
17	Inorganic emissions to industrial soil	Barium	2.02E-06	**0**	**0**

Table 30B (cont'd)

18	Heavy metals to industrial soil	Copper (+II)	5.10E-08	29,200	0.0015
19	Heavy metals to industrial soil	Zinc (+II)	2.35E-07	21,100	0.0050
20	ecoinvent long-term to fresh water	Antimony	5.47E-07	**1,222**	**0.0007**
21	ecoinvent long-term to fresh water	Barium	1.06E-05	**0**	**0**
22	ecoinvent long-term to fresh water	Beryllium	3.06E-07	3,720	0.0011
23	ecoinvent long-term to fresh water	Chromium (+VI)	2.45E-06	105,000	0.2573
24	ecoinvent long-term to fresh water	Cobalt	5.26E-06	**4,100**	**0.0216**
25	ecoinvent long-term to fresh water	Copper (+II)	1.35E-05	**55,200**	**0.7452**
26	ecoinvent long-term to fresh water	Lead (+II)	1.35E-05	375	0.0051
27	ecoinvent long-term to fresh water	Silver	2.65E-08	**194,000**	**0.0051**
28	ecoinvent long-term to fresh water	Thallium	1.16E-07	35,400	0.0041
29	ecoinvent long-term to fresh water	Tin (+IV)	1.37E-06	**2,980**	**0.0041**
30	ecoinvent long-term to fresh water	Vanadium (+III)	4.75E-06	**113,000**	**0.5368**
31	ecoinvent long-term to fresh water	Zinc (+II)	6.34E-05	**38,600**	**2.4472**
32	Heavy metals to fresh water	Antimony	4.49E-07	**1,220**	**0.0005**
33	Heavy metals to fresh water	Arsenic (+V)	3.16E-06	40,400	0.1277
34	Inorganic emissions to fresh water	Barium	4.77E-06	**0**	**0**
35	Heavy metals to fresh water	Cadmium (+II)	7.38E-07	**9,710**	**0.0072**
36	Heavy metals to fresh water	Chromium (+VI)	9.22E-07	105,000	0.0968
37	Heavy metals to fresh water	Copper (+II)	3.17E-07	**55,200**	**0.0175**
38	Heavy metals to fresh water	Mercury (+II)	6.22E-08	22,100	0.0014
39	Heavy metals to fresh water	Nickel (+II)	2.49E-05	**14,900**	**0.3710**
40	Heavy metals to fresh water	Silver	5.22E-09	**194,000**	**0.0010**
41	Heavy metals to fresh water	Tin (+IV)	3.70E-07	**2,980**	**0.0011**
42	Heavy metals to fresh water	Vanadium (+III)	3.30E-08	**113,000**	**0.0037**
43	Heavy metals to fresh water	Zinc (+II)	1.07E-06	**38,600**	**0.0413**
Total CTUe For Items In Table					4.801
Reported CTUe					4.811

[1] Items in **bold text** differ in characterization factors between SimaPro and GaBi.

11.3.2 Global Warming

TRACI 2 data for the global warming category when obtaining and disposing of 1 kg of corrugated board with 50% recycled content is given in Table 31A for SimaPro, and Table 31B for GaBi. SimaPro reported 0.984 kg CO_2 equivalent while GaBi reported 0.734 kg CO_2 equivalent, differing by a factor of 1.34. The 6 items in each table account for 99.8% of the impact reported by SimaPro, and 99.5% of the impact reported by GaBi.

The differences for this impact category came from GaBi including biotic carbon dioxide, biotic methane, and a credit for carbon sequestration in its reported impact, while SimaPro did not. The credit was taken in item 1, where carbon dioxide removed from the air and sequestered in the biomass used to produce the corrugated board got an effective characterization factor of -1.00 from GaBi, and a factor of zero from SimaPro. Item 2 covered biotic carbon dioxide where GaBi assigned a characterization factor of 1.00, and SimaPro a zero. Item 5 covered biotic methane where GaBi assigned a characterization factor of 25.0, and SimaPro another zero.

The spreadsheet version of TRACI 2.1 had characterization factors of 1.00 for carbon dioxide, and 25.0 for methane; however, there were no references for biotic carbon dioxide, biotic methane, or providing a credit for carbon sequestration. The only guideline for including biotic carbon, biotic methane, and carbon sequestration credit given in the paper discussing the TRACI 2 methodology (Bare 2011) was a reference to a 100-year time horizon for global warming potential.

Table 31A: SimaPro / TRACI 2 global warming for corrugated board

50% Recycled Content						
Item	Substance			Amount (kg)	Characterization Factor ($kg\ CO_2$ Equiv. per kg)	Impact ($kg\ CO_2$ Equiv.)
	Name	Compartment	Sub-compartment(s)			
1	Carbon dioxide, in air	air	(combined)	-1.36E+00	**0**	**0**
2	Carbon dioxide, biogenic	air	(combined)	9.53E-01	**0**	**0**
3	Carbon dioxide, fossil	air	(combined)	9.16E-01	1.00	0.916
4	Dinitrogen monoxide	air	(combined)	6.09E-05	298	0.018
5	Methane, biogenic	air	(combined)	7.13E-03	**0**	**0**
6	Methane, fossil	air	(combined)	1.95E-03	25.0	0.049
Total kg CO_2 Equiv. For Items In Table						0.983
Reported kg CO_2 Equiv.						0.984

[1] Items in **bold text** differ in characterization factors between SimaPro and GaBi.

Table 31B: GaBi / TRACI 2 global warming for corrugated board

50% Recycled Content					
Item	Substance: Category	Substance: Name	Amount (kg)	Characterization Factor (kg CO_2 eq per kg)	Impact (kg CO_2 eq)
1	Renewable Resources	Carbon Dioxide	1.38E+00	**-1.00**	**-1.380**
2	Inorganic emissions to air	Carbon Dioxide (biotic)	9.79E-01	**1.00**	**0.979**
3	Inorganic emissions to air	Carbon Dioxide	9.16E-01	1.00	0.916
4	Inorganic emissions to air	Nitrous Oxide (laughing gas)	6.10E-05	298	0.018
5	Organic emissions to air (group VOC)	Methane (biotic)	5.94E-03	**25.0**	**0.149**
6	Organic emissions to air (group VOC)	Methane	1.95E-03	25.0	0.049
Total kg CO_2 eq For Items In Table					0.730
Reported kg CO_2 eq					0.734

[1] Items in **bold text** differ in characterization factors between SimaPro and GaBi.

11.3.3 Non Carcinogens

TRACI 2 data for the non carcinogens category when obtaining and disposing of 1 kg of PET with 0% recycled content is given in Table 32A for SimaPro, and Table 32B for GaBi. SimaPro reported 4.43E-07 CTUh (**C**omparative **T**oxic **U**nits, **h**uman toxicity potential) while GaBi reported 7.96E-07 CTUh, differing by a factor of 1.80. The 17 items in each table account for 99.0% of the impact reported by SimaPro, and 99.1% of the impact reported by GaBi.

SimaPro characterization factors for chromium emissions to air in item 3 appear to be the average of the TRACI 2.1 spreadsheet factors for chromium (III) and chromium (VI), GaBi had no factor assigned for this item. SimaPro impact factors for barium emissions to water in items 9 and 14 were the same as the TRACI 2.1 spreadsheet factor for barium (II) to freshwater; GaBi had no factor assigned for these items. All 3 of these items contributed to the impact reported by SimaPro, but not to the impact reported by GaBi.

The GaBi characterization factor for vanadium ion, or vanadium (+III), emissions to water in item 10 matched the TRACI 2.1 spreadsheet factor for vanadium (V) to freshwater. No factor for vanadium (+III) was found in the TRACI 2.1 spreadsheet. SimaPro did not have a factor assigned for this item, so it did not contribute to the impact reported by SimaPro.

GaBi characterization factors for zinc ion, or zinc (+II), emissions to water in items 11 and 17 matched the TRACI 2.1 spreadsheet factor for zinc(II). The GaBi characterization factor for cadmium ion, or cadmium (+II), emissions to water in item 15 matched the TRACI 2.1 spreadsheet factor for cadmium(II). SimaPro did not have factors assigned for these items, so they did not contribute to the impact reported by SimaPro.

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Table 32A: SimaPro / TRACI 2 non carcinogens for PET

0% Recycled Content						
Item	Substance			Amount (kg)	Characterization Factor(s) (CTUh per kg)	Impact (CTUh)
	Name	Compartment	Sub-compartment(s)			
1	Arsenic [2]	air	(unspecified); high. pop.; low. pop.; low. pop., long-term	6.14E-07	1.65E-02 to 1.71E-02	1.02E-08
2	Cadmium [2]	air	(unspecified)l high. pop.; low. pop.	2.38E-07	4.45E-02 to 4.65E-02	1.09E-08
3	Chromium [3]	air	(unspecified)l high. pop.; low. pop.	8.05E-06	**4.15E-5 to 2.08E-4**	**1.55E-09**
4	Lead [2]	air	(unspecified); high. pop.; low. pop.; low. pop., long-term	1.91E-06	9.32E-03 to 9.57E-03	1.82E-08
5	Mercury [2]	air	(unspecified); high. pop.; low. pop.; low. pop., long-term	5.92E-08	8.15E-01 to 8.55E-01	4.98E-08
6	Zinc [2]	air	(unspecified); high. pop.; low. pop.; low. pop., long-term	3.55E-06	1.52E-02 to 1.60E-02	5.60E-08
7	Zinc	soil	agricultural	4.33E-08	4.35E-02	1.88E-09
8	Antimony	water	groundwater, long-term	4.64E-05	3.64E-04	1.69E-08
9	Barium	water	groundwater, long-term	6.57E-05	**9.82E-05**	**6.46E-09**
10	Vanadium, ion	water	groundwater, long-term	2.41E-04	**0**	**0**
11	Zinc, ion	water	groundwater, long-term	2.41E-04	**0**	**0**
12	Antimony	water	groundwater; river	2.05E-05	3.64E-04	7.47E-09
13	Arsenic, ion	water	groundwater; groundwater, long-term; river	9.31E-06	2.74E-02	2.55E-07

Table 32A (cont'd)

14	Barium	water	(unspecified); groundwater; river	5.21E-06	**9.82E-05**	**5.11E-10**
15	Cadmium, ion	water	groundwater; groundwater, long-term; river	4.55E-06	**0**	**0**
16	Mercury	water	groundwater; groundwater, long-term; river	2.99E-07	1.42E-02	4.25E-09
17	Zinc, ion	water	(unspecified); groundwater; river	2.67E-06	**0**	**0**
Total CTUh For Items In Table						4.39E-07
Reported CTUh						4.43E-07

[1] Items in **bold text** differ in characterization factors between SimaPro and GaBi.

[2] Characterization factors vary with sub-compartments, maximum variation does not exceed 5%.

[3] Characterization factors vary with sub-compartments by a multiple of 5.

Table 32B: GaBi / TRACI 2 non carcinogens for PET

0% Recycled Content					
Item	Substance		Amount (kg)	Characterization Factor(s) (CTUh per kg)	Impact (CTUh)
	Category	Name			
1	Heavy metals to air	Arsenic (+V)	6.14E-07	1.68E-02	1.03E-08
2	Heavy metals to air	Cadmium (+II)	2.39E-07	4.55E-02	1.09E-08
3	Heavy metals to air	Chromium (unspecified)	8.05E-06	**0**	**0**
4	Heavy metals to air	Lead (+II)	1.91E-06	9.44E-03	1.80E-08
5	Heavy metals to air	Mercury (+II)	5.92E-08	8.35E-01	4.94E-08
6	Heavy metals to air	Zinc (+II)	3.55E-06	1.56E-02	5.54E-08
7	Heavy metals to agricultural soil	Zinc (+II)	4.33E-08	4.35E-02	1.88E-09
8	ecoinvent long-term to fresh water	Antimony	4.64E-05	3.64E-04	1.69E-08
9	ecoinvent long-term to fresh water	Barium	6.57E-05	**0**	**0**
10	ecoinvent long-term to fresh water	Vanadium (+III)	2.41E-04	**1.94E-04**	**4.68E-08**
11	ecoinvent long-term to fresh water	Zinc (+II)	2.41E-04	**1.28E-03**	**3.08E-07**
12	Heavy metals to fresh water	Antimony	2.05E-05	3.64E-04	7.46E-09
13	Heavy metals to fresh water	Arsenic (+V)	9.31E-06	2.73E-02	2.54E-07
14	Inorganic emissions to fresh water	Barium	5.21E-06	**0**	**0**
15	Heavy metals to fresh water	Cadmium (+II)	4.55E-06	**4.27E-04**	**1.94E-09**
16	Heavy metals to fresh water	Mercury (+II)	3.00E-07	1.42E-02	4.26E-09
17	Heavy metals to fresh water	Zinc (+II)	2.67E-06	**1.28E-03**	**3.42E-09**
Total CTUh For Items In Table					7.89E-07
Reported CTUh					7.96E-07

[1] Items in **bold text** differ in characterization factors between SimaPro and GaBi.

11.3.4 Respiratory Effects

TRACI 2 data for the respiratory effects category when obtaining and disposing of 1 kg of aluminum with 50% recycled content is given in Table 33A for SimaPro, and Table 33B for GaBi. SimaPro reported 0.0120 kg PM10 equivalent while GaBi reported 0.0210 kg PM10 equivalent, differing by a factor of 1.75. The 5 items in each table account for 100% of the impacts reported by SimaPro and GaBi.

Perhaps the most interesting aspect of how this category was handled in SimaPro and GaBi isn't a difference that occurred between them, but rather it is a similarity; both software programs reported the impact for this category in terms of kg PM10 equivalent. This is surprising because the TRACI 2.1 spreadsheet only provides characterization factors that use kg PM2.5 equivalent as the reference substance. A check of the user's manual for TRACI 2 (Bare 2012) confirmed that the expected reference is kg PM2.5 equivalent. After further investigation, a comment was found in the paper introducing TRACI 2 (Bare 2011) that stated the original TRACI methodology for this impact category was changed for TRACI 2, going from PM10 based to PM2.5 based.

GaBi assigned a characterization factor of 1.00 to item 1, particles > 10 μm, while SimaPro had no factor assigned, so this item only contributed to the impact reported by GaBi. Item 2, particles between 2.5 μm and 10μm, is assigned a characterization factor of 1.00 by SimaPro, and a factor of 1.67 by GaBi. This means the mass for this item had proportionally more effect on the impact reported by GaBi than the impact reported by SimaPro. SimaPro and GaBi agreed the characterization factor for item 3, particles < 2.5 μm, should be 1.67. Since the spreadsheet for TRACI 2.1 listed a different reference substance, it did not provide any insight regarding the discrepancies in characterization factors between SimaPro and GaBi for this impact category.

Table 33A: SimaPro / TRACI 2 respiratory effects for aluminum

50% Recycled Content						
Item	Substance			Amount (kg)	Characterization Factor (kg PM10 Equiv. per kg)	Impact (kg PM10 Equiv.)
	Name	Compartment	Sub-compartment(s)			
1	Particulates > 10 µm	air	(combined)	6.45E-03	**0**	**0**
2	Particulates > 2.5 µm and < 10 µm	air	(combined)	3.80E-03	**1.00**	**3.80E-03**
3	Particulates < 2.5 µm	air	(combined)	2.63E-03	1.67	4.39E-03
4	Nitrogen oxides	air	(combined)	1.13E-02	0.0265	2.99E-04
5	Sulfur dioxide	air	(combined)	2.11E-02	0.167	3.51E-03
Total kg PM10 Equiv. For Items In Table						0.0120
Reported kg PM10 Equiv.						0.0120

[1] Items in **bold text** differ in characterization factors between SimaPro and GaBi.

Table 33B: GaBi / TRACI 2 respiratory effects for aluminum

50% Recycled Content					
Item	Substance		Amount (kg)	Characterization Factor (kg PM10 Equiv. per kg)	Impact (kg PM10 Equiv.)
	Category	Name			
1	Particles to air	Dust (>PM10)	6.47E-03	**1.00**	**6.47E-03**
2	Particles to air	Dust (PM2,5 - PM10)	3.80E-03	**1.67**	**6.35E-03**
3	Particles to air	Dust (PM2,5)	2.63E-03	1.67	4.39E-03
4	Inorganic emissions to air	Nitrogen oxides	1.13E-02	0.0265	2.99E-04
5	Inorganic emissions to air	Sulphur dioxide	2.11E-02	0.167	3.52E-03
Total kg PM10 Equiv. For Items In Table					0.0210
Reported kg PM10 Equiv.					0.0210

[1] Items in **bold text** differ in characterization factors between SimaPro and GaBi.

11.4 Summary Of Underlying Causes Of Dissimilar Results

A total of 14 combinations of basic materials and impact categories from 3 different impact assessment methods were examined, with the end result that all significant discrepancies between impact assessments from GaBi and SimaPro were traced to differences in the characterization factors used to implement the assessment methods. Table 34 summaries the 98 differences in characterization factors that were found. No differences were found in the LCI of the two programs for the type and amount of significant contributors to the impact assessments examined, and all calculations performed by the programs to convert LCI data to impact assessments were verified as being correct.

Table 34: Summary of differences in GaBi and SimaPro characterization factors

Characterization Factor Data	Impact 2002+	ReCiPe	TRACI 2
Number of impact categories/material combinations examined	5	5	4
Instances where GaBi had a characterization factor of zero while SimaPro had non zero.	9	21	9
Instances where GaBi had a non zero characterization factor while SimaPro had zero.	22	4	22
Instances where GaBi and SimaPro both had non zero characterization factors that differed by more than 10%.	2	0	5
Instances where SimaPro had spelling differences between substance and characterization factor names, resulting in zero being used.	4	0	0

12. RESEARCH SUMMARY & CONCLUSIONS

Through a series of tests, several life cycle assessment software programs were compared to each other to establish how consistent the results are from one program to the next. Comparisons were made involving complete packaging systems and basic packaging materials, as well as an examination of how individual substances contribute to reported environmental impact estimates. It was found that impact assessments can vary widely between software programs.

While an argument might be made that variation is to be expected when dealing with programs based on different impact assessment methodologies, comparisons done here show that even when the same methodology is used and the inputs are matched as closely as possible, implementations of a supposedly common methodology in different software can provide different results. One example of this is the global warming category in the Impact 2002+ version 2.1 assessment method; GaBi included biotic carbon dioxide and a credit for carbon sequestration while SimaPro did not. A similar issue was found between GaBi and SimaPro for the global warming category in the TRACI 2 methodology. Another example is the water depletion category in ReCiPe; GaBi includes water going through electrical generation turbines and SimaPro does not, causing GaBi to report a result that is several orders of magnitude larger than that reported by SimaPro.

For the small set of basic materials and impact categories examined, the most common cause of differences between implementations of impact assessment methods in SimaPro and GaBi is one software including characterization factors for substances that the other software excludes. There is no consistency as to which software includes a substance and which excludes it; this varies with impact category and substance. There are also instances where both SimaPro and GaBi have non-zero characterization factors for a substance, but the factors differ significantly. Whether or not a difference in characterization factors has a significant effect on reported impacts depends on the amount of the substance in the life cycle inventory. The aforementioned issue with global warming was much more noticeable when the comparison included corrugated board with a low percent of recycled fiber, meaning higher virgin fiber content, than when the percent of recycled fiber was high. The water depletion issue comes into play more as hydroelectric power use increases. Whenever there is a difference in characterization factors between software, there is the inherent possibility that impacts reported by the software will significantly disagree for some conditions and not for others.

Life cycle assessment software has the potential to simplify the often complex and time consuming task of doing life cycle analysis. For it to fulfill that potential there needs to be consistency in results that users can rely on. This is particularly true when using a common impact assessment methodology. If the implementations of an impact assessment methodology vary, then expectations of consistent results are lost, diminishing the usefulness of the software.

Providers of life cycle assessment software have commercial interests in selling their own programs, so the task of identifying differences in assessment methods between software and promoting consistency in results falls on the users. It is recommended that as new versions of software are released they should be subjected to comparison testing. For fully ISO 14040/14044 compliant software such as SimaPro and GaBi, the use of basic materials and a common database, when combined with the practice of accounting for all the mass of each substance that makes a significant contribution to the reported results, can provide a basis for such comparisons.

This paper has used a broad study of impact categories to establish that the choice of LCA software can significantly affect results. What is needed in future work on this subject is to focus on how these inconsistencies affect different areas of research that rely on LCA. Many assessment methods cover multiple environmental impact categories, yet only a subset of impact categories may be used in research on a given subject. For example, researchers on carbon footprint would be far more interested in the Global Warming impact category of Impact 2002+ than either the Ozone Layer Depletion or Terrestrial Ecotoxicity categories. Key items of interest in LCA for different subject areas need to be identified, and studies conducted to identify and rectify any inconsistencies between LCA software programs that can affect research in each subject area.

APPENDICES

APPENDIX A: Population, MSW, and Oil Consumption Data

Table A1: World population estimates

Year	Population (billions of people)
1804	1
1922	2
1959	3
1974	4
1987	5
1999	6
2013	7
2028	8
2048	9

Source: U.S. Census Bureau (U.S. Census 2002)

Table A2: U.S. Population and waste generation estimates

Year	Total Generated Municipal Solid Waste (millions of tons)	Total Containers & Packaging In Waste Stream (millions of tons)	Population (millions of people)
1960	88.12	27.37	180.67
1970	121.06	43.56	205.05
1980	151.64	52.67	227.73
1990	208.27	64.53	250.13
2000	242.54	75.84	282.39
2010	249.86	75.64	309.33
Percent Change 1960 to 2010	184%	176%	71%

Sources: U.S. Census Bureau (U.S. Census 2012, 2013)
U.S. Environmental Protection Agency (EPA 2011)

Table A3: World, U.S., and China oil consumption in thousands of barrels per day

Year	World	U.S.	China
1980	63,120	17,056	1,765
1985	60,085	15,726	1,885
1990	66,550	16,989	2,296
1995	70,132	17,725	3,363
2000	76,788	19,701	4,796
2005	84,089	20,802	6,695
2010	87,314	19,180	9,330
Percent Change 1960 to 2010	38.3%	12.5%	429%

Source: United States Energy Information Administration (EIA 2013)

APPENDIX B: Container Modeling Assumptions

Process Assumptions

1. Liners in caps were omitted from the study.
2. Label adhesives were omitted from the study.
3. Printing of labels and containers was included for selected products.
4. Filling of containers was omitted from the study.
5. Distribution center handling was omitted from the study.
6. Retail sales handling was omitted from the study.
7. Consumer use (end use) was omitted from the study.
8. Production scrap and shipping/handling damage was omitted from the study.
9. Affect of varying transport distances was included for selected products.

Functional Units and Units Of Measure

1. Functional unit for tuna in steel can and tuna in pouch was 1kg of product.
2. Functional unit for PLA bottle (water), aseptic carton (juice), glass bottle (beer), PET bottle (carbonated beverage), and aluminum Can (carbonated beverage) was 1 liter of fluid.
3. Functional unit for plastic (PP) crate (flowers) and corrugated box (flowers) was ½ box dry pack flowers.
4. Analysis was done in metric units.

Reuse

1. PP crates were modeled for 1, 10, and 100 uses.

Product Specific Assumptions

1. Refrigerated truck transport of flower boxes/crates was modeled as truck transport combined with a separate refrigeration function based on volume of material and time for transport. A transport speed of 100km per hour (62.1 miles per hour) was assumed when determining time for refrigerated truck transport. The volume of material (PP or corrugated board) used to produce the box/crate was used as shipping volume, not the volume of the container. The interior volume of the container was allocated to the product (flowers), not the package.
2. Air transport distance used for flower boxes/crates on the out going trip was 500km and 2500km. Ship transport distance used for flower crates on the return trip was 500km and 2100km. Standard truck transport distance used for flower crates on the return trip was 1200km. Air, ship, and truck transport distances between cities came from an unpublished report on distribution of cut flowers done at MSU School of Packaging. Air transport distance from Bogota, Colombia to Miami, FL is 2446km. Ship transport distance from Port Everglade, FL to Cartagena, Colombia is 2043km.
3. Rail transport distance for beer bottles was 0, 500km, and 4000km. Chicago to St. Louis by rail is 459km, or 285 miles, and Chicago to San Francisco by rail is 3927km, or 2440 miles (Rail Passenger USA 2011).

Recycling and Waste Disposal

1. At least two recycling rates, or composting rates in the case of PLA, were used with various products to see if different LCA software produced results that tracked each other (correlated).
2. Where available, typical recycling rates in US for a product, rounded to the nearest 10%, were used as one reference point.
3. What was not recycled or composted went to landfill/incineration, with the U.S. averages of 82% to landfill and 18% to incineration being used (EPA 2009).

Recycled Content In United States

1. Aluminum can (beverage): 68% (Aluminum Association 2011).
2. Aseptic carton (juice): No recycled content data found.
3. Corrugated box (flowers): 41.85% (Corrugated Packaging Alliance 2010).
4. Flexible pouch (tuna): No recycled content data found.
5. Glass bottle (beer): 27% (Glass Packaging Institute 2010).
6. PET bottle (beverage): 3% (EPA 2010).
7. PLA bottle (water): No recycled content data found.
8. PP crate (flowers): No recycled content data found.
9. Steel can (tuna): 25% (American Iron and Steel Institute 2010).

Recycling and Composting Rates For United States

1. Aluminum can (beverage): 50.7% Recycled (EPA 2009).
2. Aseptic carton (juice): 6.5% Recycled (EPA 2009).

3. Corrugated box (flowers): 81.3% Recycled (EPA 2009).
4. Flexible pouch (tuna): 0.0% Recycled (Bumble Bee Foods 2011).
5. Glass bottle (beer): 39.0% Recycled (EPA 2009).
6. PET bottle (beverage): 28.0% Recycled (EPA 2009).
7. PLA bottle (water): No composting or recycling data found.
8. PP crate (flowers): 7.4% Recycled (EPA 2009).
9. Steel can (tuna): 66.0% Recycled (EPA 2009).

APPENDIX C: Container Compositions and Material Weights

Aluminum Beverage Can

Weight information for a 12oz (354.9ml) aluminum beverage can taken from an unpublished study done at MSU School of Packaging.

Can dimensions: 12.1cm high x 6.5cm diameter (at widest point).

Cube utilization: 69.4% (based on volume occupied by fluid).

Average weight of can based on 5 samples: 13.018g

Functional unit is 1 liter of fluid (beverage).

There are 2.818 cans per functional unit.

Weight of aluminum for functional unit: 36.68g.

No area estimate for printing.

Aseptic Carton

6 cartons of juice, 200ml each, were acquired for this project.

Carton dimensions: 10.6cm high x 5.6cm long x 3.8cm wide.

Cube utilization: 88.7% (based on volume occupied by fluid).

Table C1: Weight of aseptic carton components

Carton	Unopened Weight (g)	Weight Of Empty Carton (g)	Weight Of Straw (g)	Weight of Straw Bag (g)
1	219.9	9.333	0.372	0.159
2	220.1	9.286	0.373	0.140
3	220.1	9.407	0.374	0.156
4	219.8	9.306	0.371	0.148
5	219.8	9.352	0.375	0.148
6	220.0	9.363	0.373	0.137
Average	220.0	9.341	0.373	0.148
St. Dev.	0.1	0.043	0.001	0.009

Functional unit is 1 liter of fluid (juice).

There are 5.000 cartons per functional unit.

Table C2: Packaging material used for aseptic carton

Item	Type of Material	Percent By Weight	Weight Per Container (g)	Weight Per Functional Unit (g)
Box	SBS	75	7.006	35.029
	PE	20	1.868	9.341
	aluminum foil	5	0.467	2.335
Straw	PP	100	0.373	1.865
Straw Bag	PP	100	0.148	0.740

Carton area for printing estimate: 0.200m long x 0.155m wide = 0.0310m^2.

Corrugated Box

Weight information for corrugated box taken from an unpublished study on distribution of cut flowers done at MSU School of Packaging.

Cube utilization: assume 100% for the purposes of this study.

Average weight of box based on 2 samples: 700g

Functional unit is ½ flower box (common unit in flower industry).

There is 1 corrugated box per functional unit.

Weight of corrugated board for functional unit: 700g.

No area estimate for printing.

Flexible Pouch

6 pouches of 74g net weight tuna were acquired for this project.

Pouch dimensions: 16cm long x 11.5cm wide, thickness varies.

Cube utilization: assume 100% for the purposes of this study.

Table C3: Weight of flexible pouches

Pouch	Unopened Weight (g)	Emptied Weight (g)
1	80.42	6.223
2	83.03	6.460
3	82.16	6.378
4	78.11	6.384
5	77.77	6.245
6	83.04	6.433
Average	80.76	6.354
St. Dev.	2.38	0.098

Functional unit is 1kg net weight of tuna.

There are 13.514 pouches per functional unit.

Table C4: Packaging material used for flexible pouch

Item	Type Of Material	Percent By Weight	Weight Per Container (g)	Weight Per Functional Unit (g)
Pouch	PET	40	2.542	34.345
	PP	40	2.542	34.345
	aluminum foil	15	0.953	12.879
	nylon	5	0.318	4.293

Pouch area for printing estimate: 2 x 0.160 long x 0.115m wide = 0.0368m^2.

Glass Beer Bottle

6 bottles of beer, 12oz (354.9ml) each, were acquired for this project.

Bottle dimensions: 23cm high x 5.9cm diameter (at base).

Cube utilization: 44.3% (based on volume occupied by fluid).

Table C5: Weight of bottle components

Bottle	Unopened Weight (g)	Weight of Empty Bottle (g)	Total Weight Of Labels (g)	Weight of Cap (g)
1	530.0	187.362	0.385	2.106
2	529.7	187.012	0.391	2.152
3	529.9	187.231	0.340	2.103
4	531.0	188.292	0.393	2.122
5	530.2	187.493	0.410	2.099
6	529.9	187.218	0.407	2.126
Average	530.1	187.4	0.388	2.118
St. Dev.	0.451	0.450	0.025	0.020

Functional unit is 1 liter of fluid (beer).

There are 2.818 bottles per functional unit.

Table C6: Packaging material used for beer bottle

Item	Type of Material	Weight Per Container (g)	Weight Per Functional Unit (g)
Bottle	glass (brown)	187.434	528.133
Label	bi-axially oriented PP	0.388	1.093
Cap	steel	2.118	5.969

Surface area of sheet steel needed for cap: 0.00168m^2.

Table C7: Label areas for printing estimate

Item	Length (m)	Width (m)	Area (m^2)
Front label	0.064	0.076	0.004864
Back label	0.048	0.052	0.002496
Neck label	0.038	0.017	0.000646
Total area			0.008006

PET Carbonated Beverage Bottle

Weight information for a 12oz (354.9ml) PET bottle taken from an unpublished study done at MSU School of Packaging. Bottle dimensions and cube utilization for 12oz bottle estimated from dimensions of 20oz bottle by assuming height as the only variable.

Bottle dimensions: 15.4cm high x 7.0cm diameter (at base).

Cube utilization: 47.0% (based on volume occupied by fluid).

Functional unit is 1 liter of fluid (carbonated beverage).

There are 2.818 bottles per functional unit.

Table C8: Packaging material used for PET bottle

Item	Type of Material	Weight Per Container (g)	Weight Per Functional Unit (g)
Bottle	PET	24.221	68.247
Label	PP	2.707	7.628
Cap	PP	2.870	8.087

Label area for printing estimate: 0.064m long x 0.029m wide = $0.00186m^2$.

PLA Water Bottle

6 bottles of water, 500ml per bottle, were acquired for this project.

Bottle dimensions: 21.3cm high x 6.4cm diameter (at base).

Cube utilization: 57.3% (based on volume occupied by fluid).

Table C9: Weight of PLA bottle components

Bottle	Unopened Weight (g)	Weight Of Empty Bottle and Label (g)	Weight Of Cap and Tamper Evident Ring (g)
1	473.4	24.399	2.207
2	474.1	24.540	2.183
3	474.3	24.619	2.161
4	478.1	24.550	2.200
5	473.0	24.471	2.191
6	473.6	24.491	2.163
Average	474.4	24.51	2.184
St. Dev.	1.9	0.076	0.019

Functional unit is 1 liter of fluid (water).

There are 2.000 bottles per functional unit.

Table C10: Packaging material used for PLA bottle

Item	Type Of Material	Weight Per Container (g)	Weight Per Functional Unit (g)
Bottle and Label	PLA	24.512	49.023
Cap	HDPE	2.184	4.368

Label area for printing estimate: 0.185m long x 0.076m wide = 0.0141m^2.

Label weight per container assuming 1 mil thick PLA at 1.24g/cm^3 density: 0.443g.

Estimated weight of PLA per container without label: 24.1g.

Plastic (PP) crate

Weight information for plastic crate taken from an unpublished study on distribution of cut flowers done at MSU School of Packaging.

Cube utilization: assume 100% for the purposes of this study.

Weight of plastic crate: 1.8kg.

Functional unit is ½ flower box (common unit in flower industry).

There is 1 plastic crate per functional unit.

Weight of PP for functional unit: 1.8kg.

No area estimate for printing.

Steel Food Can

6 cans of 142g net weight tuna were acquired for this project.

Can dimensions: 3.4cm high x 8.5cm diameter (at top).

Cube utilization: 78.5%.

Table C11: Weight of steel food can components

Can	Unopened Weight (g)	Emptied Weight Of Can Without Lid (g)	Emptied Weight Of Top Lid (g)	Weight Of Paper Label (g)
1	169.1	21.818	6.830	0.679
2	170.6	21.903	6.818	0.693
3	171.5	21.607	6.841	0.687
4	174.1	21.606	6.841	0.682
5	173.2	21.882	6.833	0.679
6	172.5	21.855	6.778	0.678
Average	171.8	21.78	6.824	0.683
St. Dev.	1.8	0.136	0.024	0.006

Functional unit is 1kg net weight of tuna.

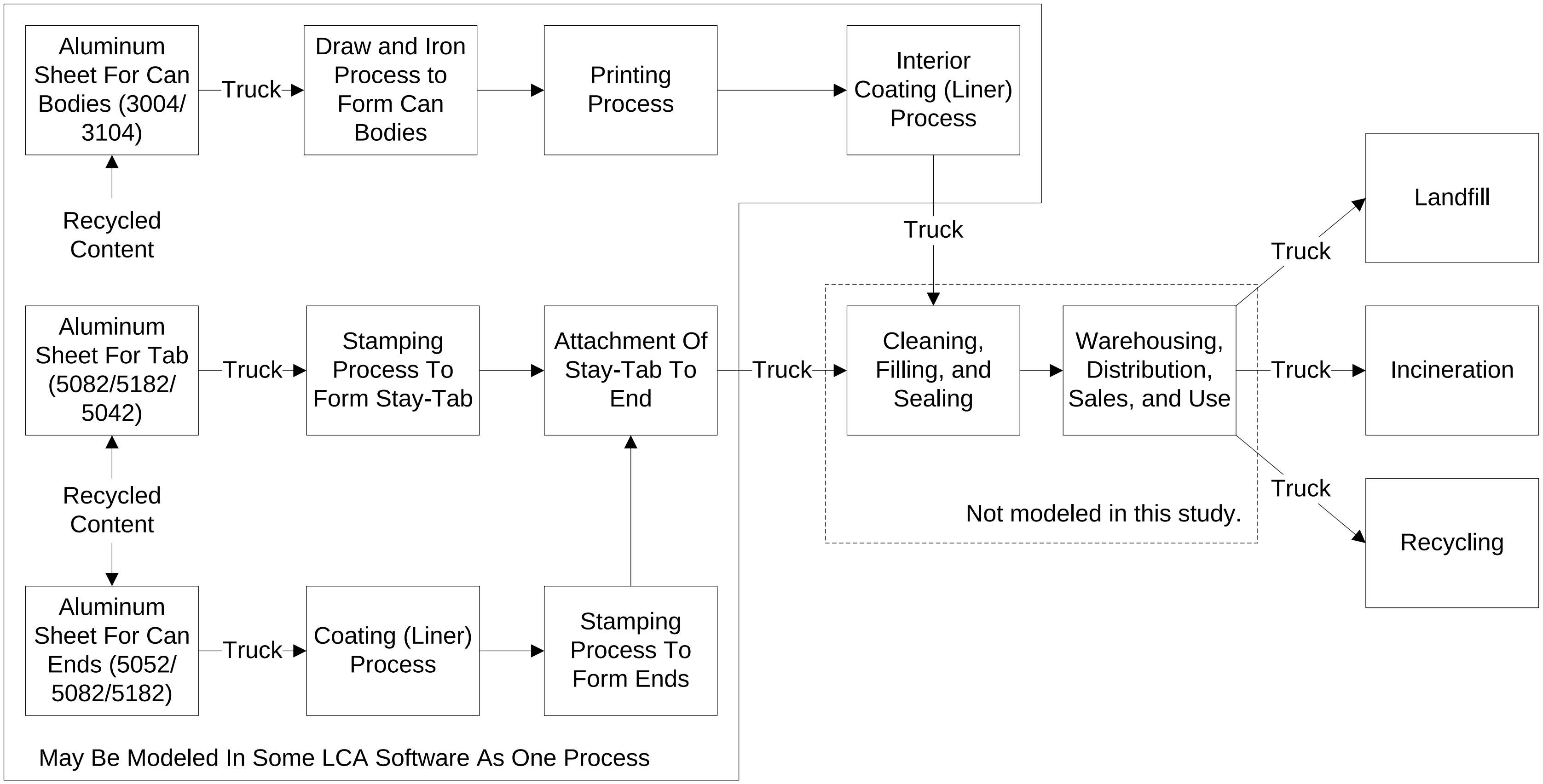
There are 7.042 cans per functional unit.

Table C12: Packaging material used for steel can

Item	Type Of Material	Weight Per Container (g)	Weight Per Functional Unit (g)
Can	steel	21.779	153.370
Lid	steel	6.824	48.053
Label	paper	0.683	4.810

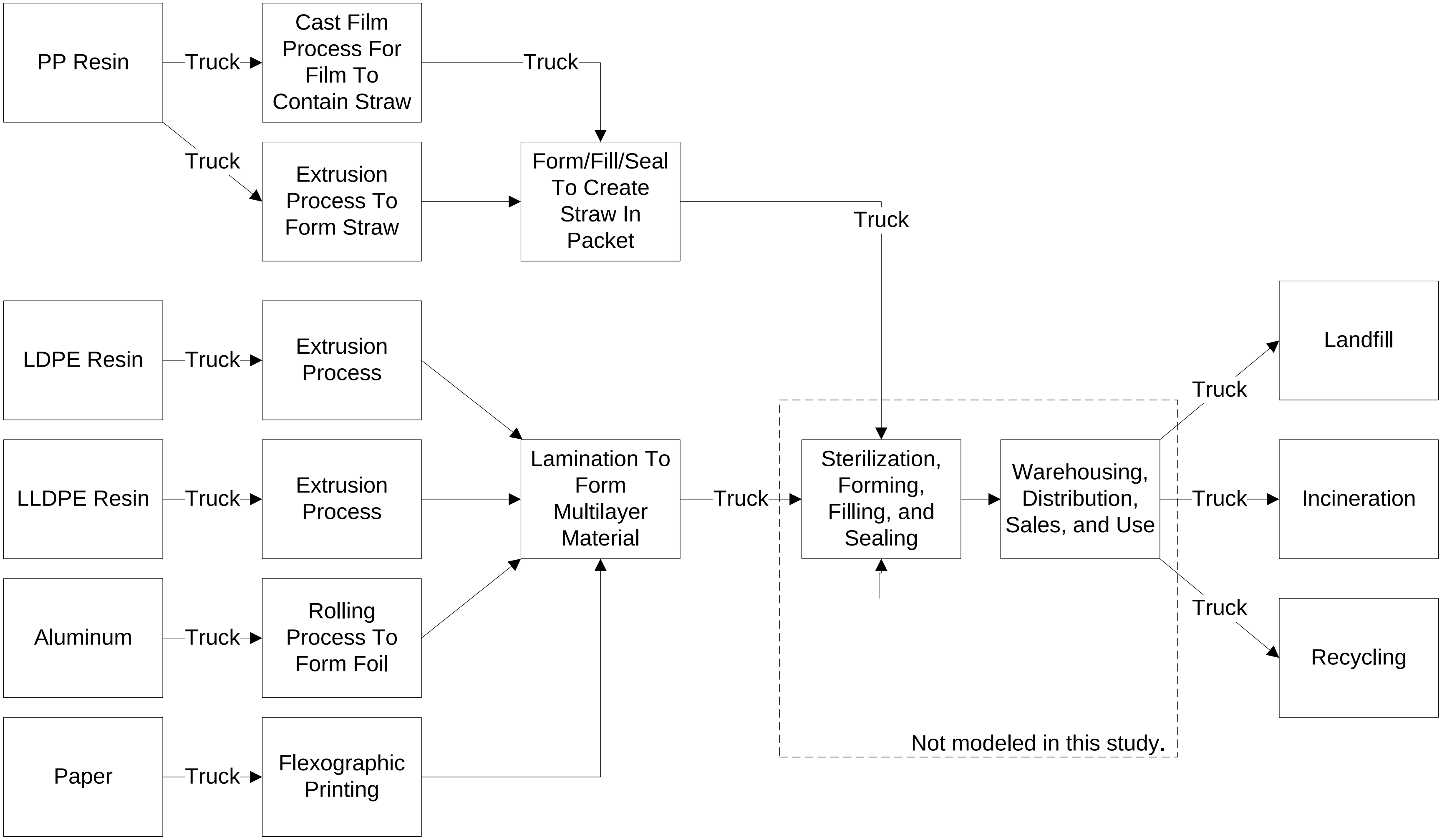
Label area for printing estimate: 0.275m long x 0.027m wide = 0.00743m^2.

APPENDIX D: Product LCA Flow Diagrams



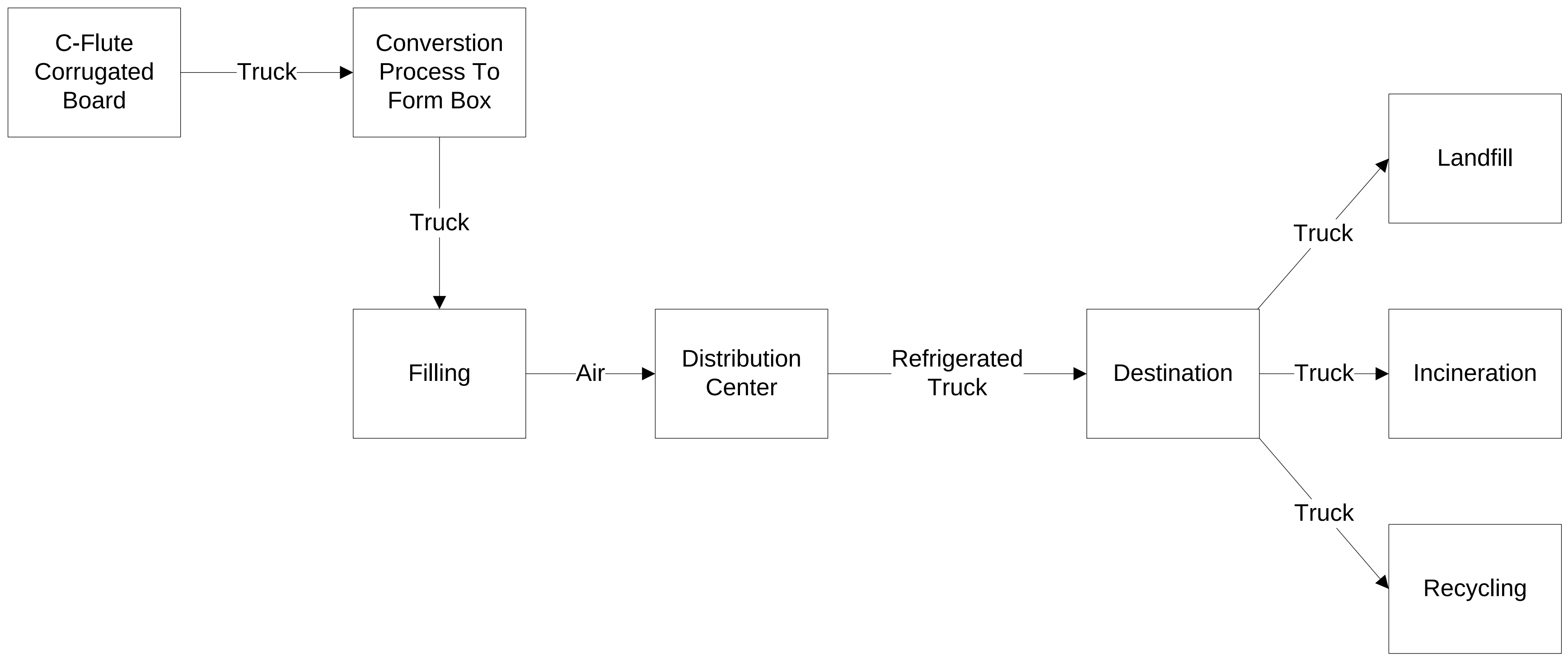
Notes: 1. Ink and sealing compound are not included in this study.
2. Cleaning, filling, and sealing are not modeled in this study.
3. Warehousing, distribution, sales, and use functions are not modeled for this study.
4. Truck transportation distances to be determined.

Figure D1: Flow diagram for aluminum can used for carbonated beverages.



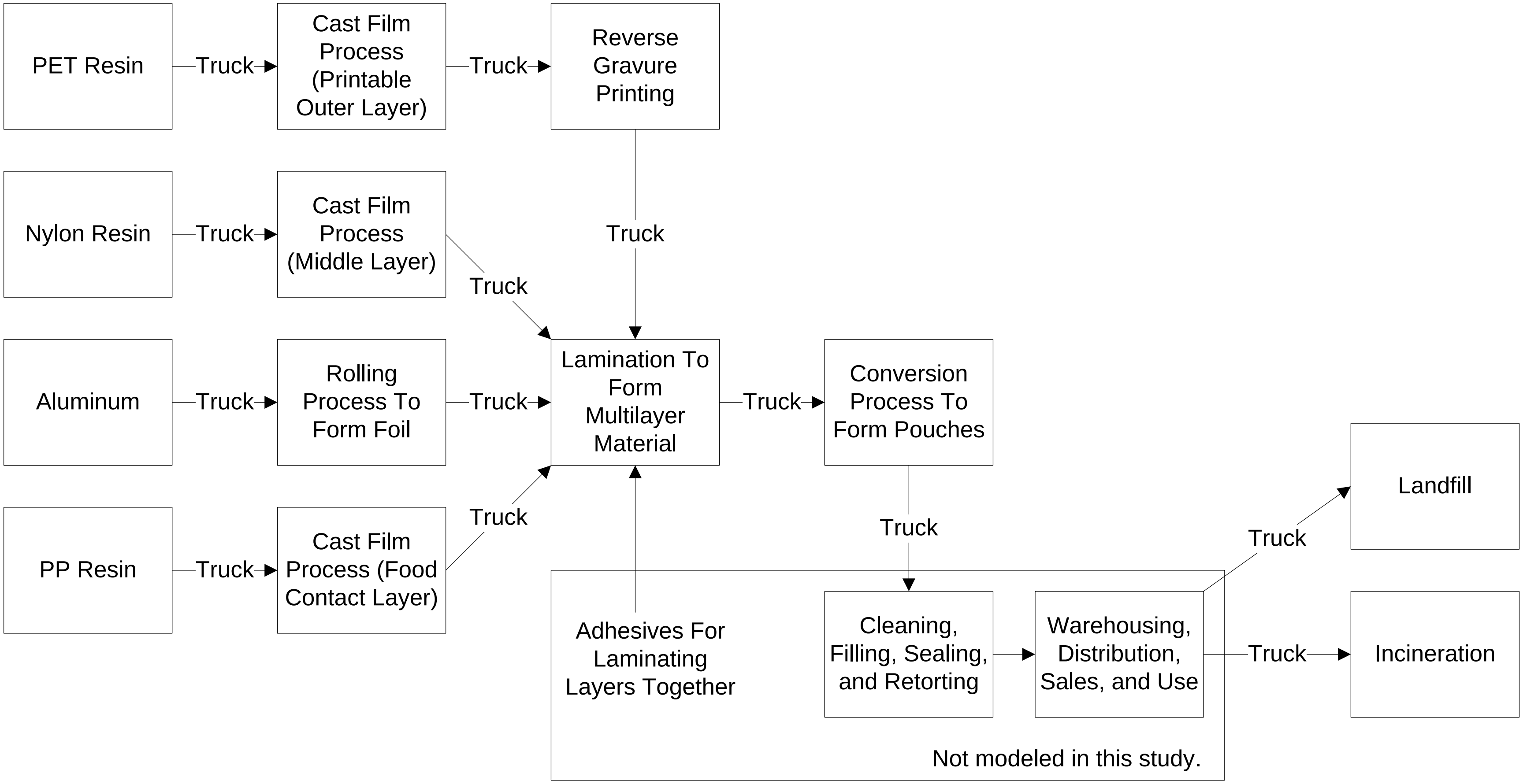
Notes:
1. Printing ink is not included in this study.
2. Sterilization, container forming, filling, and sealing are not modeled for this study.
3. Warehousing, distribution, sales, and use functions are not modeled for this study.
4. Truck transportation distances to be determined.

Figure D2: Flow diagram for aseptic carton.



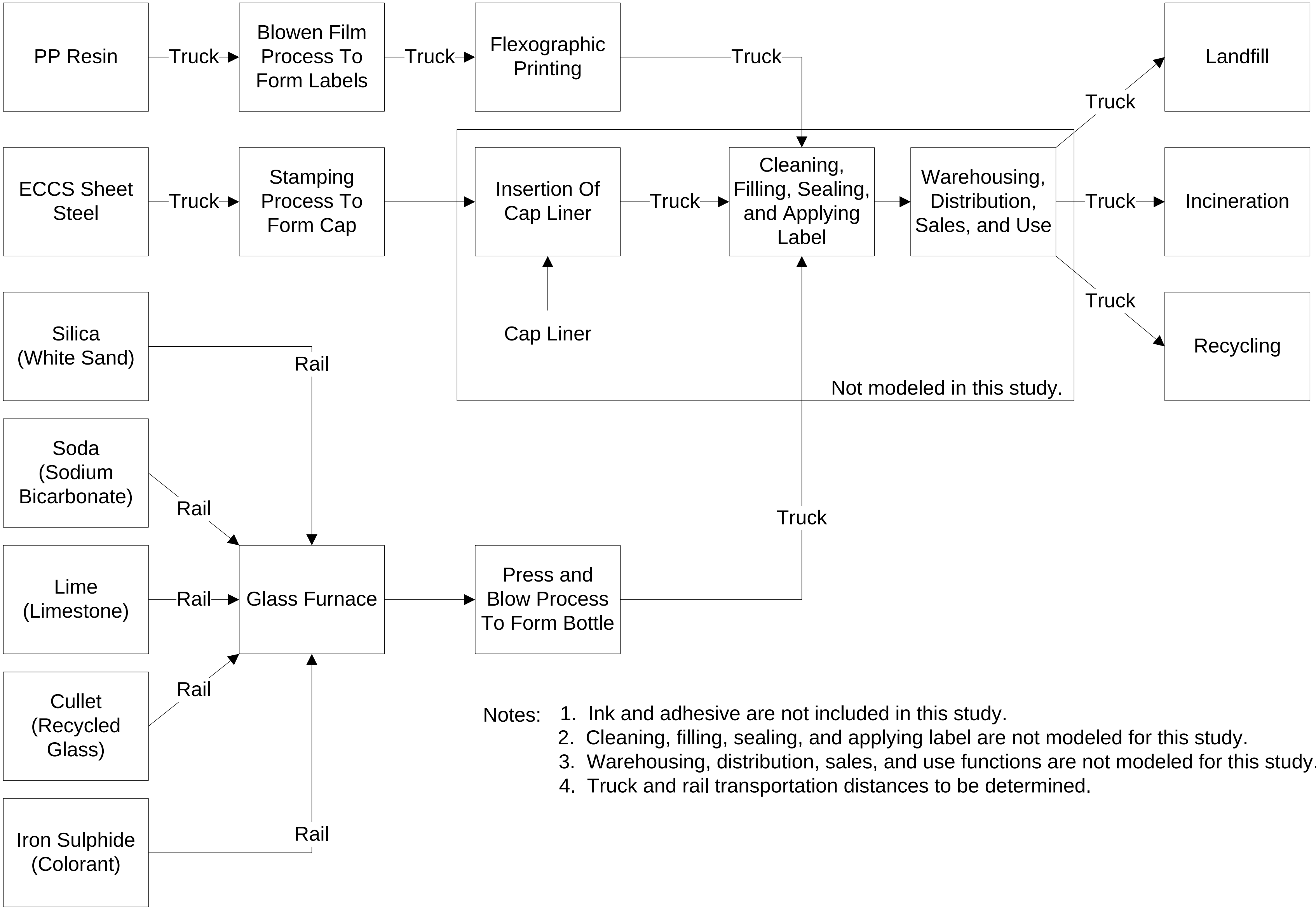
Notes:
1. No printing process or ink is included in this study.
2. Filling, distribution center, and destination processes are not modeled in this study.
3. Truck transportation distances to/from airports are rolled into other truck distances for modeling simplicity.
4. Air and truck transportation distances to be determined.

Figure D3: Flow diagram for corrugated box.



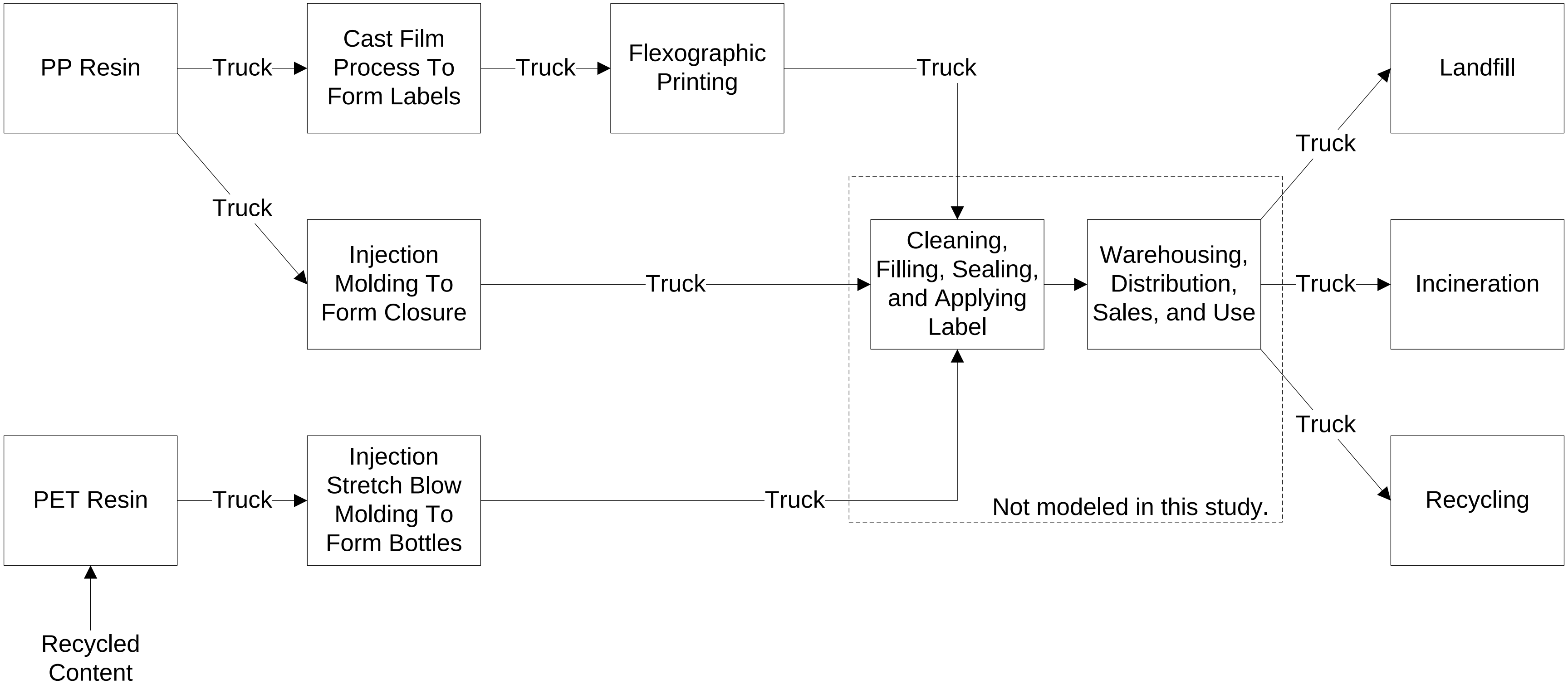
Notes:
1. Printing ink is not included in this study.
2. Cleaning, filling, sealing, and retorting are not modeled for this study.
3. Warehousing, distribution, sales, and use functions are not modeled for this study.
4. Truck transportation distances to be determined.

Figure D4: Flow diagram for flexible pouch used for packaging tuna.



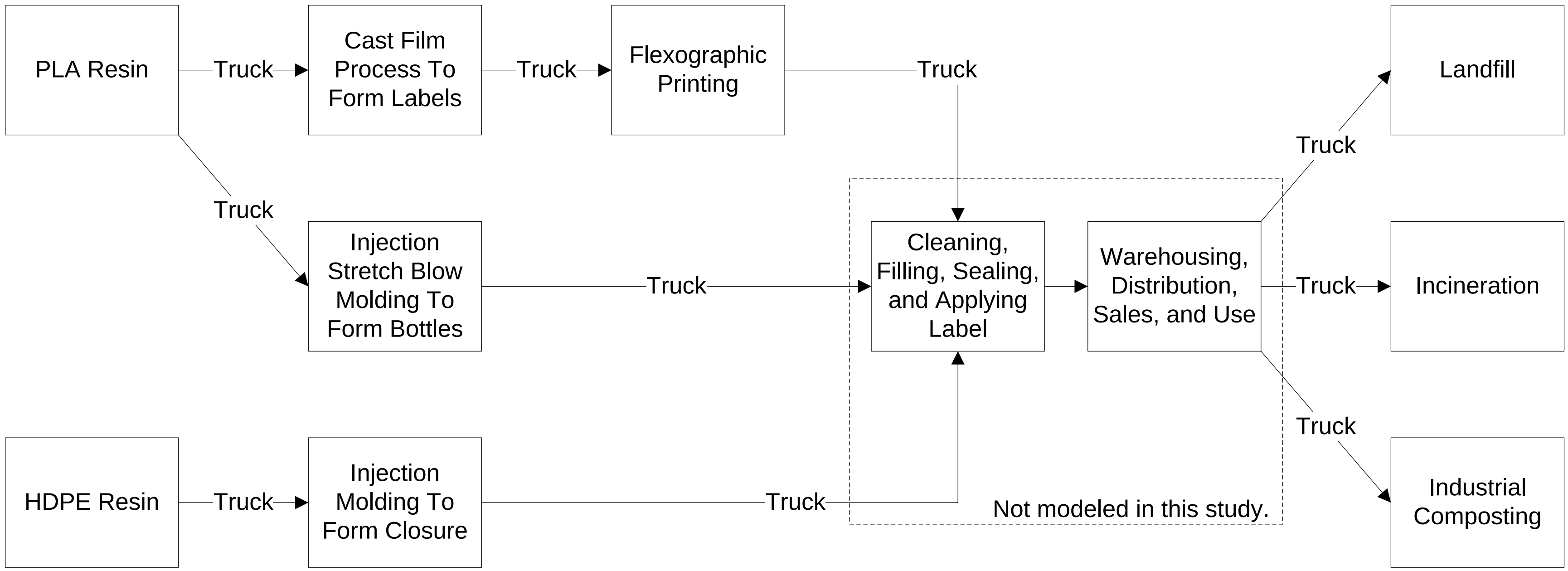
Notes:
1. Ink and adhesive are not included in this study.
2. Cleaning, filling, sealing, and applying label are not modeled for this study.
3. Warehousing, distribution, sales, and use functions are not modeled for this study.
4. Truck and rail transportation distances to be determined.

Figure D5: Flow diagram for glass (amber) beer bottle.



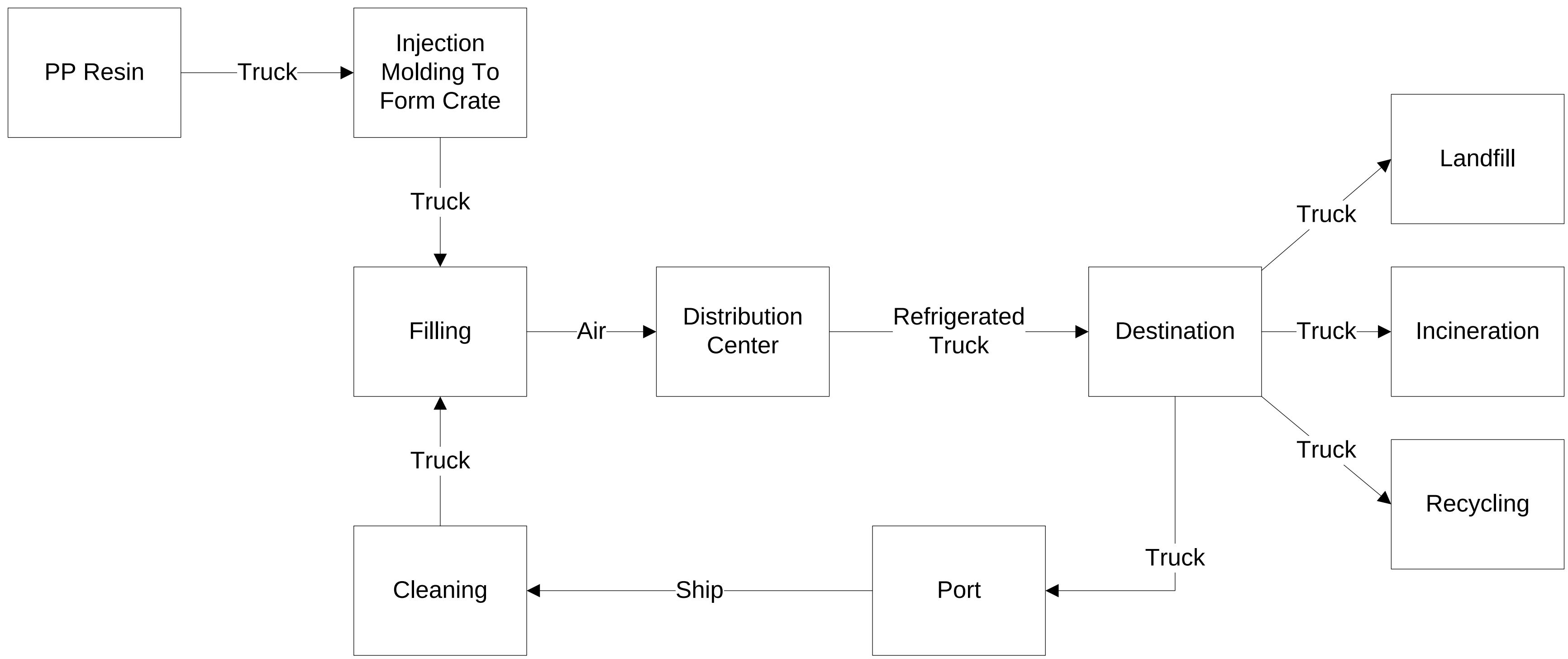
Notes:
1. Ink and adhesive used on label are not included in this study.
2. Cleaning, filling, sealing, and applying label are not modeled for this study.
3. Warehousing, distribution, sales, and use functions are not modeled for this study.
4. Truck transportation distances to be determined.

Figure D6: Flow diagram for PET carbonated beverage bottle.



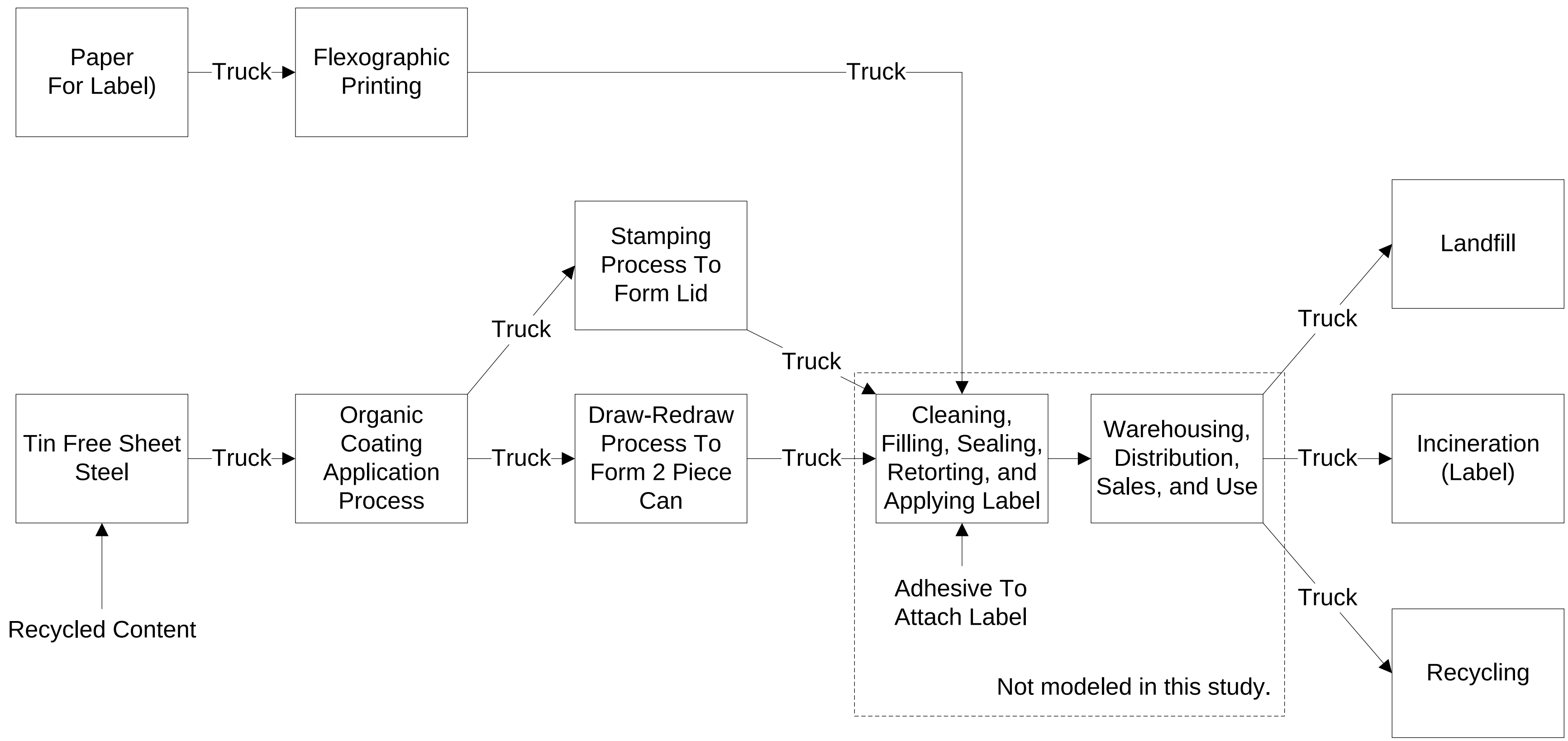
Notes:
1. Ink and adhesive used on label are not included in this study.
2. Cleaning, filling, sealing, and applying label are not modeled for this study.
3. Warehousing, distribution, sales, and use functions are not modeled for this study.
4. Truck transportation distances to be determined.

Figure D7: Flow diagram for PLA water bottle.



Notes:
1. No printing process or ink is included in this study.
2. Cleaning, filling, distribution center, destination, and port processes are not modeled in this study.
3. Truck transportation distances to/from airports and port are rolled into other truck distances for modeling simplicity.
4. Air, ship, and truck transportation distances to be determined.

Figure D8: Flow diagram for plastic (PP) crate.



Notes: 1. Ink and adhesive for label are not included in this study.
2. Cleaning, filling, sealing, retorting, and applying label are not modeled in this study.
3. Warehousing, distribution, sales, and use functions are not modeled for this study.
4. Truck transportation distances to be determined.

Figure D9: Flow diagram for steel food can used for packaging tuna.

APPENDIX E: Test Parameter Combinations For Containers

LCA Software Study
Test Parameter Combinations For Aluminum Beverage Can

Test Parameters

Aluminum recycled at end-of- life (EOL):	0, 50, and 100%
Aluminum recycled content:	0, 10, 70, and 100%.
Transport distance, rail:	0 km.
Transport distance, standard truck:	100 and 1000 km.

Note: Doing all combinations would require 3 x 4 x 1 x 2 = 24 combinations.

Parameter Combinations To Be Used

See Table E1 below.

Table E1: Aluminum beverage can test parameter combinations

Parameter	Test						
	1	2	3	4	5	6	7
Aluminum Recycled At EOL (%)	50	0	100	50	50	50	50
Aluminum Recycled Content (%)	70	70	70	0	10	100	70
Rail (km)	0	0	0	0	0	0	0
Standard Truck (km)	100	100	100	100	100	100	1000

LCA Software Study

Test Parameter Combinations For Aseptic Carton

Test Parameters

Aseptic cartons recycled at end-of-life (EOL): 0, 10, 50, and 100%
Aseptic carton recycled content: 0%.
Transport distance, rail: 0 km.
Transport distance, standard truck: 100 and 1000 km.

Note: Doing all combinations would require 4 x 1 x 1 x 2 = 8 combinations.

Parameter Combinations To Be Used

See Table E2 below.

Table E2: Aseptic carton test parameter combinations

Parameter	Test				
	1	2	3	4	5
Aseptic Carton Recycled At EOL (%)	10	0	50	100	10
Aseptic Carton Recycled Content (%)	0	0	0	0	0
Rail (km)	0	0	0	0	0
Standard Truck (km)	100	100	100	100	1000

LCA Software Study
Test Parameter Combinations For Corrugate Box

Test Parameters

Number of uses for each box:	1.
Corrugate recycled at end-of-life (EOL):	0, 80, 100%
Corrugate recycled content:	0, 25, 50, and 100%.
Transport distance, outgoing air:	500 and 2500 km.
Transport distance, outgoing refrigerated truck:	100, and 1000 km.
Transport distance, outgoing standard truck:	100 km.
Transport distance, return ship:	Not Applicable.
Transport distance, return standard truck:	Not Applicable.

Note: Doing all combinations would require 1 x 3 x 4 x 2 x 2 x 1 x1 x 1 = 48 combinations.

Parameter Combinations To Be Used

See Table E3 below.

Table E3: Corrugated box test parameter combinations

Parameter	Test							
	1	2	3	4	5	6	7	8
Number Of Uses	1	1	1	1	1	1	1	1
Corrugate Recycled At EOL (%)	80	0	100	80	80	80	80	80
Corrugate Recycled Content (%)	50	50	50	0	25	100	50	50
Outgoing Air (km)	2500	2500	2500	2500	2500	2500	500	2500
Outgoing Refrigerated Truck (km)	100	100	100	100	100	100	100	1000
Outgoing Standard Truck (km)	100	100	100	100	100	100	100	100
Return Ship (km)	0	0	0	0	0	0	0	0
Return Standard Truck (km)	0	0	0	0	0	0	0	0

LCA Software Study
Test Parameter Combinations Flexible Tuna Pouch

Test Parameters

Flexible pouch recycled at end-of-life (EOL): 0%
Flexible pouch recycled content: 0%.
Transport distance, standard truck: 100 km.

Note: Doing all combinations would require 1 x 1 x 1 = 1 combination.

Parameter Combinations To Be Used

See Table E4 below.

Table E4: Flexible pouch test parameter combinations

Parameter	Test
	1
Flexible Pouch Recycled At EOL (%)	0
Flexible Pouch Recycled Content (%)	0
Standard Truck (km)	100

LCA Software Study

Test Parameter Combinations For Glass Beer Bottle

Test Parameters

Glass recycled at end-of-life (EOL): 0, 40, 100%
Glass recycled content: 0, 25, 50, and 100%.
Transport distance, rail: 0, 500, and 4000 km.
Transport distance, standard truck: 100 and 1000 km.

Note: Doing all combinations would require 3 x 4 x 3 x 2 = 72 combinations.

Parameter Combinations To Be Used

See Table E5 below.

Table E5: Glass bottle test parameter combinations

Parameter	Test								
	1	2	3	4	5	6	7	8	9
Glass Recycled At EOL (%)	40	0	100	40	40	40	40	40	40
Glass Recycled Content (%)	25	25	25	0	50	100	25	25	25
Rail (km)	500	500	500	500	500	500	0	4000	500
Standard Truck (km)	100	100	100	100	100	100	100	100	1000

LCA Software Study
Test Parameter Combinations PET Bottle

Test Parameters

PET recycled at end-of-life:	0, 30, and 100%
PET recycled content:	0, 10, 50, and 100%.
Transport distance, rail:	0 km.
Transport distance, standard truck:	100 and 1000 km.

Note: Doing all combinations would require 3 x 4 x 1 x 2 = 24 combinations.

Parameter Combinations To Be Used

See Table E6 below.

Table E6: PET bottle test parameter combinations

Parameter	Test						
	1	2	3	4	5	6	7
PET Recycled At EOL (%)	30	0	100	30	30	30	30
PET Recycled Content (%)	10	10	10	0	50	100	10
Rail (km)	0	0	0	0	0	0	0
Standard Truck (km)	100	100	100	100	100	100	1000

LCA Software Study
Test Parameter Combinations PLA Bottle

Test Parameters

PLA composted at end-of-life (EOL): 0, 10, and 50%
PLA recycled content: 0%.
Transport distance, rail: 0 km.
Transport distance, standard truck: 100 and 1000 km.

Note: Doing all combinations would require 3 x 1 x 1 x 2 = 6 combinations.

Parameter Combinations To Be Used

See Table E7 below.

Table E7: PLA bottle test parameter combinations

Parameter	Test			
	1	2	3	4
PLA Composted At EOL (%)	10	0	50	10
PLA Recycled Content (%)	0	0	0	0
Rail (km)	0	0	0	0
Standard Truck (km)	100	100	100	1000

LCA Software Study

Test Parameter Combinations For Plastic (PP) Crate

Test Parameters

Number of uses for each crate: 1, 10, and 100.
PP recycled at end-of-life (EOL): 10, 50, and 100%
PP recycled content: 0%.
Transport distance, outgoing air: 500 and 2500 km.
Transport distance, outgoing refrigerated truck: 100, and 1000 km.
Transport distance, outgoing standard truck: 100 km.
Transport distance, return ship: 500 and 2100 km.
Transport distance, return standard truck: 1200 km.

Note: Doing all combinations would require 3 x 3 x 1 x 2 x 2 x 1 x 2 x 1 = 72 combinations.

Parameter Combinations To Be Used

See Table E8 below.

Table E8: Plastic (PP) crate test parameter combinations

Parameter	Test							
	1	2	3	4	5	6	7	8
Number Of Uses	10	1	100	10	10	10	10	10
PP Recycled At EOL (%)	10	10	10	50	100	10	10	10
PP Recycled Content (%)	0	0	0	0	0	0	0	0
Outgoing Air (km)	2500	2500	2500	2500	2500	500	2500	2500
Outgoing Refrigerated Truck (km)	100	100	100	100	100	100	1000	100
Outgoing Standard Truck (km)	100	100	100	100	100	100	100	100
Return Ship (km)	2100	0[1]	2100	2100	2100	2100	2100	500
Return Standard Truck (km)	1200	0[1]	1200	1200	1200	1200	1200	1200

[1] Distances for Return Ship and Return Standard Truck are set to 0km in Test 2 because it is assumed a single use crate will not be returned.

LCA Software Study

Test Parameter Combinations Steel Food Can (Tuna)

Test Parameters

Steel recycled at end-of- life (EOL):	10, 70, and 100%
Steel recycled content:	25 and 37%.
Transport distance, rail:	0 km.
Transport distance, standard truck:	100 km.

Note: Doing all combinations would require 3 x 2 x 1 x 1 = 6 combination.

Parameter Combinations To Be Used

See Table E9 below.

Table E9: Steel food can test parameter combinations

Parameter	Test			
	1	2	3	4
Steel Recycled At EOL (%)	70	10	100	70
Steel Can Recycled Content (%)	25	25	25	37
Rail (km)	0	0	0	0
Standard Truck (km)	100	100	100	100

APPENDIX F: Database Files Used In Software Modeling

Table F1: GaBi library/database files used

File Name	Library/Database
Aluminum Beverage Can	
CH: disposal, aluminium, 0% water, to inert material landfill	US Ecoinvent
CH: disposal, aluminium, 0% water, to municipal incineration	US Ecoinvent
RER: aluminium, primary, at plant	US Ecoinvent
RER: aluminium, secondary, from old scrap, at plant	US Ecoinvent
RER: cold impact extrusion, aluminium, 2 strokes	US Ecoinvent
RER: sheet rolling, aluminium	US Ecoinvent
US: Transport, combination Truck, average fuel mix	USLCI/PE
Aseptic Carton	
CH: disposal, aluminium, 0% water, to municipal incineration	US Ecoinvent
CH: disposal, aluminium, 0% water, to sanitary landfill	US Ecoinvent
CH: disposal, packaging paper, 13.7% water, to municipal incineration	US Ecoinvent
CH: disposal, packaging paper, 13.7% water, to sanitary landfill	US Ecoinvent
CH: disposal, polyethylene, 0.4% water, to municipal incineration	US Ecoinvent
CH: disposal, polyethylene, 0.4% water, to sanitary landfill	US Ecoinvent
RER: Aluminium foil	PE International
RER: extrusion, plastic film	US Ecoinvent
RER: extrusion, plastic film	US Ecoinvent
RER: extrusion, plastic film	US Ecoinvent
RER: kraft paper, bleached, at plant	US Ecoinvent
RNA: Linear low density polyethylene resin, at plant	USLCI/PE
RNA: Low density polyethylene resin, at plant	USLCI/PE
RNA: Polypropylene resin, at plant	USLCI/PE
US: Transport, combination truck, average fuel mix	USLCI/PE
Corrugated Box	
CH: disposal, packaging cardboard, 19.6% water, to municipal incineration	US Ecoinvent
CH: disposal, packaging cardboard, 19.6% water, to sanitary landfill	US Ecoinvent
RER: corrugated board, fresh fibre, single wall, at plant	US Ecoinvent

Table F1 (cont'd)

RER: corrugated board, recycling fibre, single wall, at plant	US Ecoinvent
RER: packaging box production unit	US Ecoinvent
US: Transport, aircraft, freight	USLCI/PE
US: Transport, combination truck, diesel powered	USLCI/PE
US: Transport, combination truck, diesel powered	USLCI/PE
Flexible Tuna Pouch	
CH: disposal, aluminium, 0% water, to municipal incineration	US Ecoinvent
CH: disposal, aluminium, 0% water, to sanitary landfill	US Ecoinvent
CH: disposal, polyethylene terephthalate, 0.2% water, to municipal incineration	US Ecoinvent
CH: disposal, polyethylene terephthalate, 0.2% water, to sanitary landfill	US Ecoinvent
CH: disposal, polyethylene, 0.4% water, to municipal incineration	US Ecoinvent
CH: disposal, polyethylene, 0.4% water, to sanitary landfill	US Ecoinvent
RER: Aluminium foil	PE International
RER: extrusion, plastic film	US Ecoinvent
RER: nylon 6, at plant	US Ecoinvent
RER: polyethylene terephthalate, granulate, amorphous, at plant	US Ecoinvent
RNA: Polypropylene resin, at plant	USLCI/PE
US: Transport, combination truck, average fuel mix	USLCI/PE
Glass Bottle (Beer)	
CH: disposal, glass, 0% water, to inert material landfill	US Ecoinvent
CH: disposal, glass, 0% water, to municipal incineration	US Ecoinvent
CH: disposal, polyethylene, 0.4% water, to municipal incineration	US Ecoinvent
CH: disposal, polyethylene, 0.4% water, to sanitary landfill	US Ecoinvent
CH: disposal, steel, 0% water, to inert material landfill	US Ecoinvent
CH: disposal, steel, 0% water, to municipal incineration	US Ecoinvent
RER: cold impact extrusion, steel, 1 stroke	US Ecoinvent
RER: extrusion, plastic film	US Ecoinvent
RER: packaging glass, brown, at plant	US Ecoinvent
RER: packaging glass, green, at plant	US Ecoinvent
RER: tin plated chromium steel sheet, 2mm, at plant	US Ecoinvent
RNA: Polypropylene resin, at plant	USLCI/PE
US: Transport, combination Truck, average fuel mix	
US: transport, freight, rail, diesel	US Ecoinvent
PET Bottle	

Table F1 (cont'd)

CH: disposal, polyethylene terephthalate, 0.2% water, to municipal incineration	US Ecoinvent
CH: disposal, polyethylene terephthalate, 0.2% water, to sanitary landfill	US Ecoinvent
CH: disposal, polyethylene, 0.4% water, to municipal incineration	US Ecoinvent
CH: disposal, polyethylene, 0.4% water, to sanitary landfill	US Ecoinvent
RER: extrusion, plastic film	US Ecoinvent
RER: injection moulding	US Ecoinvent
RER: polyethylene terephthalate, granulate, bottle grade, at plant	US Ecoinvent
RER: stretch blow moulding	US Ecoinvent
RNA: Polypropylene resin, at plant	US Ecoinvent
US: Plastic resin secondary (unspecified)	PE International
US: Transport, combination Truck, average fuel mix	USLCI/PE
PLA Bottle	
CH: compost, at plant	US Ecoinvent
CH: disposal, polyethylene terephthalate, 0.2% water, to municipal incineration	US Ecoinvent
CH: disposal, polyethylene terephthalate, 0.2% water, to sanitary landfill	US Ecoinvent
CH: disposal, polyethylene, 0.4% water, to municipal incineration	US Ecoinvent
CH: disposal, polyethylene, 0.4% water, to sanitary landfill	US Ecoinvent
RER: extrusion, plastic film	US Ecoinvent
RER: injection moulding	US Ecoinvent
RER: polyethylene, HDPE, granulate, at plant	US Ecoinvent
RER: stretch blow moulding	US Ecoinvent
US: Ingeo Polylactide (PLA) biopolymer production NatureWorks	PE/NatureWorks
US: Transport, combination truck, average fuel mix	USLCI/PE
Plastic (PP) Crate	
CH: disposal, polyethylene, 0.4% water, to municipal incineration	US Ecoinvent
CH: disposal, polyethylene, 0.4% water, to sanitary landfill	US Ecoinvent
RER: injection moulding	US Ecoinvent
RNA: Polypropylene resin, at plant	USLCI/PE
US: Transport, aircraft, freight	USLCI/PE
US: Transport, combination truck, diesel powered	USLCI/PE
US: Transport, combination truck, diesel powered	USLCI/PE
US: Transport, ocean freighter, average fuel mix	USLCI/PE

Table F1 (cont'd)

Steel Food Can (Tuna)	
CH: disposal, packaging paper, 13.7% water, to municipal incineration	US Ecoinvent
CH: disposal, packaging paper, 13.7% water, to sanitary landfill	US Ecoinvent
CH: disposal, steel, 0% water, to inert material landfill	US Ecoinvent
CH: disposal, steel, 0% water, to municipal incineration	US Ecoinvent
RER: cold impact extrusion, steel, 1 stroke	US Ecoinvent
RER: cold impact extrusion, steel, 1 stroke	US Ecoinvent
RER: kraft paper, bleached, at plant	US Ecoinvent
RER: Steel ECCS worldsteel	PE/World Steel
US: Transport, combination truck, average fuel mix	USLCI/PE
Basic Material Comparison - Aluminum	
CH: disposal, aluminium, 0% water, to sanitary landfill	US Ecoinvent
RER: aluminium, primary, at plant	US Ecoinvent
RER: aluminium, secondary, from old scrap, at plant	US Ecoinvent
Basic Material Comparison - Corrugated Board	
CH: disposal, packaging cardboard, 19.6% water, to municipal incineration	US Ecoinvent
CH: disposal, packaging cardboard, 19.6% water, to sanitary landfill	US Ecoinvent
RER: corrugated board, fresh fibre, single wall, at plant	US Ecoinvent
RER: corrugated board, recycling fibre, single wall, at plant	US Ecoinvent
Basic Material Comparison - Glass	
CH: disposal, glass, 0% water, to municipal incineration	US Ecoinvent
CH: disposal, inert material, 0% water, to sanitary landfill	US Ecoinvent
RER: packaging glass, brown, at plant	US Ecoinvent
RER: packaging glass, green, at plant	US Ecoinvent
Basic Material Comparison - PET	
CH: disposal, polyethylene terephthalate, 0.2% water, to municipal incineration	US Ecoinvent
CH: disposal, polyethylene terephthalate, 0.2% water, to sanitary landfill	US Ecoinvent
RER: polyethylene terephthalate, granulate, bottle grade, at plant	US Ecoinvent

Table F2: openLCA library/database files used

File Name	Library/Database
Basic Material Comparison - Aluminum	
Aluminium, primary, at plant/RER	Ecoinvent unit process
Aluminium, secondary, from old scrap, at plant/RER	Ecoinvent unit process
Disposal, aluminium, 0% water, to municipal incineration/CH	Ecoinvent unit process
Disposal, aluminium, 0% water, to sanitary landfill/CH	Ecoinvent unit process
Recycled Aluminum For CPIS Test	Empty Process
Basic Material Comparison - Corrugated Board	
Corrugated board, fresh fibre, single wall, at plant/RER	Ecoinvent unit process
Corrugated board, recycling fibre, single wall, at plant/RER	Ecoinvent unit process
Disposal, packaging cardboard, 19.6% water, to municipal incineration/CH	Ecoinvent unit process
Disposal, packaging cardboard, 19.6% water, to sanitary landfill/CH	Ecoinvent unit process
Recycling Corrugate For CPIS Test	Empty Process
Basic Material Comparison - Glass	
Disposal, glass, 0% water, to municipal incineration/CH	Ecoinvent unit process
Disposal, inert material, 0% water, to sanitary landfill/CH	Ecoinvent unit process
Packaging glass, brown, at plant/RER	Ecoinvent unit process
Packaging glass, green, at plant/RER	Ecoinvent unit process
Recycling Glass For CPIS Test	Empty Process
Basic Material Comparison - PET	
Disposal, polyethylene terephtalate, 0.2% water, to municipal incineration/CH	Ecoinvent unit process
Disposal, polyethylene terephtalate, 0.2% water, to sanitary landfill/CH	Ecoinvent unit process
Polyethylene terephthalate, granulate, bottle grade, at plant/RER	Ecoinvent unit process
Recycling PET For CPIS Test	Empty Process

Table F3: SimaPro library/database files used

File Name	Library/Database
Aluminum Beverage Can	
Aluminum can 100% recycled FAL	Franklin USA 98
Aluminum can FAL	Franklin USA 98
Disposal, aluminium, 0% water, to municipal incineration/CH with US electricity U	US-EI
Disposal, aluminium, 0% water, to sanitary landfill/CH with US electricity U	US-EI
Incineration/CH with US electricity U	US-EI
Landfill/CH with US electricity U	US-EI
Recycling aluminium/RER with US electricity U	US-EI
Transport, combination truck, average fuel mix/US	USLCI
Aseptic Carton	
Aluminium foil B250	BUWAL250
Cutting rolls CF	BUWAL250
Disposal, aluminium, 0% water, to municipal incineration/CH with US electricity U	US-EI
Disposal, aluminium, 0% water, to sanitary landfill/CH with US electricity U	US-EI
Disposal, packaging paper, 13.7% water, to municipal incineration/CH with US electricity U	US-EI
Disposal, packaging paper, 13.7% water, to sanitary landfill/CH with US electricity U	US-EI
Disposal, paper, 11.2% water, to municipal incineration/CH with US electricity U	US-EI
Disposal, paper, 11.2% water, to sanitary landfill/CH with US electricity U	US-EI
Disposal, polyethylene, 0.4% water, to municipal incineration/CH with US electricity U	US-EI
Disposal, polyethylene, 0.4% water, to sanitary landfill/CH with US electricity U	US-EI
Extrusion, plastic film/RER with US electricity U	US-EI
Flexography CF	BUWAL250
Incineration/CH with US electricity U	US-EI
Kraft paper, bleached, at plant/RER with US electricity U	US-EI
Landfill/CH with US electricity U	US-EI
Linear low density polyethylene resin, at plant/RNA	USLCI
Low density polyethylene resin, at plant/RNA	USLCI
Polypropylene resin, at plant/RNA	USLCI
Recycling aluminium/RER with US electricity U	US-EI

Table F3 (cont'd)

Recycling paper/RER with US electricity U	US-EI
Recycling PE/RER with US electricity U	US-EI
Recycling PP/RER with US electricity U	US-EI
Transport, combination truck, average fuel mix/US	USLCI
Corrugated Box	
Disposal, packaging cardboard, 19.6% water, to municipal incineration/CH with US electricity U	US-EI
Disposal, packaging cardboard, 19.6% water, to sanitary landfill/CH with US electricity U	US-EI
Incineration/CH with US electricity U	US-EI
Landfill/CH with US electricity U	US-EI
Packaging, corrugated board, mixed fibre, single wall, at plant/RER with US electricity U (Note: Modified into two new files, one using FRESH fiber, and one using RECYCLED fiber.)	US-EI
Recycling cardboard/RER with US electricity U	US-EI
Refrigerator, big, A	LCA Food DK
Transport, aircraft, freight/US	USLCI
Transport, combination truck, diesel powered/US	USLCI
Flexible Tuna Pouch	
Aluminium foil B250	BUWAL250
Disposal, aluminium, 0% water, to municipal incineration/CH with US electricity U	US-EI
Disposal, aluminium, 0% water, to sanitary landfill/CH with US electricity U	US-EI
Disposal, polyethylene terephtalate, 0.2% water, to municipal incineration/CH with US electricity U	US-EI
Disposal, polyethylene terephtalate, 0.2% water, to sanitary landfill/CH with US electricity U	US-EI
Disposal, polyethylene, 0.4% water, to municipal incineration/CH with US electricity (Note: Also used for disposal of polypropylene and nonspecific plastics)	US-EI
Disposal, polyethylene, 0.4% water, to sanitary landfill/CH with US electricity U (Note: Also used for disposal of polypropylene and nonspecific plastics)	US-EI
Extrusion, plastic film/RER with US electricity U	US-EI
Gravure printing CF	BUWAL250
Incineration/CH with US electricity U	US-EI

Table F3 (cont'd)

Laminating solvent free (Note: Modified to use US electricity.)	BUWAL250
Landfill/CH with US electricity U	US-EI
Nylon 6, at plant/RER with US electricity U	US-EI
Polyethylene terephthalate, granulate, amorphous, at plant/RER with US electricity U	US-EI
Polypropylene resin, at plant/RNA	USLCI
Production of pouch 100 g	BUWAL250
Transport, combination truck, average fuel mix/US	USLCI
Glass Bottle (Beer)	
Crown caps (1 million) (Note: File modified to use US electricity.)	BUWAL250
Disposal, glass, 0% water, to municipal incineration/CH with US electricity U	US-EI
Disposal, polyethylene, 0.4% water, to municipal incineration/CH with US electricity U (Note: Also used for polypropylene.)	US-EI
Disposal, polyethylene, 0.4% water, to sanitary landfill/CH with US electricity U (Note: Also used for polypropylene.)	US-EI
Disposal, steel, 0% water, to municipal incineration/CH with US electricity U	US-EI
ECCS steel sheet	BUWAL250
Extrusion, plastic film/RER with US electricity U	US-EI
Flexography CF	BUWAL250
Glass bottles FAL	Franklin USA 98
Glass bottles recycled FAL	Franklin USA 98
Incineration/CH with US electricity U	US-EI
Landfill ECCS steel B250(1998)	US-EI
Landfill Glass B250 (1998)	BUWAL250
Landfill/CH with US electricity U	US-EI
Linear low density polyethylene resin, at plant/RNA	USLCI
Polypropylene resin, at plant/RNA	USLCI
Recycling glass/RER with US electricity U	US-EI
Recycling PE/RER with US electricity U	US-EI
Recycling PP/RER with US electricity U	US-EI
Recycling steel and iron/RER with US electricity U	US-EI
Transport, combination truck, average fuel mix/US	USLCI
Transport, freight, rail, diesel/US with US electricity U	US-EI
PET Bottle	

Table F3 (cont'd)

Disposal, polyethylene terephtalate, 0.2% water, to municipal incineration/CH with US electricity U	US-EI
Disposal, polyethylene terephtalate, 0.2% water, to sanitary landfill/CH with US electricity U	US-EI
Disposal, polyethylene, 0.4% water, to municipal incineration/CH with US electricity U (Note:Also used for polypropylene.)	US-EI
Disposal, polyethylene, 0.4% water, to sanitary landfill/CH with US electricity U (Note:Also used for polypropylene.)	US-EI
Extrusion, plastic film/RER with US electricity U	US-EI
Flexography CF	BUWAL250
Incineration/CH with US electricity U	US-EI
Landfill/CH with US electricity U	US-EI
PET bottles FAL	Franklin USA 98
PET bottles recycled FAL	Franklin USA 98
Polypropylene resin, at plant/RNA	USLCI
PP caps FAL	Franklin USA 98
Recycling PET/RER with US electricity U	US-EI
Recycling PP/RER with US electricity U	US-EI
Transport, combination truck, average fuel mix/US	USLCI
PLA Bottle	
Composting organic waste/RER with US electricity U	US-EI
Disposal, polyethylene terephtalate, 0.2% water, to municipal incineration/CH with US electricity U (Note: Polyethylene terephtalate files used for PLA.)	US-EI
Disposal, polyethylene terephtalate, 0.2% water, to sanitary landfill/CH with US electricity U (Note: Polyethylene terephtalate files used for PLA.)	US-EI
Disposal, polyethylene, 0.4% water, to municipal incineration/CH with US electricity U	US-EI
Disposal, polyethylene, 0.4% water, to sanitary landfill/CH with US electricity U	US-EI
Extrusion, plastic film/RER with US electricity U	US-EI
Flexography CF	BUWAL250
Incineration/CH with US electricity U	US-EI
Injection moulding/RER with US electricity U	US-EI
Landfill/CH with US electricity U	US-EI
Polyethylene, HDPE, granulate, at plant/RER with US electricity U	US-EI

Table F3 (cont'd)

Polylactide, granulate, NatureWorks Nebraska/US with US electricity U	US-EI
Recycling PE/RER with US electricity U	US-EI
Stretch blow moulding/RER with US electricity U	US-EI
Transport, combination truck, average fuel mix/US	USLCI
Plastic (PP) Crate	
Disposal, polyethylene, 0.4% water, to municipal incineration/CH with US electricity U	US-EI
Disposal, polyethylene, 0.4% water, to sanitary landfill/CH with US electricity U	US-EI
Incineration/CH with US electricity U	US-EI
Injection moulding/RER with US electricity U	US-EI
Landfill/CH with US electricity U	US-EI
Polypropylene resin, at plant/RNA	USLCI
Recycling PP/RER with US electricity U	US-EI
Refrigerator, big, A	LCA Food DK
Transport, aircraft, freight/US	USLCI
Transport, combination truck, diesel powered/US	USLCI
Transport, ocean freighter, average fuel mix/US	USLCI
Steel Food Can (Tuna)	
Cold impact extrusion, steel, 1 stroke/RER with US electricity U	US-EI
Disposal, packaging paper, 13.7% water, to municipal incineration/CH with US electricity U	US-EI
Disposal, packaging paper, 13.7% water, to sanitary landfill/CH with US electricity U	US-EI
Disposal, paper, 11.2% water, to municipal incineration/CH with US electricity U	US-EI
Disposal, paper, 11.2% water, to sanitary landfill/CH with US electricity U	US-EI
Disposal, steel, 0% water, to municipal incineration/CH with US electricity U	US-EI
ECCS steel 100% scrap	BUWAL250
ECCS steel sheet	BUWAL250
Flexography CF	BUWAL250
Incineration/CH with US electricity U	US-EI
Kraft paper, bleached, at plant/RER with US electricity U	US-EI
Landfill ECCS steel B250(1998)	BUWAL250
Landfill/CH with US electricity U	US-EI
Recycling paper/RER with US electricity U	US-EI

Table F3 (cont'd)

Recycling steel and iron/RER with US electricity U	US-EI
Transport, combination truck, average fuel mix/US	USLCI
Basic Material Comparison - Aluminum	
Aluminium, primary, at plant/RER U	Ecoinvent unit process
Aluminium, secondary, from old scrap, at plant/RER U	Ecoinvent unit process
Disposal, aluminium, 0% water, to municipal incineration/CH U	Ecoinvent unit process
Disposal, aluminium, 0% water, to sanitary landfill/CH U	Ecoinvent unit process
Incineration/CH U	Ecoinvent unit process
Landfill/CH U	Ecoinvent unit process
Recycling aluminium/RER U	Ecoinvent unit process
Basic Material Comparison - Corrugated Board	
Corrugated board, fresh fibre, single wall, at plant/RER U	Ecoinvent unit process
Corrugated board, recycling fibre, single wall, at plant/RER U	Ecoinvent unit process
Disposal, packaging cardboard, 19.6% water, to municipal incineration/CH U	Ecoinvent unit process
Disposal, packaging cardboard, 19.6% water, to sanitary landfill/CH U	Ecoinvent unit process
Incineration/CH U	Ecoinvent unit process
Landfill/CH U	Ecoinvent unit process
Recycling cardboard/RER U	Ecoinvent unit process
Basic Material Comparison - Glass	
Disposal, glass, 0% water, to municipal incineration/CH U	Ecoinvent unit process
Disposal, inert material, 0% water, to sanitary landfill/CH U	Ecoinvent unit process
Incineration/CH U	Ecoinvent unit process
Landfill/CH U	Ecoinvent unit process
Packaging glass, brown, at plant/RER U	Ecoinvent unit process
Packaging glass, green, at plant/RER U	Ecoinvent unit process
Recycling glass/RER U	Ecoinvent unit process
Basic Material Comparison - PET	
Disposal, polyethylene terephtalate, 0.2% water, to municipal incineration/CH U	Ecoinvent unit process
Disposal, polyethylene terephtalate, 0.2% water, to sanitary landfill/CH U	Ecoinvent unit process
Incineration/CH U	Ecoinvent unit process
Landfill/CH U	Ecoinvent unit process

Table F3 (cont'd)

Polyethylene terephthalate, granulate, bottle grade, at plant/RER U	Ecoinvent unit process
Recycling PET/RER U	Ecoinvent unit process

APPENDIX G: Packaging Systems Comparison Data

Table G1: Beverage container comparison data

Impact Category	Unit	COMPASS	SimaPro	GaBi	Package Modeling
Aluminum Can					
Global Warming	kg CO_2 equiv	0.1826	0.1849	0.2437	0.3044
Fossil Fuel/Non-Renewable Energy	MJ Energy	2.3295	2.9253	3.4024	
Eutrophication	kg PO_4 equiv	7.494E-05	2.775E-05	3.819E-04	
Water Depletion	Liters	9.569E-01	1.075E-02	4.201E+03	
PET Bottle					
Global Warming	kg CO_2 equiv	0.4050	0.3313	0.3218	0.1448
Fossil Fuel/Non-Renewable Energy	MJ Energy	8.1255	7.6478	8.1523	
Eutrophication	kg PO_4 equiv	3.886E-04	4.738E-06	5.069E-04	
Water Depletion	Liters	9.274E-01	4.218E-02	1.234E+03	
Glass Bottle					
Global Warming	kg CO_2 equiv	0.5072	0.4780	0.5946	0.3149
Fossil Fuel/Non-Renewable Energy	MJ Energy	8.1489	6.9304	10.1460	
Eutrophication	kg PO_4 equiv	3.555E-04	4.220E-06	5.898E-04	
Water Depletion	Liters	5.216E+00	1.346E-01	4.180E+03	
Aseptic Carton					
Global Warming	kg CO_2 equiv	0.0958	0.1252	0.0498	0.0926
Fossil Fuel/Non-Renewable Energy	MJ Energy	1.9329	2.7602	1.8314	
Eutrophication	kg PO_4 equiv	2.190E-04	2.676E-05	5.449E-05	
Water Depletion	Liters	3.570E+00	2.277E+00	3.767E+02	
PLA Bottle					
Global Warming	kg CO_2 equiv	0.1988	0.2416	0.0644	0.0964
Fossil Fuel/Non-Renewable Energy	MJ Energy	3.9037	3.8169	1.7235	
Eutrophication	kg PO_4 equiv	6.955E-04	7.797E-05	1.086E-04	
Water Depletion	Liters	1.082E+00	1.022E+00	2.802E+02	

Table G2: Truck and rail transport comparison data for glass bottle

Transport Mode	Distance (km)	Unit	COMPASS	SimaPro	GaBi
Truck	100	kg CO_2 equiv	0.5072	0.4780	0.5946
Truck	1000	kg CO_2 equiv	0.6004	0.5218	0.6386
Rail	0	kg CO_2 equiv	0.5014	0.4640	0.5814
Rail	500	kg CO_2 equiv	0.5072	0.4780	0.5946
Rail	4000	kg CO_2 equiv	0.5473	0.5765	0.6868

Table G3: Steel can and flexible pouch comparison data

Impact Category	Unit	COMPASS	SimaPro	GaBi	Package Modeling
Steel Can - 25% to 28% recycled content[1]					
Global Warming	kg CO_2 equiv		0.8221	0.7096	0.6512
Fossil Fuel/Non-Renewable Energy	MJ Energy		10.5972	7.4115	
Eutrophication	kg PO_4 equiv		7.588E-05	2.100E-04	
Water Depletion	liters		6.413E+00	5.021E+02	
Steel Can - 37% recycled content					
Global Warming	kg CO_2 equiv	0.4796	0.7768		
Fossil Fuel/Non-Renewable Energy	MJ Energy	6.4595	10.1941		
Eutrophication	kg PO_4 equiv	3.470E-04	7.352E-05		
Water Depletion	liters	4.524E+00	6.413E+00		
Flexible Pouch					
Global Warming	kg CO_2 equiv	0.4073	0.3889	0.3466	0.2248
Fossil Fuel/Non-Renewable Energy	MJ Energy	8.0531	9.4005	7.8355	
Eutrophication	kg PO_4 equiv	4.904E-04	8.805E-05	1.719E-04	
Water Depletion	liters	1.014E+00	6.866E-01	1.459E+03	

[1] 25% recycled content for SimaPro and GaBi, 28% for Package Modeling.

Table G4: Reuse comparison data on a per use basis

Impact Category	Unit	COMPASS	SimaPro	GaBi	Package Modeling
PP crate 1 use					
Global Warming	kg CO_2 equiv	6.6544	5.9228	5.3822	2.5706
Fossil Fuel/Non-Renewable Energy	MJ Energy	186.9295	200.8648	181.6887	
Eutrophication	kg PO_4 equiv	9.040E-03	1.865E-04	4.466E-03	
Water Depletion	liters	1.259E+01	8.590E+00	1.119E+04	
PP crate 10 uses					
Global Warming	kg CO_2 equiv	1.3747	1.1062	1.0102	
Fossil Fuel/Non-Renewable Energy	MJ Energy	28.6723	27.4957	24.9602	
Eutrophication	kg PO_4 equiv	1.630E-03	2.292E-05	4.466E-04	
Water Depletion	liters	2.252E+00	8.593E-01	1.119E+03	
PP crate 100 uses					
Global Warming	kg CO_2 equiv	0.8467	0.6245	0.5995	
Fossil Fuel/Non-Renewable Energy	MJ Energy	12.8465	10.1588	9.6540	
Eutrophication	kg PO_4 equiv	8.892E-04	6.560E-06	4.466E-05	
Water Depletion	liters	1.219E+00	8.619E-02	1.119E+02	
Corrugated Box 1 use					
Global Warming	kg CO_2 equiv	0.8642	1.0803	0.4868	0.6095
Fossil Fuel/Non-Renewable Energy	MJ Energy	13.6383	16.5080	12.5507	
Eutrophication	kg PO_4 equiv	1.379E-03	2.027E-04	1.065E-03	
Water Depletion	liters	1.788E+01	1.879E+01	2.215E+03	

Table G5: Recycled content comparison data for corrugated box

Impact Category	Unit	COMPASS	SimaPro	GaBi
0% Recycled Content (12% for COMPASS [1])				
Global Warming	kg CO_2 equiv	0.5405	1.1821	0.0276
Fossil Fuel/Non-Renewable Energy	MJ Energy	13.9916	17.6705	13.0990
Eutrophication	kg PO_4 equiv	1.616E-03	3.356E-04	1.467E-03
Water Depletion	liters	2.920E+01	3.113E+01	3.559E+03
25% Recycled Content				
Global Warming	kg CO_2 equiv	0.6512	1.1312	0.2572
Fossil Fuel/Non-Renewable Energy	MJ Energy	13.8707	17.0892	12.8248
Eutrophication	kg PO_4 equiv	1.535E-03	2.692E-04	1.266E-03
Water Depletion	liters	2.533E+01	2.496E+01	2.887E+03
50% Recycled Content				
Global Warming	kg CO_2 equiv	0.8642	1.0803	0.4868
Fossil Fuel/Non-Renewable Energy	MJ Energy	13.6383	16.5080	12.5507
Eutrophication	kg PO_4 equiv	1.379E-03	2.027E-04	1.065E-03
Water Depletion	liters	1.788E+01	1.879E+01	2.215E+03
100% Recycled Content (87% for COMPASS [1])				
Global Warming	kg CO_2 equiv	1.1793	0.9784	0.9460
Fossil Fuel/Non-Renewable Energy	MJ Energy	13.2944	15.3454	12.0024
Eutrophication	kg PO_4 equiv	1.148E-03	6.978E-05	6.635E-04
Water Depletion	liters	6.855E+00	6.447E+00	8.704E+02

[1] COMPASS limited recycled content of corrugated board to range of 12% to 87%.

Table G6: Air and ship transport comparison data for corrugated box and PP crate

Container	Transport Mode	Distance [1,2] (km)	Unit	COMPASS [3]	SimaPro [3]	GaBi [3]
Corrugated Box 1 use	Air	500	kg CO_2 equiv	0.7805	0.9919	0.4019
Corrugated Box 1 use	Air	2500	kg CO_2 equiv	0.8642	1.0803	0.4868
PP Crate 10 uses	Air	500	kg CO_2 equiv	1.1600	0.8878	0.7921
PP Crate 10 uses	Air	2500	kg CO_2 equiv	1.3747	1.1062	1.0102
PP Crates 10 uses	Ship	500	kg CO_2 equiv	1.3285	1.0594	0.9634
PP Crate 10 uses	Ship	2100	kg CO_2 equiv	1.3747	1.1062	1.0102

[1] Air distances are out going transport on per use basis.

[2] Ship distances are return transport on per use basis, except no return on 10th use.

[3] kg CO_2 equivalent values are average per use.

APPENDIX H: Basic Materials Comparison Data

Table H1: Basic material comparison data

Impact Category	Unit	COMPASS	SimaPro	GaBi
Aluminum 50% recycled content				
Global Warming	kg CO_2 equiv	5.7539	5.8449	6.9588
Fossil Fuel/Non-Renewable Energy	MJ Energy	71.5823	91.6934	88.3941
Eutrophication	kg PO_4 equiv	2.600E-03	1.523E-03	9.270E-03
Water Depletion	liters	3.171E+01	3.174E+01	1.651E+05
Corrugated Board 50% recycled content				
Global Warming	kg CO_2 equiv	0.6838	0.9455	1.0262
Fossil Fuel/Non-Renewable Energy	MJ Energy	12.2068	15.2014	13.2740
Eutrophication	kg PO_4 equiv	1.464E-03	3.955E-04	9.804E-04
Water Depletion	liters	2.371E+01	2.462E+01	1.484E+03
Glass 55.5% recycled content				
Global Warming	kg CO_2 equiv	0.7831	0.8655	0.8020
Fossil Fuel/Non-Renewable Energy	MJ Energy	13.2333	15.5838	14.3383
Eutrophication	kg PO_4 equiv	1.066E-03	1.494E-04	6.620E-04
Water Depletion	liters	8.377E+00	8.641E+00	1.652E+03
PET 0% recycled content				
Global Warming	kg CO_2 equiv	3.1510	3.2656	3.2698
Fossil Fuel/Non-Renewable Energy	MJ Energy	70.1882	82.3845	76.1822
Eutrophication	kg PO_4 equiv	5.800E-03	5.818E-04	3.040E-03
Water Depletion	liters	1.151E+01	1.476E+01	6.990E+03

Table H2: Basic corrugated board recycled content comparison data

Impact Category	Unit	COMPASS	SimaPro	GaBi
12% recycled content				
Global Warming	kg CO_2 equiv	0.0927	0.9457	0.1405
Fossil Fuel/Non-Renewable Energy	MJ Energy	11.2234	15.2289	14.3315
Eutrophication	kg PO_4 equiv	1.765E-03	5.628E-04	1.755E-03
Water Depletion	liters	4.018E+01	3.703E+01	4.077E+03
50% recycled content				
Global Warming	kg CO_2 equiv	0.6838	0.9455	0.5892
Fossil Fuel/Non-Renewable Energy	MJ Energy	12.2068	15.2014	13.7957
Eutrophication	kg PO_4 equiv	1.464E-03	3.955E-04	1.363E-03
Water Depletion	liters	2.371E+01	2.462E+01	2.763E+03
87% recycled content				
Global Warming	kg CO_2 equiv	1.2594	0.9453	1.0262
Fossil Fuel/Non-Renewable Energy	MJ Energy	13.1644	15.1745	13.2740
Eutrophication	kg PO_4 equiv	1.172E-03	2.325E-04	9.804E-04
Water Depletion	liters	7.669E+00	1.254E+01	1.484E+03

Table H3: openLCA basic material comparison data

Impact Category	Unit	SimaPro	openLCA
Aluminum 50% recycled content			
Global Warming	points	5.903E-04	4.603E-04
Non-Renewable Energy	points	6.033E-04	3.733E-04
Eutrophication	kg PO_4 equiv	1.523E-03	2.524E-04
Water Depletion	liters	3.174E+01	1.600E+01
Corrugated Board 50% recycled content			
Global Warming	points	9.549E-05	5.283E-05
Non-Renewable Energy	points	1.000E-04	5.522E-05
Eutrophication	kg PO_4 equiv	1.464E-03	2.908E-04
Water Depletion	liters	2.371E+01	2.137E+01
Glass 50% recycled content			
Global Warming	points	8.781E-05	2.506E-05
Non-Renewable Energy	points	1.029E-04	4.213E-05
Eutrophication	kg PO_4 equiv	1.512E-04	5.920E-05
Water Depletion	liters	8.995E+00	7.580E-02
PET 0% recycled content			
Global Warming	points	3.298E-04	1.545E-04
Non-Renewable Energy	points	5.421E-04	3.737E-04
Eutrophication	kg PO_4 equiv	5.818E-04	1.511E-04
Water Depletion	liters	1.476E+01	4.898E+00

Table H4: openLCA corrugated board recycled content comparison data

Impact Category	Unit	SimaPro	openLCA
12% recycled content			
Global Warming	points	9.551E-05	4.812E-05
Non-Renewable Energy	points	1.002E-04	5.084E-05
Eutrophication	kg PO_4 equiv	1.765E-03	4.522E-04
Water Depletion	liters	4.018E+01	3.255E+01
50% recycled content			
Global Warming	points	9.549E-05	5.283E-05
Non-Renewable Energy	points	1.000E-04	5.522E-05
Eutrophication	kg PO_4 equiv	1.464E-03	2.908E-04
Water Depletion	liters	2.371E+01	2.137E+01
87% recycled content			
Global Warming	points	9.547E-05	5.743E-05
Non-Renewable Energy	points	9.985E-05	5.949E-05
Eutrophication	kg PO_4 equiv	1.172E-03	1.337E-04
Water Depletion	liters	7.669E+00	1.048E+01

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