Role of Uncertainty in Streamlined Life Cycle Assessment

Exploring the Case of Petrochemical Refineries and Polymer Manufacturing Units

by

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ABSTRACT

Life Cycle Assessment (LCA) is used in the chemical process sector to compare the environmental merits of different product or process alternatives. One of the tasks that involves much time and cost in LCA studies is the specification of the exact materials and processes modeled which has limited its widespread application. To overcome this, researchers have recently created probabilistic underspecification as an LCA streamlining method, which uses a structured data classification system to enable an LCA modeler to specify materials and processes in a less precise manner. This study presents a statistical procedure to understand when streamlined LCA methods can be used, and what their impact on overall model uncertainty is.

Petrochemicals and polymer product systems were chosen to examine the impacts of underspecification and mis-specification applied to LCA modeling. Ecoinvent database, extracted using GaBi software, was used for data pertaining to generic crude oil refining and polymer manufacturing modules. By assessing the variation in LCA results arising out of streamlined materials classification, the developed statistics estimate the amount of overall error incurred by underspecifying and mis-specifying material impact data in streamlined LCA. To test the impact of underspecification and mis-specification at the level of a product footprint, case studies of HDPE containers and aerosol air fresheners were conducted.

Results indicate that the variation in LCA results decreases as the specificity of materials increases. For the product systems examined, results show that most of the variability in impact assessment is due to the differences in the regions from which the environmental impact datasets were collected; the lower levels of categorization of

materials have relatively smaller influence on the variance. Analyses further signify that only certain environmental impact categories viz. global warming potential, freshwater eutrophication, freshwater ecotoxicity, human toxicity and terrestrial ecotoxicity are affected by geographic variations. Outcomes for the case studies point out that the error in the estimation of global warming potential increases as the specificity of a component of the product decreases. Fossil depletion impact estimates remain relatively robust to underspecification. Further, the results of LCA are much more sensitive to underspecification of materials and processes than mis-specification.

To my parents

Murali Srinivasan

Latha Murali

and brother Akshay Krishna Murali

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TABLE OF CONTENTS

Page

CHAPTER Page

Page

LIST OF TABLES

LIST OF FIGURES

Figure Page

CHAPTER 1

INTRODUCTION

1.1 Importance of Sustainability

It is well acknowledged that industrial growth plays a significant role in the progress and growth of a country. That being an irrefutable fact, it is also a significant contributor to pollution and environmental degradation (Samuel, Agamuthu, & Hashim, 2013). In fact global warming, energy consumption, terrestrial acidification, ecotoxicity, marine pollution, water depletion and resource depletion are some of the critical issues associated with industrial growth as highlighted by United Nations Environmental Programme (UNEP, 2008). With industrialization and globalization of markets, increasing pressure is faced by multiple stakeholders to reduce the environmental impacts associated with global consumption (TSC, 2009). As a result, global sustainability has taken a new urgency.

Industries today are faced with the challenge of balancing economic stability and process sustainability. While many industries have started to recognize the need for sustainable development, implementation of sustainability into production processes, product designs and supply chain remains a grey area. This is due to the lack of understanding of fundamental models and tools to incorporate environmental aspects into the manufacturing framework. Further, Bebbington et al., (2007) points out that there is a pressing need to effectively quantify and communicate sustainability progress. Thus, initiatives such as industrial ecology for cleaner production and green designs arose out

of such an understanding (Samuel et al., 2013). Albeit several metrics and models have recently been developed to assess sustainability, it is difficult to compare them.

1.2 Life Cycle Assessment (LCA) as a tool

The shift to sustainable practices has become indispensable to improve the environmental performance of industries. Awareness of environmental impacts of production as well as consumption patterns is crucial for manufactures, stakeholders and consumers alike for making an educated decision. With the growing demand for cleaner and greener systems, several regulatory bodies have concentrated their attention on global sustainability creating a new paradigm for sustainable production and consumption patterns. In that regard, Life Cycle Assessment (LCA) has gained widespread attraction as a decision making tool for comprehensively estimating the impacts of products, processes and materials. The International Organization for Standardization (ISO) has published several standards on the topic of LCA. Specifically, the ISO 14040 series "Environmental management- Life Cycle Assessment- Principles and Framework" specifies the main ideas of LCA. These ideas have been further detailed in other international standards and technical reports.

When presented with multiple opportunities and methods to achieve a certain function, LCA is used as a tool to rationalize and support claims for choosing a particular methodology based on its sustainability and eco-efficiency. Thus, it is critical that the LCA model encompasses all activities pertaining to a particular function analyzing the effects of choices made over a broad scope, "confirming effects anywhere in the world,

covering all relevant substances and environmental themes that are valid over a long period of time"(Guinee & Heijungs, 2005).

1.3 Uncertainty in LCA

LCA is an iterative process. The all encompassing nature of LCA demands that a large amount of relevant data be readily available to conduct a comprehensive analysis. Moreover, the level of detail required for accurate analysis might escalate with subsequent analyses. This is also one of the reasons that the LCA study is cost and resource intensive hindering its widespread application. In a quickly evolving system, the time taken to accumulate the data may restrict the relevance of the study itself. Due to such shortcomings, it has become imperative that a streamlined approach to quickly conduct an LCA is developed.

Due to the rising pressure for quick and simple methods that allow for effective evaluations, there has been an overall research effort to study streamlined LCA techniques. Several streamlining procedures have been developed over the years whose results have been compared to those reached through full LCAs (Hunt, Boguski, Weitz, & Sharma, 1998). Probabilistic underspecification is one such methodology for streamlining LCA developed by researchers at the materials science engineering group at Massachusetts Institute of Technology. The method uses a structured data classification system to enable an LCA modeler to specify materials and processes in a less precise manner, thus saving the time and cost of conducting a comprehensive LCA.

Although these streamlining methods have proven to provide some respite in terms of easing effort of conducting a complete LCA by reducing the burden of collecting

data, these could only approximate the real system. Because of the inability of streamlined systems to closely mirror the actual processes, different sources of uncertainty could result in creating large inaccuracies in the final results (Patanavanich, 2011). For example, geographic uncertainty may lead to erroneous results when the proxy data used does not coincide with the regionally specific process being modeled.

Hence, in order to use the results of streamlined LCA, it is crucial that one characterizes the associated uncertainty to make any practical contribution to the decision making process. Without modeling the uncertainty, stakeholders cannot draw meaningful conclusions from the outcome of a streamlined LCA study.

1.4 Goal of Thesis

The goal of this thesis is "*to characterize and quantify the errors associated with probabilistic underspecification as a streamlining methodology for LCA using statistical analysis*". A statistical modeling technique is used by carefully analyzing the methodology of probabilistic underspecification to quantify the variation associated with the LCA results derived from such a simplified procedure. This is done to analyze the effectiveness of underspecification in capturing all the information associated with the impacts of a system under study without resulting in substantial errors.

The specific objectives of this thesis are:

- To test underspecification as a viable streamlining approach for the LCA of petrochemicals and polymeric products. This was accomplished by:

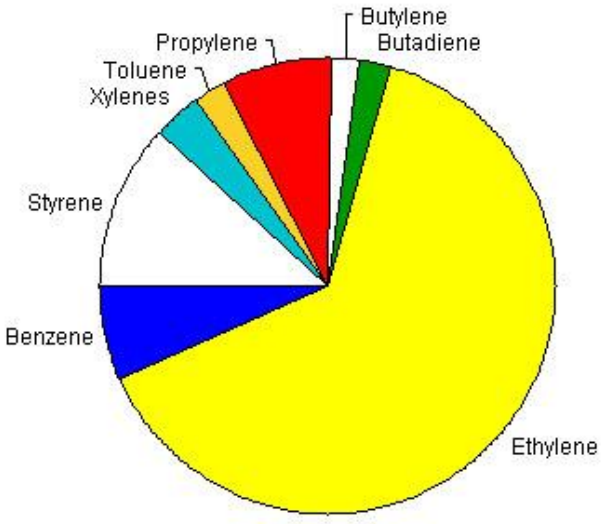
    - Classifying the products into varying levels of specificity by applying probabilistic underspecification based on Ecoinvent data structure
    - Performing extensive statistical analysis to compute the variance in the results of environmental impact estimates of the products across the different levels of specificity
- To compare the impacts of underspecification on upstream (petroleum refining) and downstream (polymer manufacturing) processes. This was accomplished by:
    - Comparing the variation in environmental impacts of petrochemicals and polymers at their generic level of specificity
- To test the effects of underspecification as well as mis-specification in LCA modeling of real life systems. This was accomplished by
    - Performing case studies on streamlined LCA of HDPE bottles and aerosol air freshener canisters

1.5 Motivation for the study

In an increasingly competitive environment, U.S. manufacturers are faced with the daunting task of reducing production costs while sustaining the product yield and quality. Increasing energy prices and uncertain markets are a major concern especially for publicly traded companies like petrochemical industries, constantly driving up the production costs and decreasing their value added. In addition, energy use is also a major source of emissions in the petrochemical industry. Therefore, industries are on the hunt

for energy efficient technologies as a cost effective investment and a sound business strategy to meet the challenge of maintaining high quality output while reducing the production costs. Moreover, the energy efficient measures always come with additional benefits for reducing environmental impacts such as emission of greenhouse gases and toxic pollutants (Neelis, Patel, Blok, Haije, & Bach, 2007)

Petroleum forms the basis for the manufacture of a wide range of fuels and chemicals. These consist of standard chemicals like acetone, ammonia, benzene etc. (Figure 1) and specialty chemicals such as plastics and synthetic polymers, lubricants, adhesives, detergents, fertilizers etc. Due to the large inventory of chemicals and associated emissions to the environment from petrochemical plants, the oil industry holds a major potential of environmental hazards such as intensification of global warming, water contamination, toxic releases to air, marine pollution and so on (Barboza Mariano & Lebre La Rovere, 2008).



Benzene	5.5
Ethylene	51.6
Butadiene	1.8
Butylene	1.6
Propylene	6.4
Toluene	1.8
Xylenes	2.8
Styrene	9.5

Figure 1. Relative Petrochemical Production (in tonnes) (IC, 2011)

The oil refining industries are a complex network of several different processes designed to produce a variety of chemicals via multiple pathways. During the initial design and development stages of petrochemical plant, the selection of the right chemical process routes is critical. Due to the increasing concern for environmental friendliness of chemical plants, process safety and risk have now become criteria in addition to economic considerations in selecting chemical process designs.

As described previously, LCA is extensively used as a decision making tool in the early stages of petrochemical plant design to evaluate design alternatives on the basis of environmental sustainability. However, a complete life cycle assessment is tedious, resource intensive and expensive. Moreover, complete information about a product or a process is not always available to LCA practitioners as industries usually hold proprietary rights to their data. Therefore, several streamlined LCA methodologies have been developed to aid in reducing the time, cost and effort expended to collect information. Probabilistic underspecification was proposed as a streamlining methodology wherein the problems associated with conducting full-fledged LCA are dealt with by specifying only certain components of the system under study using a structured classification system. As discussed earlier, streamlining methods are accompanied by several sources of uncertainty. Thus one of the main objectives of this thesis is to test the effectiveness of probabilistic underspecification as a viable streamlining option for the life cycle analysis of petrochemical products and polymers.

1.6 Contributions

This thesis seeks to add value to the existing knowledge on this topic by extending the previous research to the analysis of petrochemicals and polymers to improve confidence in probabilistic underspecification methodology. Two additional case studies on the life cycle of HDPE container/bottle production and aerosol air freshener cans are examined by partially underspecifying parts of the process chain to examine variation in impact estimates. Existing research on this topic only addressed the impacts of underspecification on cumulative energy demands of products. To further the study to additional impact categories, the methodology is extended to analyze additional environmental impact categories namely global warming potential, terrestrial acidification, freshwater eutrophication, freshwater ecotoxicity, human toxicity, marine ecotoxicity, marine eutrophication, metal depletion, photochemical oxidant formation, terrestrial ecotoxicity, fossil depletion and water depletion thereby providing valuable information on the effectiveness of this methodology across a spectrum of impact categories. To see how the differences in resolution of products affected the LCA results, petrochemicals and polymers were classified to varying levels specificity and the results were analyzed using the developed statistics. This study contributes to our understanding of when probabilistic underspecification can be used and how it impacts the overall model uncertainty when different products and a wide spectrum of environmental effects are studied.

This thesis is structured into 5 chapters. The subsequent chapter, Chapter 2 gives an overview of the petrochemical industries, its environmental concerns, a brief description about life cycle assessment and a detailed review of existing body of research

around streamlining and uncertainty assessment methodologies in LCA. Chapter 3 is much more specific to this project wherein the concept of structured underspecification is explained. Further, this chapter details the statistical analysis developed for the purpose of this thesis and the way it has been applied in the context of error quantification. Chapter 4 outlines the results of applying statistical modeling to underspecification. The life cycle models of 2 products- HDPE bottles/containers and aerosol air freshener canisters are also described. The results of underspecification and mis-specification applied to these cases are also included in this chapter. Finally, Chapter 5 summarizes and discusses the results of this thesis, conclusions as well as avenues for future research.

CHAPTER 2

LITERATURE REVIEW

2.1 The Petrochemical Industry- An Overview

The oil refining industry is energy intensive accounting for almost 10% of the total U.S energy consumption. About $10 billion was spent by petroleum refining sector on fuels and electricity in 2004. "More than 80 % of the refinery process energy is provided by the refinery products including refinery gas, petroleum coke and liquefied petroleum gas (LPG), fuel oil and other refined products" (Wang, Lee, & Molburg, 2004). This is understandable as the industry produces large volume basic and intermediate organic chemicals as well as plastics. In terms of volume, the global petrochemicals consumption was 436.86 million tons in 2011 and is expected to reach 627.51 million tons by 2018 (TransparencyMarketResearch, 2013).

The oil refining industry can be thought of as a large network of smaller interacting subsystems, such as processing technologies, connecting the basic feedstock to final products. A unit process that produces a chemical is itself a subsystem and a series of such subsystems forms the basic building blocks of a grand refinery framework. As a result, there is a complex interconnecting scheme wherein the products of one subsystem may serve as the feedstock for another. The raw materials for such petrochemical units are either sourced externally or are produced by other downstream processes in the petrochemical network (Al-Sharrah, Elkamel, & Almanssoor, 2010). Figure 2 shows a diagrammatic representation of a petrochemical refinery unit.

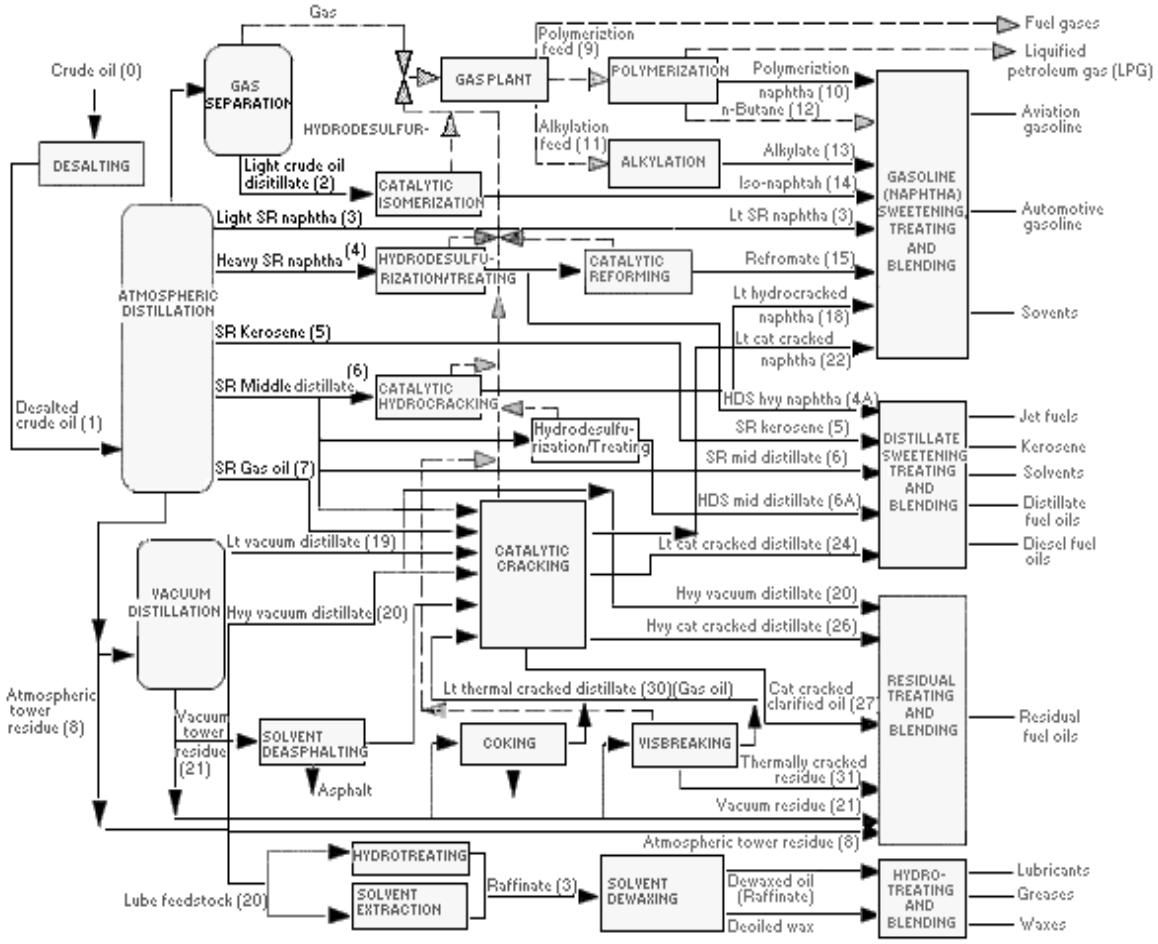


Figure 2. Petrochemical Refinery Flow Chart (SETLaboratoriesInc., 2008)

Petrochemical refining processes start with the distillation of crude oil. Distillation units fall under fractionation operations wherein crude oil is broken down into individual hydrocarbon "fractions" (also known as "cuts") based on differences in boiling points. These fractions then undergo conversion operations wherein the fractions from distillation units are converted into usable products by rearranging, dividing or combining the hydrocarbon molecules. Cracking and reforming operations are classified as conversion processes. These are the most energy intensive units of the oil refinery as they require a large amount of energy to modify long hydrocarbon chains.

The converted products then undergo further treatment to remove impurities before they are prepared into finished products. Extraction, blending, sweetening etc. are common treatment operations in the refinery which are used for the removal of sulfur, naphthenes etc. as well as other undesirable contaminants. Other refining operations include formulating, blending and other auxiliary operations to recover chemicals (SETLaboratoriesInc., 2008).

Petrochemical industries are the cause of several environmental hazards. Pollution, wastewater generation, toxic release, loss of biodiversity, global warming due to greenhouse gas intensification are some of the environmental impacts of oil refineries. Thus, oil companies are spending significant amount of money and resources in choosing chemical processing routes that are eco-friendly or at least aid in mitigating the harm caused to the environment. As a result, LCA is being extensively used to make calculated judgments about the sustainability of the processes during the planning stages as the impact of the final plant designs are dependent on the choices made during planning.

GaBi, an LCA modeling software, is extensively used to assess a products sustainability performance. The software models every element of a product system from a life-cycle perspective, equipping businesses to make the best informed decision on the manufacture and lifecycle of any product.

For the purpose of this thesis, a pre-modeled refinery module in GaBi (Figure 3) was used to gather data regarding the environmental impacts of the refinery products. The refinery supply chain was modeled by LCA experts integrating a large pre-calculated dataset from industrial research which would have otherwise been too tedious (Baitz et al., 2013).

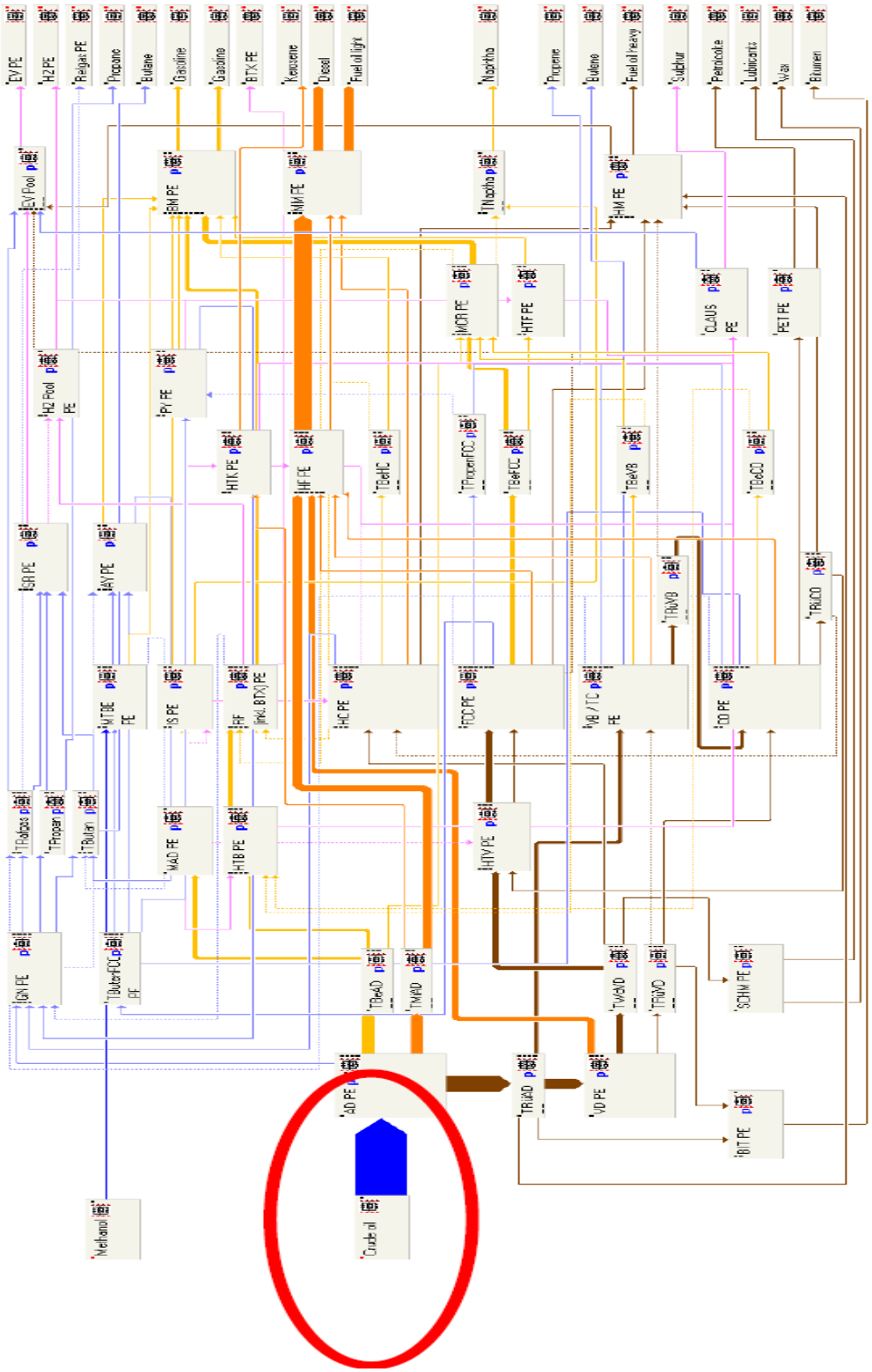


Figure 3. Refinery Module in GaBi Software (Baitz et al., 2013)

2.2 LCA Methodology

"At the outset, performing an LCA study requires several things:

- Data on the production, use and disposal of the product including materials it is made from, the energy consumption patterns etc.
- A standard method to organize and link the data in the appropriate way.
- A software to analyze the collected data
- A procedural context to use the results and apply it consequently" (Guinee & Heijungs, 2005)

Accordingly, the ISO has established a standard protocol for performing an LCA study. This methodological framework distinguishes four main phases (Figure 4).

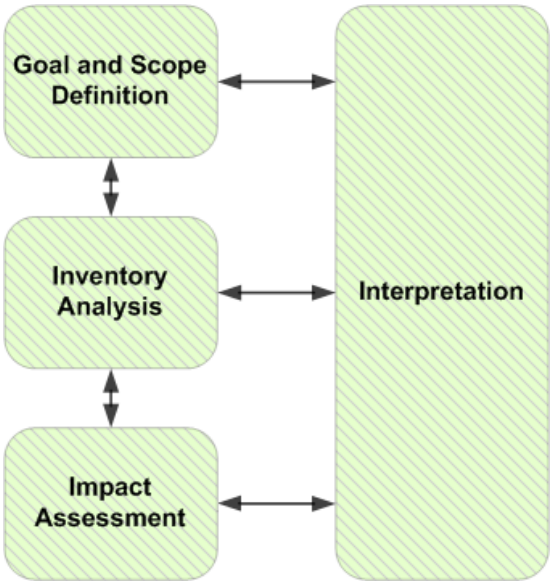


Figure 4. Illustration of LCA Phases (ISO, 2006)

An LCA starts with a precise definition of the goal and scope of the study. This sets the context of the study and the audience to whom the results are communicated. It

also draws the "boundary" for the assessment, defines the functional unit that forms the basis for comparison of systems and activities and states any assumptions and/or limitations. Further, the allocation methods for dividing the environmental impact loads and the impact categories considered are mentioned at this stage. Therefore, the definition of goal and scope of an LCA is very important as it sets the tone of the study.

The inventory analysis step involves creating a flow diagram of the product system being studied. A flow chart is used to depict the activities in the supply chain with details of flows to and from the nature and techno-sphere. It is a diagrammatic representation of inputs of energy and raw materials as well as the outputs such as emissions to air, water and soil. The data for the flows are based on an appropriate functional unit and represents all the activities in the techno-sphere and beyond depending on the goal and scope of the study.

The next stage is the life cycle impact assessment or the LCIA. According to ISO 14040, impact assessment is a "phase of LCA aimed at understanding and evaluating the magnitude and significance of the potential environmental impacts of the product system" (Guinee & Heijungs, 2005). Four main steps can be distinguished within the impact assessment: selection of impact categories, selection of category indicators and characterization models, assignment of inventories to impact categories and characterization (Guinee & Heijungs, 2005).

The life cycle impact assessment is followed by the interpretation stage wherein the results of the inventory analysis and the LCIA are quantified and summarized. These results highlight the sustainability issues from the study and relate it in a way that business decision makers can understand. Finally, the outcome of this stage is a set of

conclusions, limitations and recommendations that are used to support the decisions made by the stakeholders.

2.3 Environmental Impact Categories

As described above, one of the most important phases in life cycle assessment is impact assessment. At this stage it is very critical that the right impact categories and indicators are chosen. For the purpose of this thesis, 11 key impact categories are selected for analysis. A brief description of each of those is given below.

Global warming potential is an index to measure the contribution of a substance released to the atmosphere to global warming. It is impacted mainly by the emission of greenhouse gases such as carbon dioxide and methane. It is measured in terms of kg CO_2 equivalents for a time horizon of 100 years.

Terrestrial acidification refers to the increase in acidity of the soil and associated ecosystems due to chemical emissions. It is measured in terms of kg SO_2 equivalents.

Freshwater eutrophication is an abnormal increase in concentration of chemical nutrients in a freshwater system resulting in hindered productivity of aquatic life due to reduction of available oxygen. It is expressed in terms of kg PO_4 equivalents.

Freshwater ecotoxicity refers to the impact on freshwater ecosystems due to the addition of toxic substances to air, water and soil. It is expressed in terms of kg 1,4-dichlorobenzene equivalents.

Human toxicity is the impact on humans due to toxic emissions to the environment based on their inherent toxicity and potential dosages. This however does

not include occupational exposure to toxic chemicals. These by-products are mainly caused from electricity production from fossil sources. It is expressed in terms of kg 1,4-dichlorobenzene equivalents.

Marine ecotoxicity refers to the impact on marine life due to the addition of toxic chemical substances to marine systems. It is expressed in terms of kg 1,4-dichlorobenzene equivalents.

Marine eutrophication is similar to freshwater eutrophication in that it refers to the addition of nutrients from agricultural and urban sources to marine systems resulting in the reduction of oxygen available to support aquatic life. It is measured in terms of kg N equivalents.

Metal depletion refers to the impact of consuming non-renewable metal resources. It is measured in terms of kg Fe equivalents.

Fossil depletion refers to the exhaustion of non-renewable fossil resources such as crude oil. It is measured in terms of kg oil eq.

Photochemical oxidant formation refers to the contribution to air pollution due to smog formation as a result of reactions that take place between NO_x and volatile organic compounds (VOC) when exposed to UV radiations. It is measured in terms of kg NMVOC (non-methane volatile organic compounds).

Terrestrial ecotoxicity refers to the impact of toxic substances on terrestrial ecosystems. It is measured in terms of kg 1,4- dichlorobenzene equivalents.

Water depletion refers to the depletion of water resources resulting from the use of freshwater for various purposes throughout a products' life cycle. It is measured in terms of volume of water used i.e. m^3 (Osram, 2014).

2.4 LCA Applications

Life cycle assessment is a systematic procedure for developing the environmental profile of a product system. "LCA techniques range from full-scale comprehensive assessments to streamlined methodologies. The appropriate technique will depend on the specific design application as indicated in the table below" (Keoleian, 1993).

Table 1

Applications of LCA to Product Design (Keoleian, 1993)

Evaluation of project designs
• Use streamlined LCAs for screening projects based on environmental performance. • Identify improvement opportunities to reduce environmental burdens and improve process sustainability. • Conduct a detailed life cycle assessment to create benchmark profiles for future designs.
Specification of requirements
• Use information from existing LCAs to drive improvements and innovation in new sustainable product designs. • Conduct LCAs to assess product performance and observe perceivable improvements. • Achieve and exceed benchmarked performance standards.
Evaluation of design alternatives
• Conceptual design: use streamlined LCAs to conduct preliminary evaluations at this stage. The system is not fully specified for a comprehensive analysis. • Detailed design: After filtering and selecting the main projects, conduct comprehensive full scale LCAs to compare designs. At this stage, there is limited room for process/product modifications and design changes.

Today, LCA is applied at different stages. Broadly, the two levels at which LCA is applied is at the operational level and at the strategic level.

At an operational level, LCA finds applications in stages of product design, development and product improvement as well as comparison of systems based on environmental performance. On the other hand, LCAs can be used at a strategic level for providing guidance on types of products to develop and investments to make for new products, systems and waste handling (Guinee & Heijungs, 2005). Moreover, when

companies are presented with numerous options for providing a particular service or function, results from an LCA prove to be extremely useful to pick the one that presents maximum benefit in terms of economic feasibility and environmental safety.

Life cycle assessment is a versatile tool. Depending upon the purpose for which LCA is put to use, it can be categorized into two types: product specific LCAs and non-product LCAs. Today, LCA has been applied to a gamut of product categories such as electronics, general merchandize, toys, plastic products, and home & personal care products and so on and so forth. It has been applied to something as simple as a pencil to complex products like cars. Some non-product LCA studies include those on transportation and logistics sectors, waste management options, business cycle studies and so on (Guinee & Heijungs, 2005).

Sustainability and sustainable development has become the interest of several businesses and companies around the world. Multiple companies and industries are currently funding several projects related to sustainability measurement and reporting. Life cycle assessment forms the core of such initiatives. For instance, Wal-Mart, the world's largest retailer of consumer products, in collaboration with The Sustainability Consortium, has integrated sustainability into their businesses to identify hotspots and improvement opportunities in their supply chains and communicates the issues to buyers and suppliers of their products. Further, sustainability indices developed by the consortium is being put to use to create internal tools to track and measure sustainability progress in their business practices and product supply chains (TSC, 2009).

2.5 Limitations of LCA

Although the conceptual structure for LCA is well-developed, several limitations obstruct the practical implementation of a comprehensive LCA. Both cost and time constraints limit the usage of LCA. The benefits of conducting a full-fledged LCA may not be immediately evident for small and large companies alike. As mentioned earlier, the effort required to gather data remains rigorous and expensive. One of the most crucial hindrances for conducting an LCA is the lack of availability of data. Proprietary data and lack of access to accurate information, precision and completeness are some of the common issues that have slowed down the implementation of LCA into the existing environmental management systems.

Due to the prohibitive costs, resource intensiveness and time constraints for conducting a complete analysis, several streamlining methods have been proposed over the years. Some of them are highlighted below.

2.6 Streamlined LCA- A Possible Solution?

Most of the streamlined LCA techniques studied could be broadly classified into two types – qualitative and quantitative. Qualitative techniques are usually either pattern based or matrix based. The matrix based approach uses a predefined survey of questions in conjunction with streamlined LCA to provide a systematic scoring system as an environmental impacts evaluating tool. On the other hand, the pattern based LCA uses results of existing LCAs to compare products' environmental impact maps based on product characteristics. The results of the comparison in combination with a weighting

ratio enable the LCA modeler to develop a qualitative LCA of environmental impacts of new innovative designs and product operations (Chen & Chow, 2003).

Several applications today demand a quantitative assessment of their processes and systems. Consequently a slew of quantitative assessment procedures have been developed that are fundamentally more difficult to streamline (Patanavanich, 2011).

Essentially, qualitative LCA is a form of streamlined LCA that requires less data collection as opposed to quantitative methods. To balance the need for quantitative systems that could deliver accurate results with greater confidence as well as qualitative systems for ease of data gathering, semi-quantitative approaches have been proposed. For instance, one of the methods involves assessing the entire product system to identify parts of the life cycle that have a relatively smaller weight associated to the LCA results. These parts are then dropped to derive semi-quantitative estimates without introducing huge errors in the LCI results (Hunt et al., 1998).

One other streamlining approach involves the use of surrogate data for those processes for which data are not readily available. These heavily rely on existing information and predefined data. Further, this method requires that the substitute data closely resembles the process described. More often than not, the data available may not match the process being studied that leads to erroneous results (Hunt et al., 1998).

Hunt et al., (1998) has summarized some of the procedures for applying streamlining methods to conduct LCA studies. Table 2 gives an overview of the approaches used to streamline LCAs. These methods can be roughly assembled into three types: reduction of scope by excluding classes of materials, reduction of data by substituting surrogates for data that may not be readily available to the practitioner and

reduction of data by using qualitative or less accurate information where better data are not accessible.

Table 2

Summary of Procedures for Applying Streamlining Methods

Type	Streamlining Method	Procedure
Reduction of scope by	removal of all upstream components	Includes all processes starting from primary manufacture & processing of raw materials to final products, consumer use, and end-of-life treatment methods. Does not include preliminary processes such as raw material extraction, transportation to processing plants etc.
	removal of some upstream components	Includes all processes starting from the step just preceding the primary manufacture & processing of raw materials at plants and the steps following it. All other preliminary upstream processes are dropped.
	removal of all downstream components	Includes all preliminary stages such as extraction of raw materials, transportation to plants and so on up to the manufacture of final products at plant. All processes post manufacture of finished goods is dropped. Cradle-to-gate scope.
	removal of all upstream and downstream components	Only primary material processing and manufacture into finished products are included. All upstream and downstream processes are not scoped in. Gate-to-gate scope.
	excluding classes of inputs by contribution (<10%)	All raw materials contributing less than 10% by mass of the LCI totals are not inventoried and included for the analysis.
	excluding classes of inputs by contribution (<30%)	All raw materials contributing less than 30% by mass of the LCI totals are not inventoried and included for the analysis.
Using surrogates for	representing impacts	Based on mass (and expertise of the modeler), only certain entries are used as proxies for 24 impact categories. Other entries are dropped.
	representing life cycle inventories	Comprehensive and partial LCIs are compared. Only those entries from partial LCIs that closely match those from full LCIs are used as proxies; other entries are excluded.
	representing processes	Certain processes are replaced by other processes based on similarity of functionalities, physical & chemical properties and data availability.
Using qualitative data	Or less accurate data depending upon the need	Only data for those processes that significantly impact the final results are included. Other process steps are either dropped from the analysis or marked as less accurate data based on initial screening of LCI data.

After a thorough review of the methodologies, the “sensitivity analysis” approach was declared the most successful procedure. It involves the study of a model of the product system under consideration and the formation of a preliminary LCI after which

the percentage contribution of each process to the total can be assessed for further scrutiny.

Society for Environmental Toxicology and Chemistry (SETAC) also established similar approaches that in essence dealt with altering the goal and scope of the LCA based on relative contributions of different stages in the process chain to the overall environmental impacts (Todd et al., 1999).

As already discussed before, Chen & Chow (2003) described two simplified approaches for LCA of eco-innovative design of products viz. matrix-type and pattern based LCAs. The matrix type qualitative approach developed by Graedel (1998) uses a predefined scoring list combined with streamlined LCA and matrix approach. The scoring is based on a rating system ranging from 0 (highest impact) to 4 (lowest impact). The pattern based LCA maps out a products characteristic as a qualitative LCA value. The basic idea is that a product under consideration would have the same environmental impacts as a product studied previously that has similar properties. Thus, this methodology relies on existing LCA studies to match product characteristics to conduct LCA studies.

Ines Sousa & David Wallace (2006) recognized the need for analytically based conceptual design methods for integrated LCA. They developed an "automated classification system to support the specialization of surrogate LCA models for different groups of products". Surrogate LCAs are used for preliminary assessments wherein learning algorithms are trained to generalize on product characteristics and environmental data using pre-existing LCA studies. Using the "trained" artificial model, approximate environmental performance for a new product concept is obtained without defining new

LCA models. These results could then be used in combination with other models to predict environmental performance, trade-off analysis and concept selection.

The review conducted by Hunt et al., (1998) showed that most of the streamlining methods gave incorrect ranking of the products at least 50% of the time or more as compared to results arrived through full LCAs. Moreover, it was concluded that the results were unpredictable more often than not making it impossible to validate results based on a specific method.

The use of proxy data in place of actual ones, although widely followed, proved to be detrimental as it increases the uncertainty in the LCAs due to inaccurate representation of real systems. Additionally, this procedure is prone to errors as it relies heavily on the practitioners' subjective judgment for data match.

A quick literature survey shows several other research projects that have focused on developing innovative approaches for streamlining LCAs. Although significant effort has gone in to finding alternatives for comprehensive LCA studies, lack of accuracy of results proves to be a major cause for concern.

2.7 Uncertainty Analysis

Since LCA plays a key role in environmental decision making, it is natural that LCA experts and decision makers show interest in increasing the credibility of the results of the LCA study through efficient procedures. Results from life cycle assessments may lead to misleading conclusions about the significance of outcomes if the LCA is not supported by uncertainty evaluations (Heijungs & Huijbregts, 2004).

As highlighted previously, results from streamlined LCA studies have associated uncertainties that have to be quantified for making reliable conclusions. Table 3 lists a few types of uncertainties.

Table 3

Types of Uncertainty (Heijungs & Huijbregts, 2004)

Bevington & Robinson (1992)	**Morgan &Henrion (1990), Hoffstetter (1998)**	**Huijbregts (2001)**
Systematic and random errors	Statistical variation, subjective judgment, linguistic imprecision, variability, inherent randomness, disagreement and approximation	Parameter uncertainty, model uncertainty, uncertainty due to choices, spatial variability, temporal variability, variability between sources and objects
Funtowicz & Ravetz (1990)	**Bedford & Cooke (2001)**	**US-EPA (1989)**
Data uncertainty, model uncertainty, completeness uncertainty	Aleatory uncertainty, epistemic uncertainty, parameter uncertainty, data uncertainty, model uncertainty, ambiguity, volitional uncertainty	Scenario uncertainty, parameter uncertainty, model uncertainty

From Table 3, it can be seen several different types of uncertainty have been recognized over the years. However, many factors affect the application of uncertainty assessments to compliment a comprehensive study. Maximum amount of research has been focused on those aspects of uncertainty pertaining to parameter uncertainty or data uncertainty. Due to the complex nature of other types such as epistemic uncertainty or volitional uncertainty, these have not received widespread attention (Heijungs & Huijbregts, 2004).

Ross et al., (2002) argue that some of these uncertainties are pervasive in full fledged LCAs as well. Further, they point out that these uncertainties arise due to poor data quality, non-transparent assumptions and failure to do sensitivity analyses. The quantification of uncertainty to support LCA results has been mired due to the need for additional data and the necessity to perform additional complex calculations thereby

making the whole process cumbersome in terms of cost and resources (Patanavanich, 2011).

Ross et al., (2002) have conducted extensive research on how practitioners have dealt with the problem of uncertainty in their studies. They conducted a review of 30 LCA studies to identify those studies that reported uncertainty in their results and those that performed quantitative or qualitative uncertainty analysis. The results of the survey indicated that more than half of the studies made no reference to problems commonly associated with uncertainty. 14 (47 %) studies identified these problems but only 4 among those explicitly mentioned uncertainty. It was found that only 1 study performed quantitative analysis of the uncertainties linked to impact assessment. Finally, it was concluded that the limitations on impact assessment imposed by the inventory step of LCA went largely unrecognized and that LCA studies must at least include a qualitative discussion of the limitations of the study to improve credibility of the results.

Huijbregts (1998) pointed out that probabilistic simulation could be used as a means to address parametric uncertainty and variability in both the inventory and impact assessment stages of the LCA. Further, scenario analysis or standardization and peer review could be performed to mitigate uncertainty due to choices. Non-linear inventory models in the inventory and multi-media models in the characterization phase were cited as advanced procedures to deal with other model uncertainties. Parametric uncertainty and variability quantification is mostly dependant on the product system under review thus leading to the need for development of a structured framework for conducting such studies. Data uncertainty is caused due to lack of representative data and data inaccuracy. In order to address the need to express and propagate uncertainty, classical statistical

analysis was proposed as a potential tool. Using the available data points, a probability distribution could be developed to calculate the uncertainty associated with the results. Expert judgment using parametric distributions already established for similar processes could be used when statistical analysis is not possible. Distinct scenarios could be used to perform sensitivity analysis to deal with choice based uncertainty (Bjorklund, 2002).

Another approach involves the use of "fuzzy numbers to propagate data uncertainty in LCI calculations and results in fuzzy distribution of inventory results". Epistemological uncertainty could be modeled with high efficiency and lesser number of iterations using this approach. Further, this serves as an alternative to probabilistic or Monte Carlo analysis (Tan, 2008). However, it was noted that additional work was needed for modeling correlations of variability of parameters using fuzzy numbers.

A survey of recent developments in LCA was conducted by Finnvedan et al., (2009). The paper highlighted three techniques to deal with uncertainty viz. scientific, social and statistical. The scientific/mathematical way to deal with uncertainty and improve reliability is to find better data and models (Heijungs, 1996). Heijungs (1996) highlighted that "the structured procedure of LCA can be described in mathematical terms, so that standard mathematical techniques for the study of propagation of uncertainties could be employed".However, such practices often are often too rigorous and in fact contradict the whole point of performing a streamlined LCA. The urgency of finding quick answers to solving uncertainty therefore forbids the decision makers to wait for complete evidence. The social way, a variant of the "legal way", involves dealing with uncertainty by collaborating with authoritative bodies and stakeholders for reaching

a consensus in terms of data quality, models and choices. Parametric variation and scenario analysis along with classical statistical theory already highlighted previously could form the basis of dealing with uncertainty the "statistical way" (Finnveden et al., 2009).

One other popular approach for dealing with uncertainty associated with data quality is by the use of pedigree matrix (Weidema & Wesnæs, 1996). It can be used to ascertain how accurately the surrogate data/proxy represents the actual product system by assigning quantitative scores to qualitative judgment of an LCA practitioner. The data quality characteristics are classified into six categories (Table 4). The LCA practitioner can assign a semi-quantitative indicator score ranging from 1 to 5, 1 being the best, by assessing the quality of the data against each of these characteristics. These scores are then converted into a geometric standard deviation with associated uncertainty factors to give an idea of the overall data quality (Patanavanich, 2011).

Although substantial research has been carried out over the years to propose novel streamlining strategies for life cycle assessments and associated uncertainty quantification methods, there is still an impending need for an integrated as well as automated processes for performing the evaluations efficiently.

This thesis proposes a statistical methodology to evaluate the effectiveness of probabilistic underspecification as a viable streamlining approach for LCA studies. By quantifying data variability across the streamlining process, a quantitative judgment can be made by the LCA modeler about data quality and assessment. An overview of probabilistic underspecification streamlining methodology is given in the following section.

Table 4

Pedigree Matrix (Frischknecht et al., 2007).

Indicator score	1	2	3	4	5	Remarks
Reliability	Verified data based on measurements	Verified data partly based on assumptions OR non-verified data based on measurements	Non-verified data partly based on qualified estimates	Qualified estimate (e.g. by industrial expert); data derived from theoretical information (stoichiometry, enthalpy, etc.)	Non-qualified estimate	verified means: published in public environmental reports of companies, official statistics, etc unverified means: personal information by letter, fax or e-mail
Completeness	Representative data from all sites relevant for the market considered over an adequate period to even out normal fluctuations	Representative data from >50% of the sites relevant for the market considered over an adequate period to even out normal fluctuations	Representative data from only some sites (<<50%) relevant for the market considered OR >50% of sites but from shorter periods	Representative data from only one site relevant for the market considered OR some sites but from shorter periods	Representativeness unknown or data from a small number of sites AND from shorter periods	Length of adequate period depends on process/technology
Temporal correlation	Less than 3 years of difference to our reference year (2000)	Less than 6 years of difference to our reference year (2000)	Less than 10 years of difference to our reference year (2000)	Less than 15 years of difference to our reference year (2000)	Age of data unknown or more than 15 years of difference to our reference year (2000)	less than 3 years means: data measured in 1997 or later; score for processes with investment cycles of <10 years; for other cases, scoring adjustments can be made accordingly
Geographical correlation	Data from area under study	Average data from larger area in which the area under study is included	Data from smaller area than area under study, or from similar area		Data from unknown OR distinctly different area (north america instead of middle east, OECD-Europe instead of Russia)	Similarity expressed in terms of enviornmental legislation. Suggestion for grouping: North America, Australia; European Union, Japan, South Africa; South America, North and Central Africa and Middle East; Russia, China, Far East Asia
Further technological correlation	Data from enterprises, processes and materials under study (i.e. identical technology)		Data on related processes or materials but same technology, OR Data from processes and materials under study but from different technology	Data on related processes or materials but different technology, OR data on laboratory scale processes and same technology	Data on related processes or materials but on laboratory scale of different technology	Examples for different technology: - steam turbine instead of motor propulsion in ships - emission factor Bi(a)P for diesel train based on lorry motor data Examples for related processes or materials: - data for tyles instead of bricks production - data of refinery infrastructure for chemical plants infrastructure
Sample size	>100, continous measurement, balance of purchased products	>20	> 10, aggregated figure in env. report	>=3	unknown	sample size behind a figure reported in the information source

2.8 Probabilistic Underspecification

Specification of exact materials and the processes modeled is usually tedious, expensive and in some cases, impossible. Thus, LCA modelers rely on surrogate/proxy data for their studies. However, the use of surrogate data is almost always accompanied by the uncertainty that the data proxy does not mirror product system under

consideration. In other words, the results are affected by inaccuracies arising out of erroneous judgment of the LCA modeler that introduces a bias into the analysis. To mitigate such errors, probabilistic underspecification was proposed by Patanavanich (2011) as a streamlining methodology to conduct LCA studies.

Information about the system or process is categorized in the form of "levels" or "steps" with every subsequent level corresponding to smaller spectrum of possible parametric values necessary to describe the system. The idea is to reduce the effort needed to carry out a tedious LCA study by streamlining the same using different levels of data specificity. In doing so, one can compare the results obtained from the study across the different levels of classification thus giving a rough sense of the amount of effort necessary to gather better information where uncertainty comes from underspecifying a product life cycle.

The process involves breaking down the information into levels of increasing specificity based on system or materials properties and indexing materials information in a way that LCA practitioners "can understand the degree of uncertainty of different materials specificity about a component" (Patanavanich, 2011). This streamlining methodology has been adapted for the classification of refinery and polymeric products for the purpose of this thesis.

2.8.1 Overview of the Streamlining Methodology

When carrying out a conventional LCA, the evaluation of the environmental impacts of a system or material of interest involves the investigation of the specifics of the material by collecting primary data or looking for exact matches in existing database

of inventories. However, such a procedure would require the expertise of the modeler or additional effort in the form of research to be able to correctly select a data proxy for the system or product under study. To overcome this, probabilistic underspecification could be used wherein a product will be specified at lower levels of specificity and the inventory data will be collected based on the distribution of data associated with similar processes or activities (Patanavanich, 2011). For example, consider the refinery product diesel. Underspecification in this case would classify diesel as a refinery product precluding the need for further specification and collect the data associated with all refinery products and perform additional characterization of the uncertainty associated with such a simplification.

The general structured classification scheme for underspecification adapted from Patanavanich (2011) is illustrated in Figure 5 below. Each of the levels below represents information about the system under study at different levels of specificity. Here the most underspecified level is L0 and the most specified level is L4. Accordingly, L0 is associated with maximum uncertainty and L4 the least. From the figure, it can be seen that for a component when specified at L1, any database entry from L4-A through L4-F can be chosen as a data proxy. However, as the component gets further specified, to say L3-A, the corresponding proxies from the database are only L4-A and L4-B (Patanavanich, 2011). Thus, in going from "left" to "right", the possible options for data associated with similar processes or activities become narrower and therefore more specific and credible. In doing so, the modeler can estimate if a complete assessment with a certain degree of uncertainty could be made at any of the underspecified levels thereby aiding in achieving cost saving targets.

For the purpose of this thesis, refinery products as well as polymers were classified into different levels of increasing specificity on the basis of factors such as material families, properties, types and the geographic locations from which the respective products were derived. The most specific level in our case is level 4 (L4) which contains individual entries from the Ecoinvent database extracted with the LCA software GaBi. Then, the error in impact assessment associated with each level of specificity was statistically characterized to observe the penalty of losing precision in impact assessment at each of those levels.

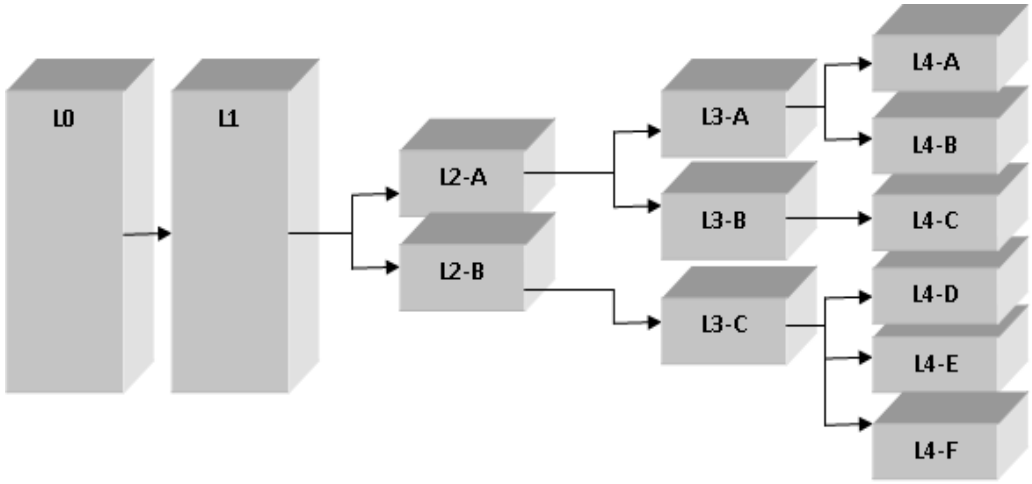


Figure 5. Structured Underspecification (adapted from Patanavanich 2011)

It should be noted that the most specific entries from the database themselves carry some level of uncertainty as they are merely ballpark figures or "best estimates for surrogate data" (Patanavanich, 2011). These uncertainties may be in the form of geographic variations, temporal variations and so on. These aspects can lead to vague results and thus have to be factored in when characterizing the uncertainty. Different sources of uncertainty in the data are discussed in detail in the next chapter.

CHAPTER 3

METHODOLOGY

3.1 Problem Statement

Researchers in materials systems laboratory at MIT have proposed a novel streamlining methodology for carrying out LCA studies. The concept, called probabilistic underspecification, incorporates a structured classification of life cycle activities and/or materials to leverage the fact the only some activities/materials must be well specified to gather complete information about the environmental performance of the entire system (Patanavanich, 2011). Essentially, this system aids in quantifying the effort necessary to carry out a full-fledged assessment of the products' life cycle.

The work developed herein adds value to the proposed streamlining methodology by characterizing the error in terms of variability in the LCA results arising out of structured underspecification. Moreover, this project seeks to explore the different sources that significantly affect the precision of the estimate of the environmental performance of a product system. By doing so, this thesis answers the question of how effective underspecification is as a viable LCA streamlining option.

3.2 Structured Underspecification of Refinery Products and Polymers

Some of the common outputs of the refinery are fuel gases, liquefied petroleum gas (LPG), aviation gasoline, automotive gasoline, solvents, jet fuels, kerosene, distillate fuel oils, diesel fuel oils, residual fuel oils, lubricants, greases and waxes. Of these, some specific products like greases, waxes and lubricants are further refined in several downstream processes before being sold for consumer use. In this thesis, refinery

products have been grouped together into meaningful sets to highlight just the key products that are common to any refinery around the globe. The main products considered in this thesis are petrol (unleaded and low sulphur), diesel, fuel oil (heavy and light), kerosene, naphtha, sulphur, electricity (produced within the refinery), propane/butane and other refinery gases.

As described in the previous section, the inventory data for the 10 key refinery products was compiled and categorized into hierarchical levels of specificity. Only 3 refinery products (diesel, heavy fuel oil and light fuel oil) are shown as an example in Table 5 below. A complete list of all the refinery products analyzed is shown in Chapter 4 of this document. The functional unit was considered to be 1 kg of the product produced. Since L0 was labeled to be the least specific/most generic level, the products of the refinery were classified into one superset called "Refinery Products". L1 is the next higher level of specificity and thus refinery products were further categorized into "Fuels" and "Chemicals". Fuels are then categorized into "Oil" and "Gases" and Chemicals into "Inorganic". Moving further, the oil, gases and inorganic chemicals categories have been further specified to individual refinery products viz. "Diesel", "Petrol" and so on depending upon the appropriate category they fall under. For example, diesel is classified as an oil where as propane/butane as a gaseous fuel. Finally, these refinery products are classified based on the geographic location of the refinery itself viz. Switzerland (CH) and Rest of Europe (RER) which forms the most specific level L4. Entries for L4 are individual entries extracted from life cycle inventory Ecoinvent database.

Table 5

Underspecification of Refinery Products

L0	L1	L2	L3	L4
Refinery Products	Fuels	Oil	Diesel	Diesel, at refinery/CH U
Refinery Products	Fuels	Oil	Diesel	Diesel, at refinery/RER U
Refinery Products	Fuels	Oil	Diesel	Diesel, low-sulphur, at refinery/CH U
Refinery Products	Fuels	Oil	Diesel	Diesel, low-sulphur, at refinery/RER U
Refinery Products	Fuels	Oil	Fuel Oil	Heavy fuel oil, at refinery/CH U
Refinery Products	Fuels	Oil	Fuel Oil	Heavy fuel oil, at refinery/RER U
Refinery Products	Fuels	Oil	Fuel Oil	Light fuel oil, at refinery/CH U
Refinery Products	Fuels	Oil	Fuel Oil	Light fuel oil, at refinery/RER U

Since petrochemicals form the basis for the manufacture of several polymers and plastics, polymeric materials were also underspecified to see how such a classification system affected downstream processes as opposed to upstream processes in the supply chain. In other words, refinery impacts and polymer manufacturing impacts were compared at their least specific level to see if all the impacts of upstream refinery operations were fully captured while evaluating the impacts of downstream polymer manufacturing operations.

An approach similar to the classification of refinery products was taken to classify polymers. In this case, different polymers were classified into 4 levels, level 1 (L1) to level 4 (L4). Here, L1 is the least specific level and L4 the most specific level consisting of individual entries from the database. It is to be noted that in this case, only polymers from European plants were considered. This was due to the lack of environmental impact information for polymers from Swiss plants. Thus, while comparing the variation in impacts of refinery products and polymers, only data from European refineries and polymer manufacturing plants are analyzed.

8 polymers were selected for the analysis viz. Nylon, PMMA, Polyethylene, Polystyrene, Polyvinylchloride, Polyurethane, Epoxy resins and Formaldehyde resins. At level 1, all these polymers were classified into a superset named "Polymers". In the next level, L2, they were further subdivided on the basis of their properties into "Thermoplastics" and "Thermosets". L3 being the next higher level of granularity signifies classification of individual polymers based on their types. Accordingly they are assorted by the characteristic of that category. Finally, L4 consisted of individual entries for polymers from European polymer manufacturing plants and their variations. Table 6 below shows an example of polymer classification system.

Table 6

Underspecification of Polymers

L1	L2	L3	L4
Polymers	Thermoplastic	Nylon	Nylon 6, at plant/RER U
Polymers	Thermoplastic	Nylon	Nylon 6, glass-filled, at plant/RER U
Polymers	Thermoplastic	Nylon	Nylon 66, at plant/RER U
Polymers	Thermoplastic	Nylon	Nylon 66, glass-filled, at plant/RER U
Polymers	Thermoplastic	PMMA	Polymethyl methacrylate, beads, at plant/RER U
Polymers	Thermoplastic	PMMA	Polymethyl methacrylate, sheet, at plant/RER U

Since the classification follows a hierarchical structure, each entry in the most specified level is linked to all preceding levels without introducing statistical bias (Patanavanich, 2011). For the purpose of this project, 11 different environmental impact categories were selected viz. global warming potential, terrestrial acidification, freshwater eutrophication, freshwater ecotoxicity, human toxicity, marine ecotoxicity, marine eutrophication, metal depletion, petrochemical oxidant formation, terrestrial

ecotoxicity and water depletion. The impact data for each of the refinery outputs as well as polymers was extracted using GaBi software with inbuilt Ecoinvent database.

3.3 Mis-specification

In this work, one other interesting study has been introduced and tested. Suppose an LCA modeler had access to all the data associated with the characteristics of a material under consideration. However, to model a particular component, he/she is faced with the task of choosing a material proxy from a whole slew of options available in the database. How much penalty in terms of error will he/she incur by choosing the wrong substitute from the database?

Refer to table 6 above. For example, imagine a product made of Nylon 6 material. If the LCA modeler only knows it is made of Nylon (L3) but does not know the exact variety, he/she is faced with the 4 similar data proxies belonging to the Nylon family (L4) to choose from to model the life cycle of the product. Therefore, by choosing the wrong variety of Nylon viz. "Nylon 6 glass filled" or variations of Nylon 66, the modeler, in actuality, is "mis-specifying" the material. As a result, the environmental impacts of the product being modeled may vary depending on the material chosen and hence affect the LCA results. This concept is termed mis-specification. Mis-specification has been tested as part of analysis of two case studies in this thesis wherein certain components in the life cycle of a product are wrongly specified and the LCA results are analyzed.

3.4 Statistical Characterization of Uncertainty

As stated previously, the quantification of the variability across and within the different levels of classification will provide the modeler with vital information on the

effectiveness of probabilistic underspecification. This can therefore be used to analyze the different sources of variation and make a calculated judgment about how the LCA results are affected because of underspecifying certain components of a product system. Moreover, these results can be used to further refine the streamlining process to obtain results with better certainty without performing a complete LCA. These results arising out of characterization of errors in the streamlining procedure could be used to earmark and handpick only those factors that need further "specification", thus reducing the effort needed for data collection.

3.4.1 Estimation of Error

Standard deviation is used as a measure of dispersion from average values. Thus, it is used to quantify the margin of error in the environmental impact estimation arising out of underspecifying a material or a product system. In other words, it gives us an idea of the amount of information lost in moving from L4 to L0. Therefore, to capture the variability throughout the entire classification system, it is vital that the error within the individual levels and across the levels is calculated.

Accordingly, the standard deviations are calculated as follows:

$$\sigma_{Level\ 4} = \sqrt{Average\ (\sigma^2{}_4)} \quad (1)$$

$$\sigma_{Level\ 3} = \sqrt{Weighted\ Average\ (\sigma^2{}_{Pooled\ Level\ 3})} \quad (2)$$

$$\sigma_{Level\ 2} = \sqrt{Weighted\ Average\ (\sigma^2{}_{Pooled\ Level\ 2})} \quad (3)$$

$$\sigma_{Level\ 1} = \sqrt{Weighted\ Average\ (\sigma^2{}_{Pooled\ Level\ 1})} \quad (4)$$

$$\sigma_{Level\ 0} = \sqrt{\sigma^2{}_{Level\ 0}} \quad (5)$$

"$\sigma_{Level\,4}$" from equation 1 above represents the average error within the most specific level L4. In this thesis, for the case of refinery products, L4 represents the variation in the product environmental impacts due to difference in geographic location. For example, the calculated numerical value for each impact category represents the difference in impacts between kerosene produced in refineries in Switzerland and rest of Europe. Thus, the average variance of impacts between the two locations is calculated for each unique product of the refinery. The square root of the variance gives the measure of standard deviation. However, for the case of polymer manufacturing, data is collected only from plants located in Europe. As a result, for the purpose of calculations, the standard deviation in impacts is calculated only up until level 3. Nevertheless, this does not eliminate the possibility of uncertainty within level 4 of polymers classification. These individual entries from Ecoinvent database might not be the right substitute for the material under study and as a result might carry some level of underlying uncertainty along with the data itself.

Similarly, "$\sigma_{Level\,3}$","$\sigma_{Level\,2}$" and "$\sigma_{Level\,1}$" indicate the variations within each of those respective levels. Specifically, $\sigma_{Level\,3}$ represents the average error in the impact values among L3 categories. For the case of refinery products, within L3, there are 9 different product categories viz. diesel, fuel oil, kerosene, naphtha, petrol, electricity, propane/butane, refinery gas and sulfur. Similarly, for the case of polymers, L3 constitutes Nylon, PMMA, Polyethylene, Polystyrene, Polyvinylchloride, Epoxy, Formaldehyde resins and Polyurethane. Thus, $\sigma_{Level\,3}$ indicates the difference in the impacts between each of these product categories. Going by the same logic, $\sigma_{Level\,2}$ yields a measure of error in impacts of oil vs. gases vs. organics for refinery products,

and thermoplastic vs. thermosets for polymers. Similarly, $\sigma_{Level\ 1}$ represents the difference between fuel and chemical impacts. $\sigma_{Level\ 0}$ represents the error associated with impacts of refinery products as a whole. In the case of polymers, this numerical value ($\sigma_{Level\ 0}$ is equivalent to $\sigma_{Level\ 1}$ for polymers) indicates the grand error associated all the polymer products.

Note that for levels 3, 2 and 1weighted average is used for the calculation of error in place of regular average. The weighted average is similar to a regular average, where instead of each of the data points contributing equally to the final average, some data points contribute more than the others. In other words, weighted average is used to account for the difference in the sample sizes in the individual categories within each of those levels. For example, within level 3 of refinery products, fuel oil has 4 data points whereas kerosene has just 2 data points.

Thus, the pooled average weighted variance is calculated as

$$Weighted\ mean\ of\ variance\ \sigma_{pooled}^2 = \frac{\sum Sum\ of\ Squares}{\sum Degrees\ of\ Freedom} = \frac{\sum (n_i - 1) * \sigma_i^2}{\sum (n_i - 1)}$$

In the above equation, "n_i" represents the number of data points in a specific product category within that particular level of specificity and "σ_i^2" represents the variation in impacts of that product category.

The ratio of the standard deviation to the grand mean of the data at the lowest level of specificity of all the refinery products (as well as polymers) gives the percentage of overall error associated with the environmental impact data of entire product category for all the impact categories.

3.4.2 Analysis of Variance (ANOVA)

In order to clearly see the distinctions in contribution of different sources to the variation in the environmental impact values, an analysis of variance was performed. The different levels were used as input factors and the impact data across a variety of impact categories was used as the response variable. The most significant sources of variation could be identified across different impact categories. In other words, it gives a clear picture as to whether underspecifying materials to lower levels of specificity introduces a bias or a significant error in the life cycle impact assessment. Since multiple impact categories are compared and contrasted with each other, this analysis also explains whether underspecification affects all the impact categories alike. One important advantage of ANOVA is that it is robust to the distribution of data set. In other words, normality of the data is not entirely critical for performing ANOVA analyses. ANOVA was also done in the context of this work to understand the fact that different impact categories are characterized and evaluated differently and that different parts of the life cycle of a product might contribute to different extents to each of these impacts.

Further, for ease of interpretation of data, box plots for each of the levels were generated. These box and whisker diagrams conveniently depict the mean, median, spread (dispersion) and skewness in groups of numerical data through their quartiles. Very large differences in the mean impact values of different product groups in moving from one level to the other could easily be identified using these plots. One other important use of such box plot diagrams is to spot conspicuous outliers in the raw data. In theory, the width of the box plots also illustrates the size of each group whose data by making the width proportional to the sample size of the group in each level. This could

additionally be used to refine the streamlining process by modifying the granularity within the levels or across them to enhance the credibility of the results. JMP software was used to perform the statistical modeling and variance studies.

3.5 Case Studies

In order to investigate the usefulness of structured underspecification in working models, the life cycle of High Density Polyethylene bottles/containers and aerosol air freshener cans were studied. The effects of mis-specification were also studied for each of these cases.

3.5.1 High Density Polyethylene Containers

Polyethylene is one of the most extensively used commodity polymers in the world. The plants that manufacture polyethylene are usually found in the vicinity of the refineries that produce the monomer ethylene for polymerization reactions. Polyethylene is classified into three types on the basis of their physical and chemical properties: high density polyethylene, low density polyethylene and linear low density polyethylene. LDPE and LLDPE are widely used as films for packaging or plastic bags. On the other hand, due to the extremely stable, robust and moisture resistant properties of HDPE, they find applications as plastic bottles, containers, canisters etc. These polyolefins also find uses in various other consumer merchandise and household applications, furniture, electronics, agriculture and so forth (PlasticsEurope, 2014). Polyethylene is formed by the addition polymerization of ethylene through repeated addition of free radicals.

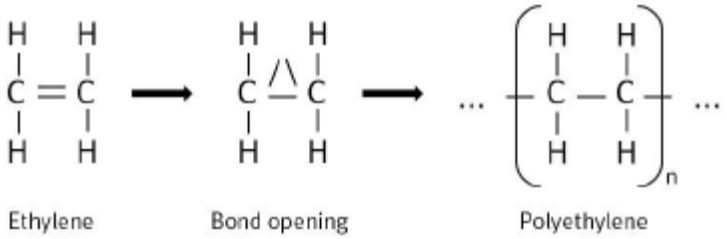


Figure 6. Schematic of Ethylene Polymerization (PlasticsEurope, 2014)

By varying the process conditions (temperature, pressure and catalysts), different properties could be achieved viz. branching, density and polymerization factor, thereby yielding different grades of polyethylene. HDPE is the most rigid of all, with very few side branches. Its density is between 0.94-0.97 g/cm^3 (PlasticsEurope, 2014).

HDPE is one of the most widely used polymeric resins for the manufacture of plastic bottles and containers due to its superior properties. They are lightweight, robust and provide a good moisture barrier. Moreover, they are cost effective in terms of manufacturing and production costs and thus have replaced glass bottles for a variety of applications.

The process flow for the manufacture of HDPE bottles is shown in Figure 7 below. The scope of the process was considered to be cradle-to-grave with recycling streams. Therefore, all the steps right from crude oil extraction to production of HDPE bottles are included in the life cycle analysis of HDPE bottles. Ethylene for polymerization reactions are produced by steam cracking process. Naphtha, produced by the refining of crude oil as well as processed natural gas are usually the feedstock for the steam cracking process. Cracking takes place at extremely high temperatures of about 875^{o}C wherein the dehydrogenation i.e. the breaking up of larger hydrocarbon molecules to shorter chains takes place.

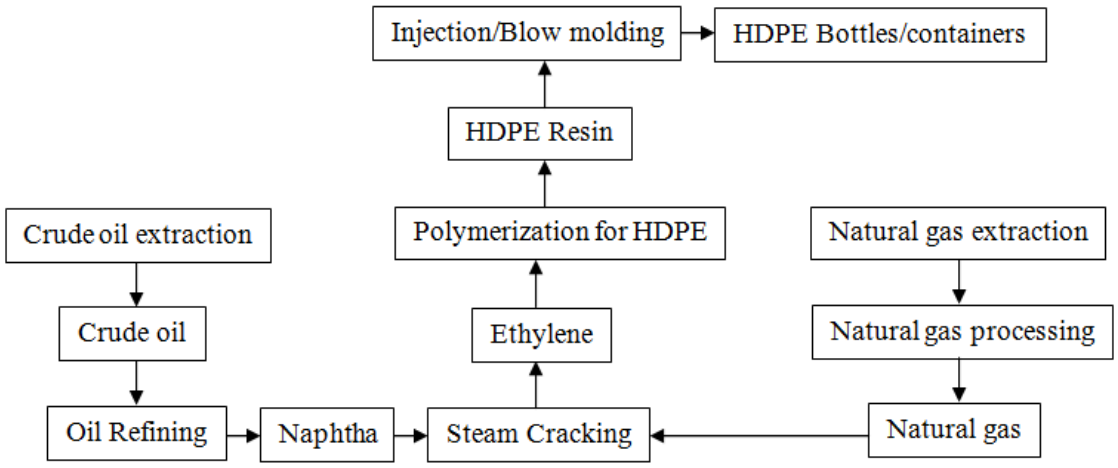


Figure 7. Manufacture of HDPE Bottles (adapted from PlasticsEurope, 2014)

The ethylene produced is then transported to polymerization plants for the production of polyethylene. Specifically, for the production of HDPE, polymerization reactions take place in the presence of Ziegler-Natta catalyst at temperatures of around 100^{o}C-120^{o}C and atmospheric pressures (PlasticsEurope, 2014).

For the purpose of this thesis, the life cycle of a 1 gallon HDPE plastic container was modeled using GaBi software. The functional unit for this study was one bottle/container. Three different variations in terms of end-of-life scenarios in the life cycle are studied- one with 100% recycling rate & 85% recycling efficiency, another with 30% recycling rate & 50% recycling efficiency and finally one with no recycling stream.

3.5.2 Aerosol Air Freshener Cans

Air fresheners are consumer products designed to counteract the effect of foul odor by emitting fragrance. Typically, such aerosol air fresheners consist of an aluminum body with a HDPE trigger which when depressed releases pleasant fragrance. A pre-built model of an aluminum aerosol spray canister with an HDPE trigger was selected. The

functional unit for this study was set at one canister and model was scoped to be from raw material extraction to retail.

In both these models, the HDPE granulates are converted into HDPE bottles and HDPE triggers respectively via a series of manufacturing steps which are elaborated in the next chapter. For the purpose of this study, the HDPE granulate manufacturing step is underspecified to lower levels and the impact assessment was redone to see the effect of such a procedure. For instance, in this case, "HDPE granulates" were underspecified to "polyethylene granulates" (L3) followed by "thermoplastic granulates" (L2) and finally just "polymeric granulates" (L1). Keeping the mass balance consistent, the environmental impact assessment was repeated at each level to observe if the underspecification introduced a huge error in the final result. The percentage differences in the impacts of the product when the component was specified at the most granular level and at lower levels in the hierarchy were also reported. In actuality, the error quantified gives a measure of how far away one is from the actual result.

To test the effects of mis-specification, the HDPE component in the model in both cases was mis-specified as LDPE (low density polyethylene) and LLDPE (linear low density polyethylene). Again, keeping the mass balance consistent, the environmental impacts of the products were recalculated to see if mis-specifying the components from the same material family had a significant effect on the life cycle impact assessment of the overall product. Sample calculations are included in appendix F to better explain the concepts.

CHAPTER 4

RESULTS AND DISCUSSION

This chapter outlines the results obtained by applying probabilistic underspecification to refinery products and polymers. First, the detailed classification schemes for both the product categories are highlighted. The results of performing statistical uncertainty analyses are then explained in detail. The concepts of underspecification and mis-specification applied to two product case studies are also discussed.

4.1 Classification of Refinery Products and Polymers

Table 7 and Table 8 below show a complete list of refinery products and polymers categories respectively categorized based on probabilistic underspecification streamlining methodology. The column to the extreme right shows the values for global warming potential impact category for each of these products, extracted from Ecoinvent database built in with GaBi software. These values essentially represent the amount of greenhouse gases (in terms of carbon dioxide equivalents) released to the atmosphere during the course of production of each of these products. For instance, the global warming potential data for "Diesel, at refinery/ CH U" takes into account the greenhouse gases emitted during oil field exploration, crude oil extraction, transportation of crude oil to refineries and oil refining. That is, the scope considered here is cradle-to-gate. Airborne emissions inventoried comprise CO, CO_2, SO_2, NO_x and other particulates (Dones et al., 2007). The data collected for other impact categories is attached in appendices A and B.

Table 7

Structured Underspecification of Refinery Products

L0	L1	L2	L3	L4	GWP
Ref Products	Fuels	Oil	Diesel	Diesel, at refinery/CH U	6.56E-04
Ref Products	Fuels	Oil	Diesel	Diesel, at refinery/RER U	1.25E-03
Ref Products	Fuels	Oil	Diesel	Diesel, low-sulphur, at refinery/CH U	0.00E+00
Ref Products	Fuels	Oil	Diesel	Diesel, low-sulphur,at refinery/RER U	0.00E+00
Ref Products	Fuels	Oil	Fuel Oil	Heavy fuel oil, at refinery/CH U	5.81E-04
Ref Products	Fuels	Oil	Fuel Oil	Heavy fuel oil, at refinery/RER U	1.16E-03
Ref Products	Fuels	Oil	Fuel Oil	Light fuel oil, at refinery/CH U	6.56E-04
Ref Products	Fuels	Oil	Fuel Oil	Light fuel oil, at refinery/RER U	1.24E-03
Ref Products	Fuels	Oil	Kerosene	Kerosene, at refinery/CH U	6.57E-04
Ref Products	Fuels	Oil	Kerosene	Kerosene, at refinery/RER U	1.24E-03
Ref Products	Fuels	Oil	Naphtha	Naphtha, at refinery/CH U	5.56E-04
Ref Products	Fuels	Oil	Naphtha	Naphtha, at refinery/RER U	1.13E-03
Ref Products	Fuels	Oil	Petrol	Petrol, low-sulphur, at refinery/CH U	0.00E+00
Ref Products	Fuels	Oil	Petrol	Petrol, low-sulphur, at refinery/RER U	0.00E+00
Ref Products	Fuels	Oil	Petrol	Petrol, unleaded, at refinery/CH U	8.57E-04
Ref Products	Fuels	Oil	Petrol	Petrol, unleaded, at refinery/RER U	1.46E-03
Ref Products	Fuels	Oil	Electricity	Electricity, at refinery/CH U	1.10E-03
Ref Products	Fuels	Oil	Electricity	Electricity, at refinery/RER U	7.30E-04
Ref Products	Fuels	Gases	Propane/Butane	Propane/ butane, at refinery/CH U	7.81E-04
Ref Products	Fuels	Gases	Propane/Butane	Propane/ butane, at refinery/RER U	1.38E-03
Ref Products	Fuels	Gases	Refinery gas	Refinery gas, at refinery/CH U	7.81E-04
Ref Products	Fuels	Gases	Refinery gas	Refinery gas, at refinery/RER U	1.38E-03
Ref Products	Chemicals	Inorganic	Sulphur	Secondary sulphur, at refinery/CH U	3.69E-04
Ref Products	Chemicals	Inorganic	Sulphur	Secondary sulphur, at refinery/RER U	4.17E-04

The polymer manufacturing units have been scoped to be from cradle-to-gate. Thus, the impact data for polymers represents all the steps right from raw material extraction (including crude oil refining to produce monomers) to polymer production at the plant. However, aggregated data has been used for all processes from raw material

extraction up until delivery at polymer manufacturing plants. Datasets are aggregated together due to lack of access to industry protected proprietary information.

Table 8

Structured Underspecification of Polymers

L1	L2	L3	L4	GWP
Polymers	Thermoplastic	Nylon	Nylon 6, at plant/RER U	9.19E+00
Polymers	Thermoplastic	Nylon	Nylon 6, glass-filled, at plant/RER U	7.25E+00
Polymers	Thermoplastic	Nylon	Nylon 66, at plant/RER U	7.97E+00
Polymers	Thermoplastic	Nylon	Nylon 66, glass-filled, at plant/RER U	6.98E+00
Polymers	Thermoplastic	PMMA	Polymethyl methacrylate, beads, at plant/RER U	7.04E+00
Polymers	Thermoplastic	PMMA	Polymethyl methacrylate, sheet, at plant/RER U	8.28E+00
Polymers	Thermoplastic	Polyethylene	Polyethylene, HDPE, granulate, at plant/RER U	1.91E+00
Polymers	Thermoplastic	Polyethylene	Polyethylene, LDPE, granulate, at plant/RER U	2.08E+00
Polymers	Thermoplastic	Polyethylene	Polyethylene, LLDPE, granulate, at plant/RER U	1.83E+00
Polymers	Thermoplastic	Polyethylene	Fleece, polyethylene, at plant/RER U	0.00E+00
Polymers	Thermoplastic	Polyethylene	Polyethylene terephthalate, granulate, amorphous, at plant/RER U	0.00E+00
Polymers	Thermoplastic	Polyethylene	Polyethylene terephthalate, granulate, bottle grade, at plant/RER U	0.00E+00
Polymers	Thermoplastic	Polyethylene	Polyester resin, unsaturated, at plant/RER U	0.00E+00
Polymers	Thermoplastic	Polystyrene	Polystyrene, expandable, at plant/RER U	3.32E+00
Polymers	Thermoplastic	Polystyrene	Polystyrene, general purpose, GPPS, at plant/RER U	3.47E+00
Polymers	Thermoplastic	Polystyrene	Polystyrene, high impact, HIPS, at plant/RER U	3.46E+00
Polymers	Thermoplastic	Polyvinylchloride	Polyvinylchloride, emulsion polymerised, at plant/RER U	2.48E+00
Polymers	Thermoplastic	Polyvinylchloride	Polyvinylchloride, suspension polymerised, at plant/RER U	1.89E+00
Polymers	Thermoplastic	Polyvinylchloride	Polyvinylidenchloride, granulate, at plant/RER U	4.52E+00
Polymers	Thermoset	Epoxy	Epoxy resin, liquid, at plant/RER U	6.68E+00
Polymers	Thermoset	Epoxy	Epoxy resin, liquid, disaggregated data, at plant/RER U	7.70E-01
Polymers	Thermoset	Formaldehyde resin	Melamine formaldehyde resin, at plant/RER U	0.00E+00
Polymers	Thermoset	Formaldehyde resin	Urea formaldehyde resin, at plant/RER U	0.00E+00
Polymers	Thermoset	Polyurethane	Polyurethane, flexible foam, at plant/RER U	5.10E-02
Polymers	Thermoset	Polyurethane	Polyurethane, rigid foam, at plant/RER U	0.00E+00

4.2 Error Characterization in Structured Underspecification

As explained in section 3.4.1, the consequence of losing precision regarding the estimates of impacts of the materials due to underspecification is quantified with the help

of standard deviation. Tables 9 and 10 below depict the standard deviation values across the different levels of structured classification system for the GWP impact category for refinery products and polymers respectively. The complete list of standard deviation values for other impact categories is included in appendices A and B.

Table 9

Error Characterization of GWP of Refinery Products

L0		
CATEGORY	**STD DEV**	**L0(STD DEV)/GRAND AVERAGE**
Ref. Products	0.000469	6.13E-01

L1	
CATEGORY	**STD DEV**
Fuels	0.000465
Chemicals	

L2	
CATEGORY	**STD DEV**
Oil	0.000456
Gases	
Inorganic Chemicals	

L3	
CATEGORY	**STD DEV**
Diesel	0.000497
Fuel Oil	
Kerosene	
Naphtha	
Petrol	
Electricity	
Propane/Butane	
Refinery Gas	
Sulphur	

L4	
CATEGORY	**STD DEV**
Diesel, from CH & RER	0.000348
Diesel, low-sulphur, from CH & RER	
Heavy fuel oil, from CH & RER	
Light fuel oil, from CH & RER	
Kerosene, from CH & RER	
Naphtha, from CH & RER	
Petrol, low-sulphur, from CH & RER	
Petrol, unleaded, from CH & RER	
Electricity, at CH & RER	
Propane/Butane, from CH & RER	
Refinery gas, from CH & RER	
Secondary Sulphur, from CH & RER	

Table 10

Error Characterization of GWP of Polymers

L1		
CATEGORY	**STD DEV**	**L1(STD DEV)/GRAND AVERAGE**
Polymers	3.151	9.95E-01

L2	
CATEGORY	**STD DEV**
Thermoplastic	3.017
Thermoset	

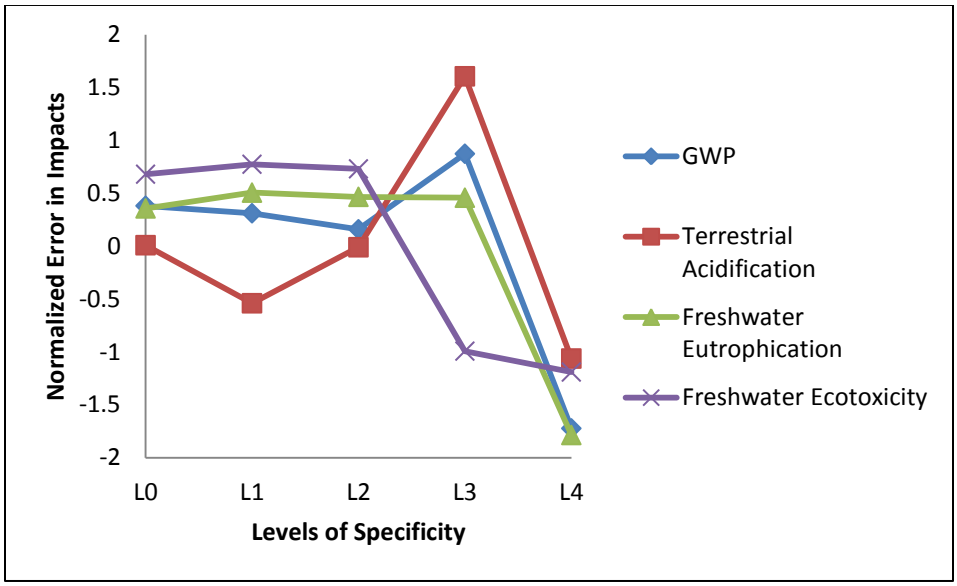
L3	
CATEGORY	**STD DEV**
Nylon	1.360
PMMA	
Polyethylene	
Polystyrene	
Polyvinylchloride	
Epoxy	
Formaldehyde resin	
Polyurethane	

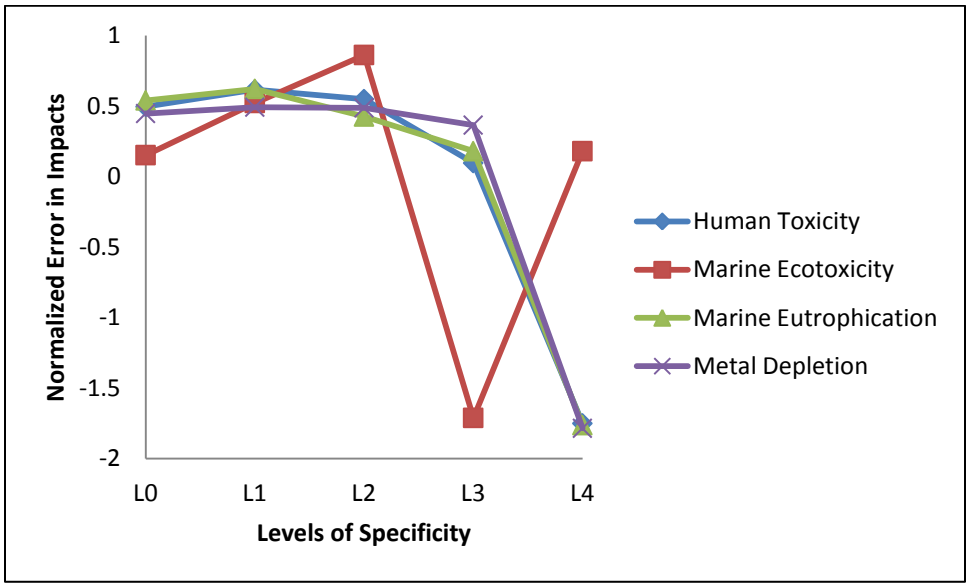
Each of the levels in Tables 7 and 8 signifies a certain amount of effort that must be spent in order to characterize the components at that level of specificity. Accordingly, the amount of information gathered at each of those levels has a certain level of uncertainty associated with it. This uncertainty reduces as the modeler specifies the component to the maximum extent. As the components are approaching maximum specificity, the domain of possibilities decreases and so does the error associated with the selection of proxy data for the estimation of environmental impact of that system.

From Tables 9 and 10, it can be seen that the standard deviation in the data significantly reduces in moving from the most underspecified level to the most specified level (L0 → L4 for refineries and L1 → L3 for polymers). Thus, it can be concluded that the penalty of losing precision of LCA results across the streamlined classification system decreases as the components of the system are completely specified. The uncertainty across structured underspecification is characterized in terms of the deviation of the impacts evaluated at each of those levels from the accurate results obtained by choosing the right proxy from the most specific level. This demonstration conveys the information that when accurate data associated with the characteristics of the system under study are not readily available to the LCA practitioner, underspecification, although effective in reducing the bias due to human judgment, introduces a considerable error in the impact assessment.

Figures 8 and 9 below help visualize the decline in standard deviation across increasing levels of specificity. From the graphs it can be seen that the trend is similar for all the impact categories in spite of a few discontinuities for certain impact categories. For example, in Figure 8, the normalized error for the marine ecotoxicity impact category

to increases between L3 and L4. However, looking at the raw data, it can be noticed that this phenomenon is caused due to the outlier with an unusually large impact value for marine ecotoxicity in the kerosene product category within L3. Similarly, abnormally large values for terrestrial acidification impact category (Figure 8) for sulphur cause the increase in error at L3.





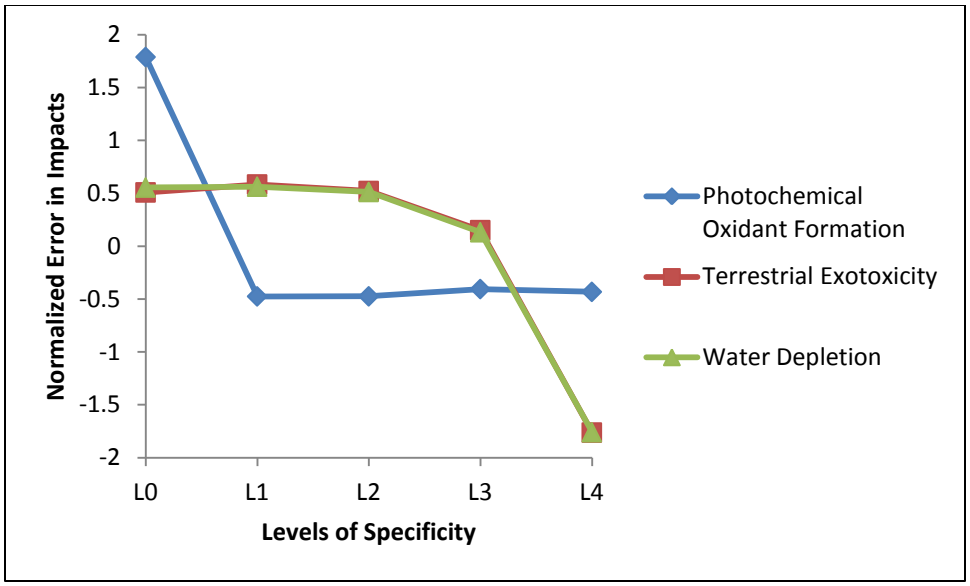
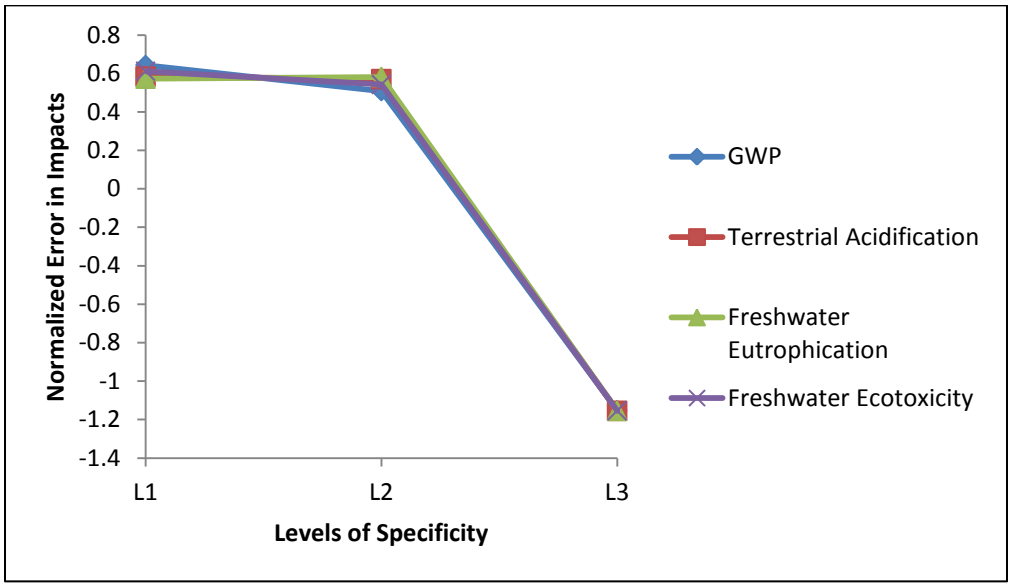
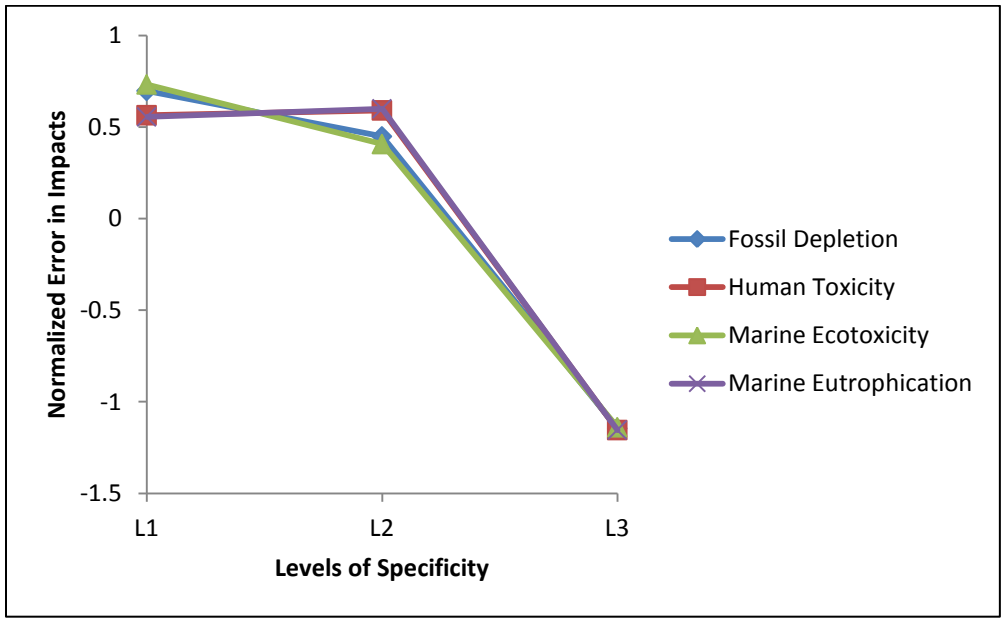


Figure 8. Standard Deviation vs. Levels of Specificity for Refinery Products

It is clear from the plots above that there is a steep decline in the error in life cycle impact assessment between levels 3 and 4. As can be seen, underspecification introduces a substantial amount of residual variation in the impact assessment. However, across levels 0 through 3, the decline is consistent although not very substantial. This phenomenon indicates that even by increasing the resolution of information steadily from L0 to L3, there is no considerable improvement in the results of the LCA. In other words, the impacts evaluated by underspecifying components at each of the levels 0, 1, 2 and 3 are almost similar. Also, the differences between impact evaluation at level 4 and each of the levels from 0 through 3 are almost similar. Level 4 signifies specific proxies that are chosen from the database for LCA modeling. However, oversimplification of material specificity at the lower levels widens the range of proxies to choose from thus escalating the error. In other words, data at lower levels are averaged out over a broad spectrum of possible material choices/types leading to the divergence from accurate results.

This occurrence, however, is purely a function of the way the materials are classified. That is, the effects of underspecification may become more pronounced by adopting a much more granular structure wherein the differences between individual levels become notable. Similar trends are observed for the polymers category.





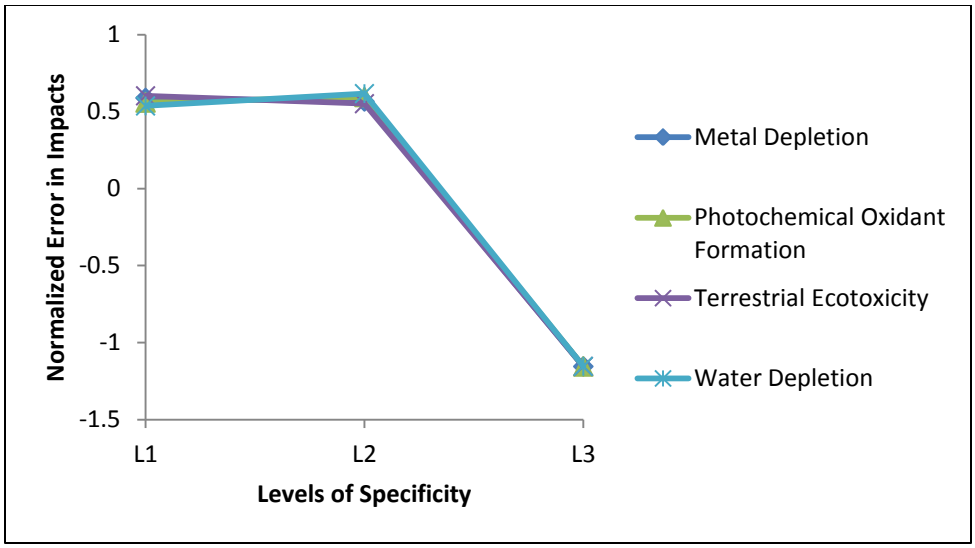


Figure 9. Standard Deviation vs. Levels of Specificity for Polymers

4.3 Analysis of Variance on Impacts of Refinery Products

The ratio of standard deviation calculated with respect to the grand average at the least specific level gives a sense of magnitude of error associated with the entire data set across all the impact categories.

Table 11

Magnitude of Error in Impact Assessment

IMPACT CATEGORY	MAG. OF EROR (Std Dev/ Average at L0)
Global Warming Potential	6.13E-01
Terrestrial Acidification	3.33E+00
Freshwater Eutrophication	7.51E-01
Freshwater Ecotoxicity	7.29E-01
Human Toxicity	6.66E-01
Metal Depletion	2.29E+00
Marine Ecotoxicity	4.37E+00
Marine Eutrophication	5.59E-01
Photochemical Oxidant Formation	1.90E+00
Terrestrial Ecotoxicity	6.95E-01
Water Depletion	5.90E-01

Table 11 shows the magnitude of error in impact assessment for the refinery products category. From the table, it can be seen that the average error is about 60-70% of the mean values for most of the impact categories. In fact, for other impact categories such as terrestrial acidification and metal depletion it is much higher. Further, looking at the patterns in Figures 8 and 9, it can be deciphered that most of the variability is due to the location (L4 represents the differences in impacts of the products obtained from refineries in Switzerland and other European locations); other levels of distinction have a relatively smaller influence on the variability in the impact estimates.

In order to directly quantify the contribution of each variance source, ANOVA analysis was done by using location as a binary variable. The results of the analyses are shown in Table 12 below.

The *p*-value or "probability > | t |" is computed from the F-ratio. The *p*-value tests the null hypothesis that data from all groups are drawn from population with identical means. If the overall *p*-value is large, it means that the means do not differ all that much and if the *p*-value is small, then the null hypothesis that all the populations have identical means can be rejected. In a nutshell, the *p*-value gives a measure of significance of a parameter. For our case, the level of significance was set at 5%. Thus, for all *p*-values that is less that 5%, the null hypothesis can be rejected and the parameter could be declared significant and vice versa.

From the results highlighted in the table below, it can be seen that the variability due to structured underspecification is not very significant among the lower levels. That is, the *p*-values of levels 1 through 3 are much larger than the 0.05 significance level. This substantiates the argument made in section 4.2 that the location from which the

datasets are derived (L4) is the most significant parameter causing maximum variance in the results; the other levels of distinction (L0 to L3) have a smaller influence on the variability or in other words, relatively insignificant.

Table 12

ANOVA Across Different Impact Categories

Parameter Estimates

Term		Estimate	Std Error	t Ratio	Prob>|t|
Intercept	Biased	0.0012094	0.000652	1.85	0.0850
L1[Chemicals]	Biased	0.0003796	0.00078	0.49	0.6339
L2[Gases]	Biased	0.0002506	0.000197	1.27	0.2251
L2[Inorganic]	Zeroed	0	0	.	.
L3[Diesel]	Biased	-0.000103	0.000322	-0.32	0.7547
L3[Electricity]	Biased	0.0003357	0.000395	0.85	0.4096
L3[Fuel Oil]	Biased	0.00033	0.000322	1.02	0.3235
L3[Kerosene]	Biased	0.0003692	0.000395	0.93	0.3657
L3[Naphtha]	Biased	0.0002637	0.000395	0.67	0.5151
L3[Petrol]	Zeroed	0	0	.	.
L3[Propane/Butane]	Biased	-5.37e-19	0.000456	-0.00	1.0000
L3[Refinery gas]	Zeroed	0	0	.	.
L4[CH U]		-0.000183	0.000093	-1.97	0.0694

GWP

Parameter Estimates

Term		Estimate	Std Error	t Ratio	Prob>|t|
Intercept	Biased	0.0260591	0.033009	0.79	0.4430
L1[Chemicals]	Biased	0.0259352	0.039438	0.66	0.5215
L2[Gases]	Biased	3.1125e-5	0.009991	0.00	0.9976
L2[Inorganic]	Zeroed	0	0	.	.
L3[Diesel]	Biased	-0.000041	0.016314	-0.00	0.9980
L3[Electricity]	Biased	-0.000057	0.019981	-0.00	0.9978
L3[Fuel Oil]	Biased	0.0257136	0.016314	1.58	0.1373
L3[Kerosene]	Biased	0.0000101	0.019981	0.00	0.9996
L3[Naphtha]	Biased	-3.08e-5	0.019981	-0.00	0.9988
L3[Petrol]	Zeroed	0	0	.	.
L3[Propane/Butane]	Biased	-5e-7	0.023072	-0.00	1.0000
L3[Refinery gas]	Zeroed	0	0	.	.
L4[CH U]		-0.004669	0.00471	-0.99	0.3383

Terrestrial Acidification

Parameter Estimates

Term		Estimate	Std Error	t Ratio	Prob>|t|
Intercept	Biased	2.1691e-7	9.771e-8	2.22	0.0434*
L1[Chemicals]	Biased	1.0039e-7	1.167e-7	0.86	0.4043
L2[Gases]	Biased	3.8887e-8	2.957e-8	1.31	0.2097
L2[Inorganic]	Zeroed	0	0	.	.
L3[Diesel]	Biased	1.25e-10	4.829e-8	0.00	0.9980
L3[Electricity]	Biased	-7.763e-8	5.915e-8	-1.31	0.2105
L3[Fuel Oil]	Biased	7.77e-8	4.829e-8	1.61	0.1299
L3[Kerosene]	Biased	7.7675e-8	5.915e-8	1.31	0.2102
L3[Naphtha]	Biased	7.8175e-8	5.915e-8	1.32	0.2074
L3[Petrol]	Zeroed	0	0	.	.
L3[Propane/Butane]	Biased	-1.5e-10	6.83e-8	-0.00	0.9983
L3[Refinery gas]	Zeroed	0	0	.	.
L4[CH U]		4.6038e-8	1.394e-8	3.30	0.0052*

Freshwater Eutrophication

Parameter Estimates

Term		Estimate	Std Error	t Ratio	Prob>|t|
Intercept	Biased	0.0000412	1.825e-5	2.26	0.0405*
L1[Chemicals]	Biased	0.000019	2.18e-5	0.87	0.3980
L2[Gases]	Biased	7.4125e-6	5.522e-6	1.34	0.2008
L2[Inorganic]	Zeroed	0	0	.	.
L3[Diesel]	Biased	2.5e-8	9.017e-6	0.00	0.9978
L3[Electricity]	Biased	-1.478e-5	0.000011	-1.34	0.2023
L3[Fuel Oil]	Biased	0.000015	9.017e-6	1.66	0.1184
L3[Kerosene]	Biased	1.4525e-5	0.000011	1.32	0.2096
L3[Naphtha]	Biased	1.4775e-5	0.000011	1.34	0.2023
L3[Petrol]	Zeroed	0	0	.	.
L3[Propane/Butane]	Biased	-5e-8	1.275e-5	-0.00	0.9969
L3[Refinery gas]	Zeroed	0	0	.	.
L4[CH U]		0.0000081	2.603e-6	3.11	0.0077*

Freshwater Ecotoxicity

Parameter Estimates

Term		Estimate	Std Error	t Ratio	Prob>|t|
Intercept	Biased	0.0004172	0.000187	2.23	0.0424*
L1[Chemicals]	Biased	0.0001753	0.000223	0.79	0.4454
L2[Gases]	Biased	8.0625e-5	5.655e-5	1.43	0.1759
L2[Inorganic]	Zeroed	0	0	.	.
L3[Diesel]	Biased	2.5e-7	9.235e-5	0.00	0.9979
L3[Electricity]	Biased	-0.000161	0.000113	-1.43	0.1759
L3[Fuel Oil]	Biased	0.000166	9.235e-5	1.80	0.0939
L3[Kerosene]	Biased	0.0001502	0.000113	1.33	0.2053
L3[Naphtha]	Biased	0.0001612	0.000113	1.43	0.1759
L3[Petrol]	Zeroed	0	0	.	.
L3[Propane/Butane]	Biased	-1.62e-19	0.000131	-0.00	1.0000
L3[Refinery gas]	Zeroed	0	0	.	.
L4[CH U]		0.0000615	2.666e-5	2.31	0.0369*

Human Toxicity

Parameter Estimates

Term		Estimate	Std Error	t Ratio	Prob>|t|
Intercept	Biased	0.0003932	0.000393	1.00	0.3339
L1[Chemicals]	Biased	0.0003853	0.000469	0.82	0.4255
L2[Gases]	Biased	2.6712e-6	0.000119	0.02	0.9824
L2[Inorganic]	Zeroed	0	0	.	.
L3[Diesel]	Biased	2.25e-8	0.000194	0.00	0.9999
L3[Electricity]	Biased	-5.298e-6	0.000238	-0.02	0.9825
L3[Fuel Oil]	Biased	5.4675e-6	0.000194	0.03	0.9779
L3[Kerosene]	Biased	0.0007623	0.000238	3.21	0.0064*
L3[Naphtha]	Biased	5.2925e-6	0.000238	0.02	0.9826
L3[Petrol]	Zeroed	0	0	.	.
L3[Propane/Butane]	Biased	-4.5e-8	0.000275	-0.00	0.9999
L3[Refinery gas]	Zeroed	0	0	.	.
L4[CH U]		-0.000067	0.000056	-1.19	0.2522

Marine Ecotoxicity

Parameter Estimates

Term		Estimate	Std Error	t Ratio	Prob>|t|
Intercept	Biased	2.4075e-5	1.055e-5	2.28	0.0387*
L1[Chemicals]	Biased	7.325e-6	1.261e-5	0.58	0.5704
L2[Gases]	Biased	4.85e-6	3.193e-6	1.52	0.1511
L2[Inorganic]	Zeroed	0	0	.	.
L3[Diesel]	Biased	-5.8e-6	5.215e-6	-1.11	0.2848
L3[Electricity]	Biased	0.0000129	6.387e-6	2.02	0.0630
L3[Fuel Oil]	Biased	1.45e-6	5.215e-6	0.28	0.7850
L3[Kerosene]	Biased	0.0000052	6.387e-6	0.81	0.4292
L3[Naphtha]	Biased	0.000003	6.387e-6	0.47	0.6458
L3[Petrol]	Zeroed	0	0	.	.
L3[Propane/Butane]	Biased	-5e-8	7.375e-6	-0.01	0.9947
L3[Refinery gas]	Zeroed	0	0	.	.
L4[CH U]		1.7042e-6	1.505e-6	1.13	0.2766

Marine Eutrophication

Parameter Estimates

Term		Estimate	Std Error	t Ratio	Prob>|t|
Intercept	Biased	1.4162e-8	1.533e-8	0.92	0.3713
L1[Chemicals]	Biased	1.4162e-8	1.832e-8	0.77	0.4523
L2[Gases]	Biased	-7.9e-24	4.641e-9	-0.00	1.0000
L2[Inorganic]	Zeroed	0	0	.	.
L3[Diesel]	Biased	1.4175e-8	7.578e-9	1.87	0.0825
L3[Electricity]	Biased	-9.93e-24	9.282e-9	-0.00	1.0000
L3[Fuel Oil]	Biased	1.415e-8	7.578e-9	1.87	0.0830
L3[Kerosene]	Biased	-9.93e-24	9.282e-9	-0.00	1.0000
L3[Naphtha]	Biased	-9.93e-24	9.282e-9	-0.00	1.0000
L3[Petrol]	Zeroed	0	0	.	.
L3[Propane/Butane]	Biased	6.781e-24	1.072e-8	0.00	1.0000
L3[Refinery gas]	Zeroed	0	0	.	.
L4[CH U]		-1.71e-10	2.188e-9	-0.08	0.9389

Metal Depletion

Parameter Estimates

Term		Estimate	Std Error	t Ratio	Prob>|t|
Intercept	Biased	0.0012463	0.000195	6.39	<.0001*
L1[Chemicals]	Biased	0.0010993	0.000233	4.71	0.0003*
L2[Gases]	Biased	0.0000465	0.000059	0.79	0.4443
L2[Inorganic]	Zeroed	0	0	.	.
L3[Diesel]	Biased	-1.025e-5	9.646e-5	-0.11	0.9169
L3[Electricity]	Biased	-3.665e-5	0.000118	-0.31	0.7610
L3[Fuel Oil]	Biased	0.0000755	9.646e-5	0.78	0.4468
L3[Kerosene]	Biased	0.0000795	0.000118	0.67	0.5119
L3[Naphtha]	Biased	0.0000675	0.000118	0.57	0.5768
L3[Petrol]	Zeroed	0	0	.	.
L3[Propane/Butane]	Biased	-1.89e-19	0.000136	-0.00	1.0000
L3[Refinery gas]	Zeroed	0	0	.	.
L4[CH U]		-0.000027	2.785e-5	-0.97	0.3472

Photochemical Oxidant Formation

Parameter Estimates

Term		Estimate	Std Error	t Ratio	Prob>|t|
Intercept	Biased	4.2894e-7	1.844e-7	2.33	0.0356*
L1[Chemicals]	Biased	1.9781e-7	2.204e-7	0.90	0.3846
L2[Gases]	Biased	7.6875e-8	5.583e-8	1.38	0.1901
L2[Inorganic]	Zeroed	0	0	.	.
L3[Diesel]	Biased	2.5e-10	9.116e-8	0.00	0.9979
L3[Electricity]	Biased	-1.543e-7	1.117e-7	-1.38	0.1888
L3[Fuel Oil]	Biased	1.5375e-7	9.116e-8	1.69	0.1138
L3[Kerosene]	Biased	1.5425e-7	1.117e-7	1.38	0.1888
L3[Naphtha]	Biased	1.5475e-7	1.117e-7	1.39	0.1874
L3[Petrol]	Zeroed	0	0	.	.
L3[Propane/Butane]	Biased	5e-10	1.289e-7	0.00	0.9970
L3[Refinery gas]	Zeroed	0	0	.	.
L4[CH U]		7.2333e-8	2.632e-8	2.75	0.0157*

Terrestrial Ecotoxicity

Parameter Estimates

Term		Estimate	Std Error	t Ratio	Prob>|t|
Intercept	Biased	0.0062794	0.00244	2.57	0.0221*
L1[Chemicals]	Biased	0.0028981	0.002915	0.99	0.3370
L2[Gases]	Biased	0.0011337	0.000738	1.54	0.1470
L2[Inorganic]	Zeroed	0	0	.	.
L3[Diesel]	Biased	0.000015	0.001206	0.01	0.9903
L3[Electricity]	Biased	-0.002248	0.001477	-1.52	0.1503
L3[Fuel Oil]	Biased	0.002265	0.001206	1.88	0.0813
L3[Kerosene]	Biased	0.0022475	0.001477	1.52	0.1503
L3[Naphtha]	Biased	0.0022475	0.001477	1.52	0.1503
L3[Petrol]	Zeroed	0	0	.	.
L3[Propane/Butane]	Biased	0.00001	0.001705	0.01	0.9954
L3[Refinery gas]	Zeroed	0	0	.	.
L4[CH U]		2.2083e-5	0.000348	0.06	0.9503

Water Depletion

The fact that these conclusions arise out of this exclusive classification of refinery products adopted for this thesis and that different classification schemes could yield different results is reiterated.

From Figures 8 and 9, it can be seen that there is a steep drop in error from level 3 to level 4. Hence, the change in variance of impact data in moving from a less granular level to a more granular highly specific level is significant. In the present case, at level 4, the main differentiator is the location from which the respective products are derived. Therefore, results from the ANOVA analyses could also be used to observe the significance of location as a factor affecting the variability in the environmental impact assessment.

Interestingly enough, it can be seen from Table 12 above that not all the impact estimates were affected alike by the differences in location. Except for GWP, freshwater eutrophication, freshwater ecotoxicity, human toxicity and terrestrial ecotoxicity impact categories whose *p*-values are almost close to or less than the level of significance; all other environmental impact categories remain relatively immune to geographic variations.

Environmental impacts are representative of the emissions that arise out of products' life cycle. Different characterization factors are used to quantitatively evaluate the impacts from each emission/resource that comes from the life cycle of the system and are expressed as category indicator results. In essence, different substances contribute to different impact categories via different environmental mechanisms and pathways. Moreover, the life cycle stages that lead to these emissions may vary from one impact category to the other. For example, the extraction of crude oil, the transportation of crude oil to the refineries as well as combustion of fuels for energy may individually contribute to different extents to the global warming potential. However, these stages may have a relatively smaller effect in terms of contribution to freshwater eutrophication

which is essentially caused due to an overload of nutrients into the freshwater system. Similarly, within a refinery, processes like de-sulphurization might contribute significantly more towards terrestrial acidification due to the release of relatively larger amounts of sulphur from this stage as opposed to processes like cracking or polymerization. Additionally, within a single life cycle stage, the different sub-systems operating under different process conditions may individually add to the overall emissions thereby making the allocation of inventories extremely complex. Finally, the technological variations across different locations, temporal variations, underlying uncertainty in data collection and measurement, extrapolations and aggregation of data due to lack of access to proprietary information may lead to data inaccuracies thus explaining the patterns regarding significance of parameters for impact estimation.

In the present case, the inventory data for refineries in Switzerland has been collected by investigation for the refineries in Collombey and Cressier. Emission factors and energy uses for the two Swiss refineries were based on available information from questionnaires. Some other data and indicators were based on older literature data. In comparison, the inventory data for European refineries were based on assumptions for the European average. Average emission factors for the European refineries were estimated based on available information for about 10% of the refineries. Further, other data and indicators were estimated based on different environmental reports as well as extrapolated from information collected only from 1 to 5 plants. For both these situations, assumptions about the average technology for petrochemical refineries were made and a large chunk of data was averaged out over a period of time based on literature surveys of journal articles as well as available statistical data. The reliability and representativeness

of the data sources are important aspects to ensure data quality and accuracy of impact assessment. These basic differences in data collection, uncertainty associated with consistency of the literature data in comparison to actual refineries studied, extrapolations, assumptions and data validity may lead to considerable errors in the overall impact assessment.

Due to different pieces of information from different sources for a variety of processes spliced together, the results might not be fully representative of the actual situation. Thus, fundamental technological differences in terms of variations in process conditions, geographic variations, and average supply situations for different countries might become relevant and vital.

As a result of several sources of uncertainties in impact assessment discussed above, it might not be entirely accurate to compare the results of ANOVA across all the impact categories as a whole and a case by case investigation is necessary. It might not be erroneous to surmise that different methodologies may have been followed for the allocation of inventories for calculating environmental impacts from each of these refineries explaining the variations in the significance of parameters from ANOVA assessment. For instance, for European refineries, the demand for fossil energy resources was inventoried with the crude oil and natural gas exploration. Moreover, NO_x emissions during crude oil production were assumed to be significant mainly in low populated areas. Cadmium emissions to soil were caused by several background processes in European refineries. These allocations may not exactly match the ones from Swiss refineries thereby leading to differences in impact assessments. Other possible explanations include aggregation of data or “underspecification” of the datasets itself.

In other words, data for different subsystems might have been substituted using proxies from existing databases leading to technological disparities.

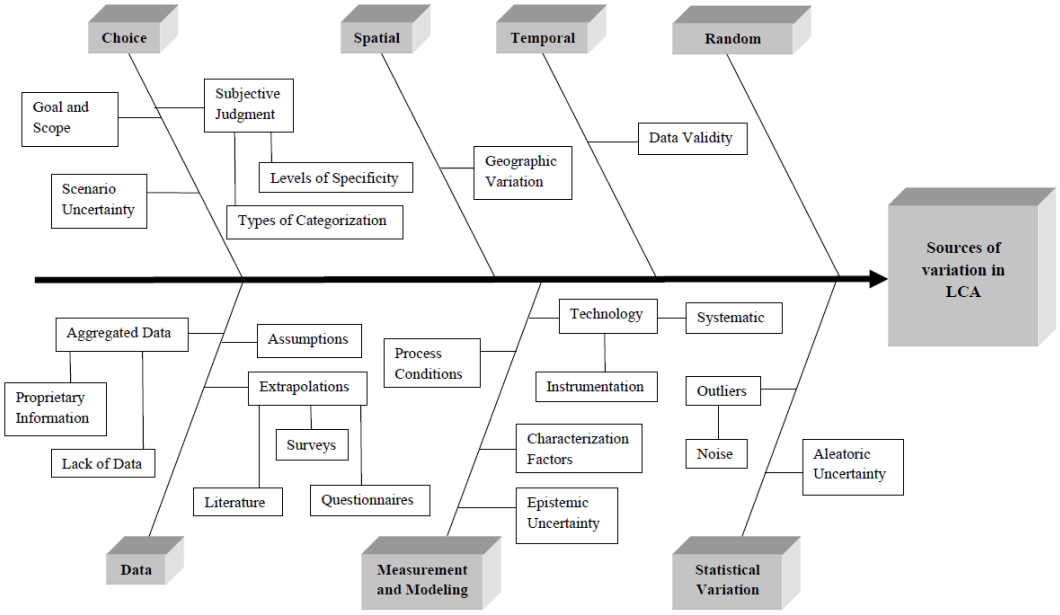


Figure 10. Fishbone Diagram for Sources of Variation in LCA

It is clear from this demonstration that the environmental impact categories must be treated individually and that several sources of uncertainty (Figure 10) have to be taken into account when comparing their contributions to the variation in LCA results. The results of the study may have been entirely different had a different scheme of classification been followed or high quality data fully representative of the systems studied were collected firsthand without assumptions or extrapolations. It is safe to conclude that the uncertainty introduced due to underspecification is the same order of magnitude as introduced by other sources of uncertainty. Nevertheless, it accounts for another level of ambiguity that has to be taken into account when probabilistic underspecification is used as a streamlining opportunity for LCA.

4.4 Variation in Impacts of Upstream and Downstream Processes

Figure 11 below shows the comparison of variation in impacts between petrochemicals and polymeric products. As can be seen from the graph below, the variation in environmental impacts for polymer manufacturing and processing is higher than that of refinery products for most of the impact categories. This may be because of the fact that additional steps beyond the refining of crude oil (upstream processes) are necessary for the production of polymers (downstream processes). For example, HDPE is manufactured by steam cracking of naphtha obtained by refining the crude oil and natural gas at temperatures of up to 875^{o}C to form ethylene which is then polymerized at atmospheric pressures and approximately at 100^{o} C. Ecoinvent database, from which the data for the analyses was extracted, has scoped the polymer production plants to include all processes, aggregated together, from raw material extraction up until delivery at plant. This all inclusive nature of the scoping mechanism indicates that the impacts of production of petrochemicals necessary for the manufacture of polymers are also included in the impact assessment of polymers itself. Further, other life cycle stages such as transportation of petrochemicals to the polymer manufacturing plants may have been scoped in thereby contributing to the overall impact assessment.

Again, in this case each of the impact categories has to be treated individually. Some impacts such as terrestrial acidification, marine ecotoxicity, metal depletion and photochemical oxidant formation have a higher variation at the refinery level. Looking at the raw data (see appendices A and B) for these impact categories, some conclusions regarding these results could be made. For example, the terrestrial acidification refers to the increase in acidity of ecosystems measured in terms of SO_2 eq. From the impact data

for refineries, it can be seen that the production of secondary sulphur at the refineries contributes the maximum to terrestrial acidification. This may be because of the emission and disposal of waste sulphur to the surrounding environment from this stage in the production chain. Moreover, certain processes such as de-sulphurization or treating and blending that are exclusive for oil refineries might add up to terrestrial acidification impacts. Similarly, the extraction of crude oil and natural gas leads to non-renewable metal depletion. These impacts, when assessed at the polymer production level, may have a relatively lower effect on the overall assessment.

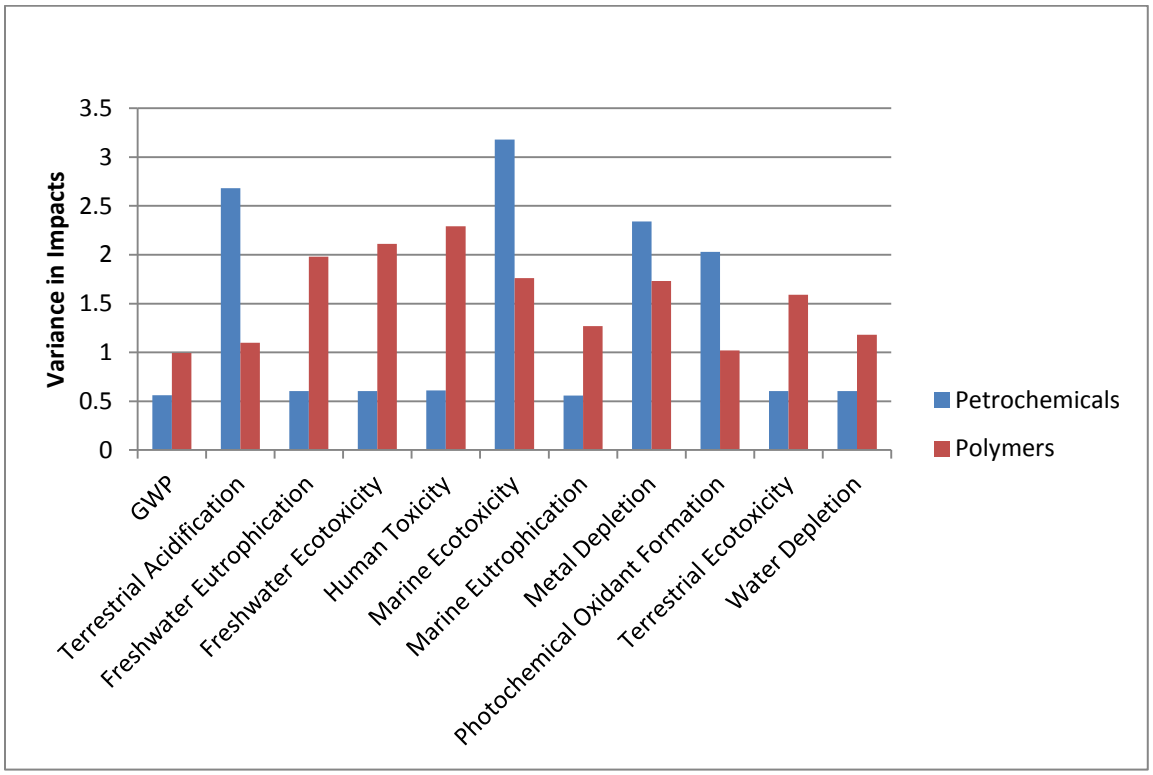


Figure 11. Variation in Environmental Impacts of Petrochemicals and Polymers

It should be noted that not all products from the oil refineries are used for the manufacture of polymers. Although the scope of the polymer production plants includes all the steps from the extraction of raw materials to the production of polymers, only

those steps relevant to the manufacture of polymeric products may have been considered. In other words, oil refining plants and polymer production plants may share common processes up until a certain "point" in the process chain depending on the scope of the analysis beyond which fundamental technological variations at these industries may play a big role in the variations in life cycle impact assessment.

However, due to lack of granularity regarding the amounts of emissions from individual processes at refinery and polymer production levels, the results from this analysis may not be entirely precise. Further resolving the supply chain into individual levels may provide better answers to questions regarding relative allocation of emissions from every individual processes. Unfortunately, due to the aggregation of processes for the protection of proprietary information derived from European industries, individual break down of processes could not be done and is beyond the scope of this thesis.

Turning a blind eye to the nature of manufacturing processes and only considering the raw data available, one can spot outliers that may be the reason for variations in statistical analyses. Structured underspecification, being a statistical approach, may be sensitive to outliers in the data. Future work will focus on refining data analysis procedures to increase the robustness of this streamlining methodology.

4.5 Comparison of Variance Across Different Product Categories

In order to see large differences in variances clearly, box plots for each environmental impact category were generated for every level of classification of petrochemicals. Box plots were not generated for polymer products as there are only two

distinct levels of unique product categories (L2 and L3) whose variances could easily be compared.

Figure 12 below shows box and whisker diagrams generated for global warming potential impacts at the refinery level.

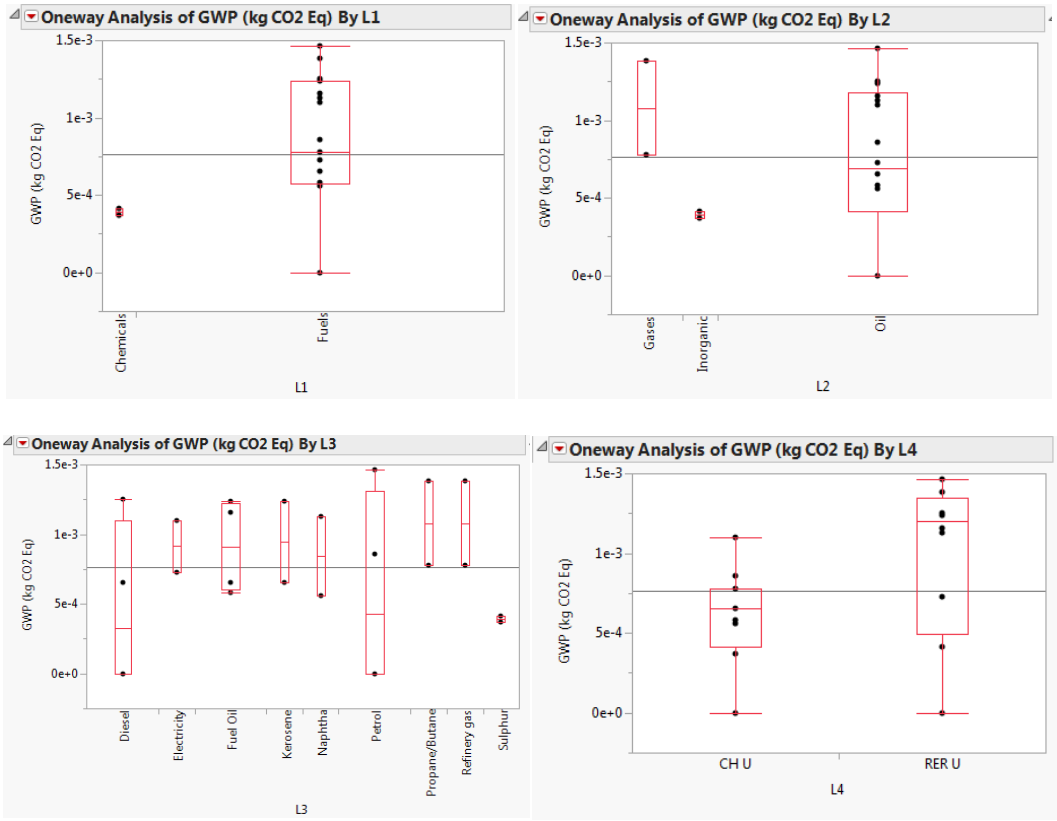


Figure 12. Box Plots for Comparison of Variances

From the above figures, it can be immediately seen that the variance in GWP values caused due to the production of both liquid and gaseous fuels is much greater than that caused due to the production of inorganic chemicals like sulphur. As highlighted in Chapter 2, more than 80% of the energy required for the operation of refineries is generated by the combustion of liquid as well as gaseous fuels. This process in turn releases a large amount of greenhouse gases thereby intensifying the GWP. Therefore,

the production of secondary sulphur has a relatively smaller impact on the variation of GWP impact assessment results. Further, from the plots generated for L3 categories, it can be seen that diesel and petrol; propane/butane and other refinery gases; kerosene, fuel oils and naphtha categories have comparable variances. This may be due to the similarity of chemical properties and compositions of each of these product groups. For example, liquid fuels such as diesel, petrol, fuel oil and naphtha are essentially composed of carbon, hydrogen, oxygen, nitrogen and sulphur. However, the relative amounts of these elements in each of those fuels may vary. Due to these elemental variations, the heating values and densities of each of these products are also different from one another though not drastically. Table 13 below shows the chemical composition, heating values and densities of some refinery fuels.

Table 13

Chemical Properties of Fuels (adapted from Dones et al., 2007)

		Petrol	Diesel	Kerosene	Light Fuel Oil
		kg	kg	kg	kg
Main Elements					
C	kg	0.865	0.865	0.850	0.862
H	kg	0.135	0.133	0.150	0.134
O	kg	0.003	0	0	-
N	kg	-	0	0	0.00014
S	kg	0.00216	0.0035	0.0005	0.001
Heating values					
LHV	MJ	42.8	42.8	43.25	42.7
UHV	MJ	45.8	45.5	46.0	45.4
Density					
Density	kg/l	0.75	0.84	0.795	0.84

LHV- Lower heating value (net calorific value), UHV- upper heating value (gross calorific value)

As can be seen from the table above, the properties of diesel and petrol are almost the same. Likewise, the properties of kerosene and fuel oils are also similar. For the same reasons, variations in the impacts of propane/butane and refinery gases are also comparable. Due to these common traits, variation in impacts of these products may also be alike. Note that the sulphur category relatively has very little impact in terms of variation in GWP values (see L3 graphs in Figure 12).

Box diagrams generated for other impact categories are attached in appendix E. Similar analyses on the basis of physical and chemical properties for each of those product categories within each level of categorization could be done to observe large differences across different environmental impact categories.

4.6 Case Studies

The results of applying structured underspecification and mis-specification to the two case studies- HDPE bottles and aerosol air freshener canisters are discussed in the following sections.

4.6.1 Life Cycle of HDPE Containers

In Chapter 3, the manufacturing process of HDPE bottles was discussed. The process begins with the extraction and refining of crude oil to produce ethylene which is then polymerized to form HDPE. The process flow for the production of ethylene was modeled in GaBi as shown in Figure 13 below.

Energy for the purpose of cracking is fed in the form of electricity. The product of this process is 1 kg of ethylene. This is further fed to the polymerization plants for the production of HDPE resin. This is then fed in the form of granulates to the injection

molding plants for the production of HDPE containers/bottles. HDPE bottles are then supplied to the consumer for their use.

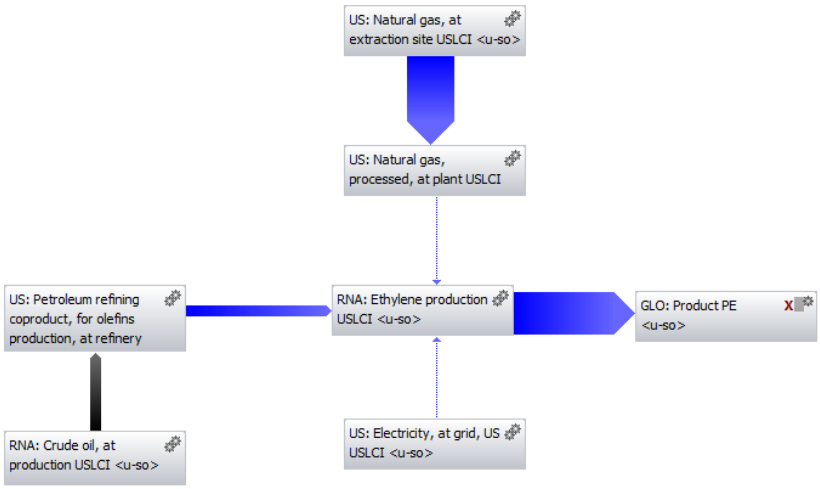


Figure 13. Ethylene production

As mentioned in Chapter 3, for the purpose of this thesis, three end-of-life scenarios are studied. The life cycle of HDPE bottles/containers are modeled with no recycling streams, 100% recycling rates and 30% recycling rates post the use phase. The process flows for each of these cases are shown in Figures 14, 15 and 16.

As can be seen from each of these figures, HDPE granulates produced at polymerization plants are transported by trucks to the injection molding units. Diesel required for the trucks are also included. Injection molding, being a mechanical process, requires electricity. Electricity production and distribution systems are interlinked and cannot be separated easily. The fuels needed to produce electricity are usually not disclosed and therefore US national average grid mix was used as the input for injection molding process. The output of this process is HDPE bottles/containers which are then

transported to retail facilities. This marks the beginning of the use phase in the life cycle system. Post use phase, the bottles are then disposed of. A quick survey of the recycling rates of HDPE bottles shows that the recycling rates for HDPE bottles rose from 29.9 in 2012 to 31.6 % in 2013(Killinger & Alexander, 2013). Hence, two scenarios in terms of recycling rates are studied. Figure 15 shows the recycling stream with 100% recycling rate and 85% recycling efficiency. This is an ideal case as 100% recycling rates with 85% recycling efficiencies of recycling plants are indicative of the fact that almost all the HDPE bottles produced and used are recycled. However, this is rarely the case. Figure 16 shows the life cycle flow with 30% recycling rate with an assumed efficiency of 51%. This scenario more closely represents the real case. The other 70% of the bottles are either incinerated or end up as landfill/solid wastes.

The functional unit used is one bottle. The mass of a typical empty one gallon HDPE container is 65 grams or 0.065 kg (Singh, Krasowski, & Singh, 2011). The flow quantities calculated with respect to this functional unit are shown in the figures. Note that flows from disposal facilities and waste recovery systems are also scoped in as inputs to the polymerization units. These inputs, however, constitute a very meager amount and as such do not have a significant contribution to the overall impacts of producing the HDPE polymer.

The individual unit processes were extracted using the Ecoinvent database. Due to its modular structure, the scope of the polymerization units already covers the entire supply chain from raw material acquisition, including all transportation, up to the factory gate. Therefore, separate streams for crude oil extraction, refining and production of ethylene need not be linked here and are shown separately in Figure 13.

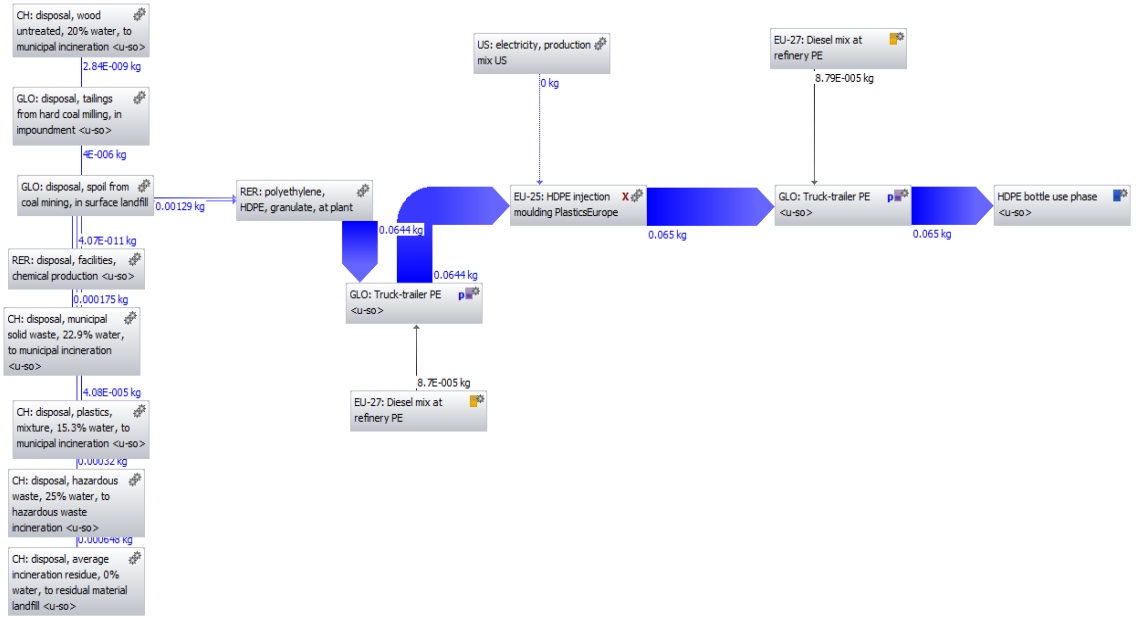


Figure 14. Life Cycle of HDPE Bottles with No Recycling

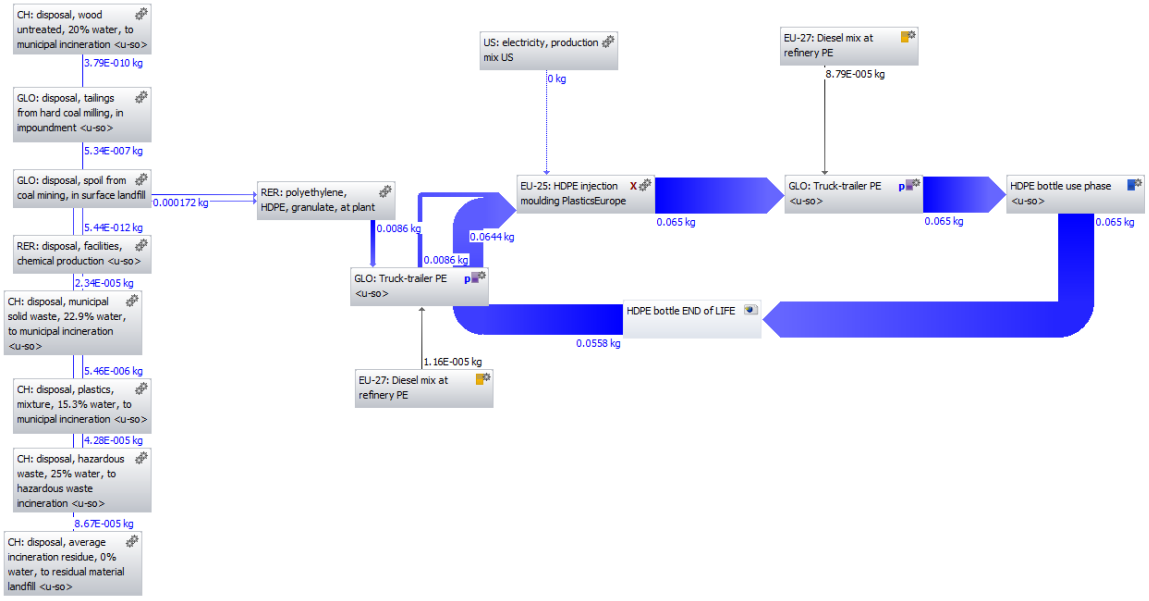


Figure 15. Life Cycle of HDPE Bottles with 100% Recycling Rate

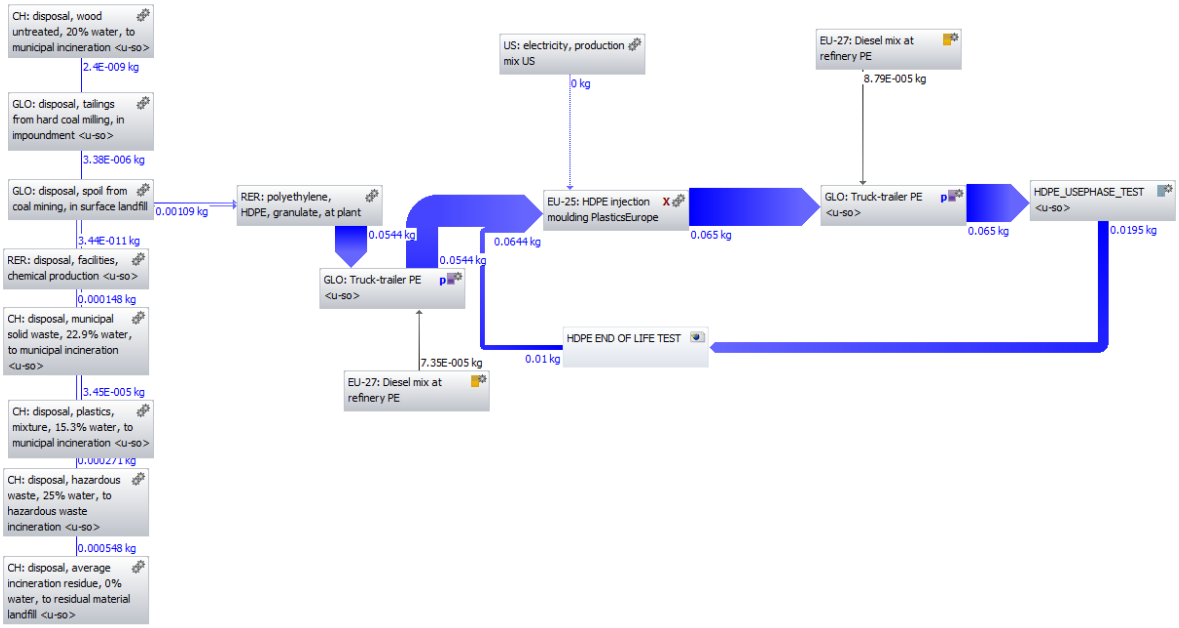


Figure 16. Life Cycle of HDPE Bottles with 30% Recycling Rate

It was assumed that the use phase of the bottles produces no environmental impacts. Note from Figure 15 the "output" of the use phase is 0.065 kg. This shows that all the bottle(s) that are disposed go into the recycling stream. Similarly, from Figure 16, note that only 0.0195 kg (30% of 0.065kg) of HDPE plastic comes out of the use phase. This indicates a 30% recycling rate. Moreover, in each of these cases, it can be seen that the presence of recycling streams decreases the relative output of virgin HDPE from the polymerization plants. It should be noted that there may be inherent uncertainties due to geographic variations between the different components in the model.

The results of the impact assessment of the three models are summarized in Table 14. ReCiPe impact assessment methodology was used to normalize and characterize the results. It was found that among all the impact categories, GWP and Fossil Depletion had

the greatest effects. As a result, only these two impact categories are selected for further assessment.

Table 14

Impact Assessment of HDPE Bottles

Scenario	GWP (kg CO_2 eq/FU)	Fossil Depletion (kg oil eq/FU)
No recycling	0.222	0.137
100% recycling, 85% efficiency	0.153	0.0512
30% recycling, 51% efficiency	0.21	0.122

From literature, it was found that the average GWP of producing one HDPE bottle along with the production of LDPE cap and transportation to storage as well as an end of life scenario of 40% recycling, 30% incineration and 30% landfill is about 1.27 kg CO_2 eq. (Singh et al., 2011). However, in the present case, the manufacture of LDPE caps, adhesive labels and the effects of incineration and landfill were not scoped in. This may explain the relatively smaller values of 0.21 kg CO_2 eq. from the model with ~30% recycling scenario herein (Table 14). Buhner (2012) reported the GWP from the life cycle of one 1 gallon bottle made of virgin HDPE (i.e. no recycling) as 0.516 kg CO_2 eq. These values approximately validate the results of 0.22 kg CO_2 eq. for GWP from the model (Table 14). The values from literature and the model developed herein could be roughly extrapolated to other situations depending on the scope of the model being studied.

Figures 17, 18, 19 below show the life cycle impact assessment for each of the models developed. From the assessment, it was found that the HDPE granulate manufacturing step had large impacts (excluding the effects of producing electricity) in

the whole life cycle of the bottle for the cases studied. The electricity mix used for injection molding showed comparable impacts. This may be due to the combustion of non-renewable sources to produce electricity. However, due to lack of access to proprietary information regarding the production of electricity, it could not be stated with confidence in this case.

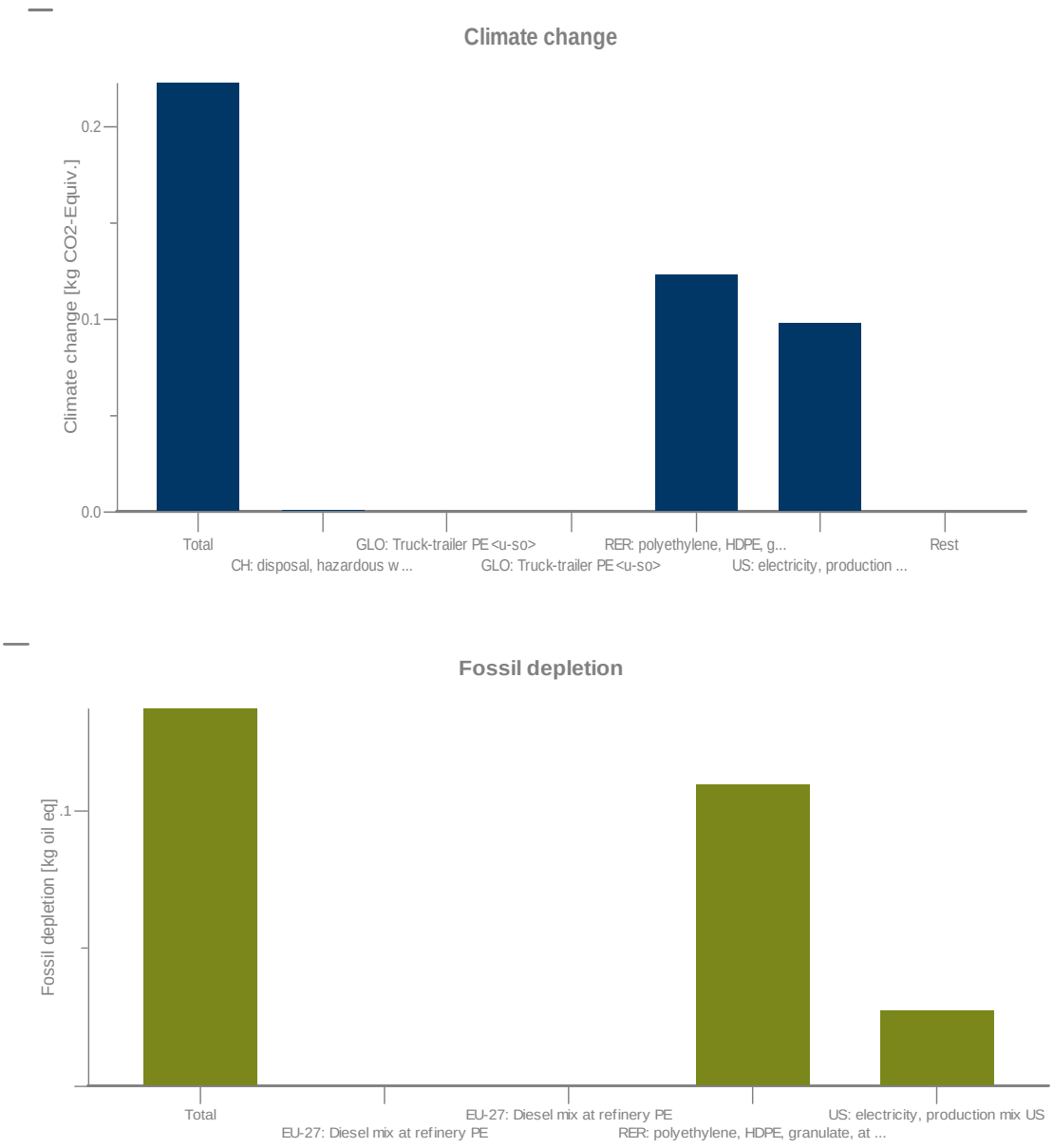


Figure 17. Impacts from Scenario without Recycling

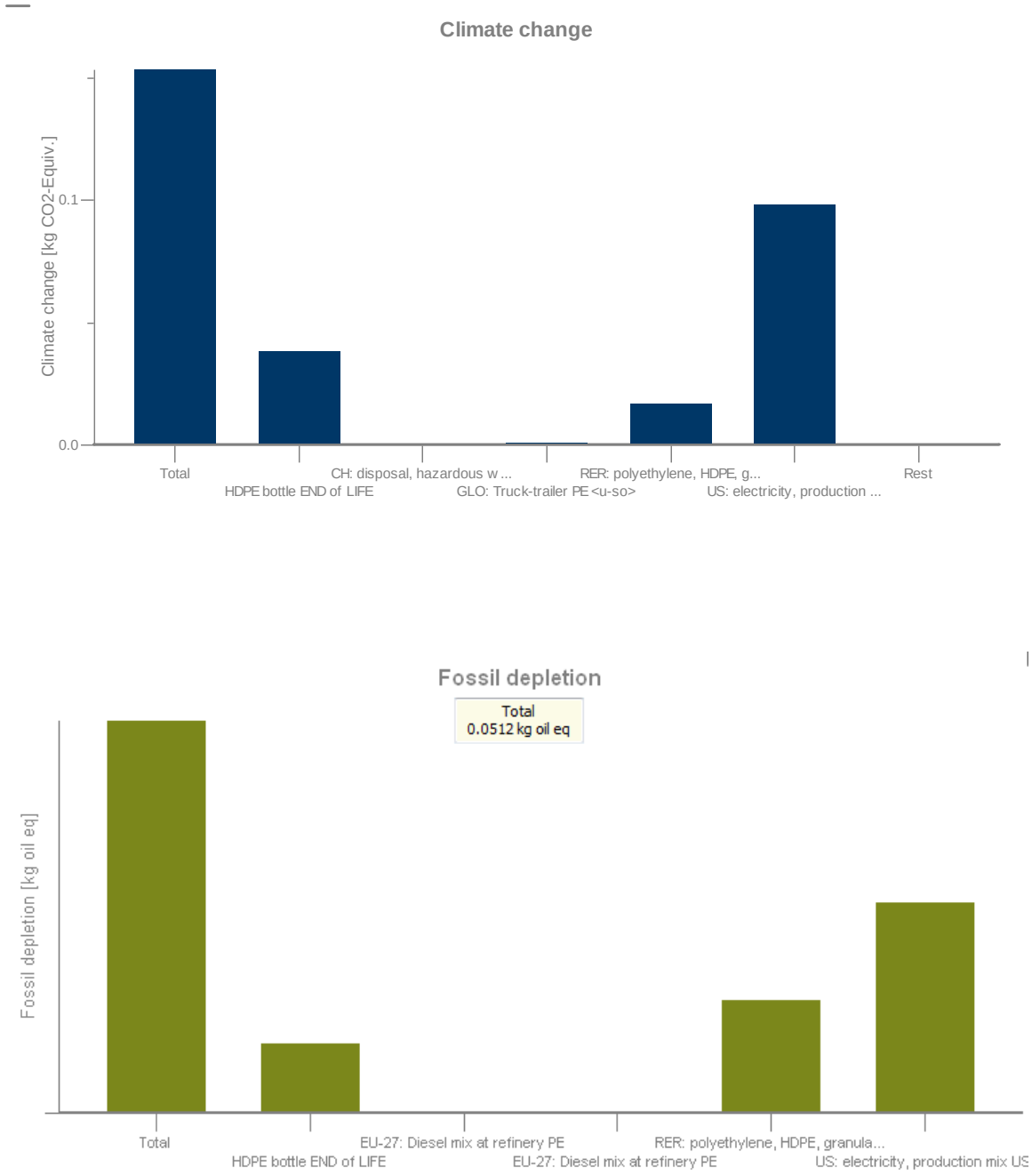


Figure 18. Impacts from Scenario with 100% Recycling Rate

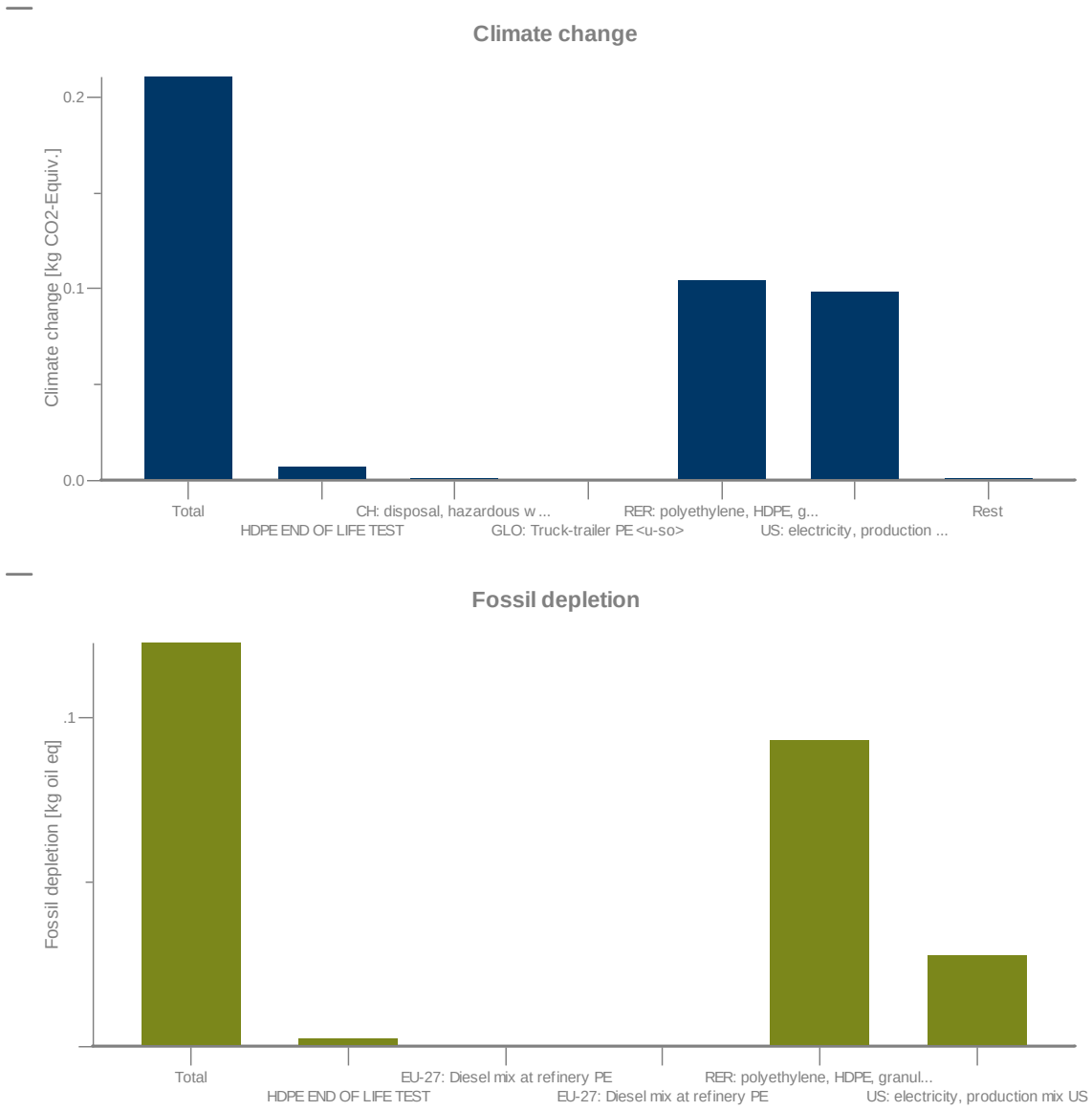


Figure 19. Impacts from Scenario with 30% Recycling Rate

Comparing the two end-of-life scenarios, the impacts of recycling HDPE bottles are higher for the case with 30% recycling rate with 50% efficiency compared to that with 100% recycling rate with 85% recycling efficiency. This is understandable because as more and more plastic bottles are recycled, the overall environmental burdens are reduced. In the present case, 100% recycling rate indicates that all the bottles that are

disposed are recycled thus reducing the impact of plastics on the environment. However, for the case with 30% recycling rate, only a fraction of the bottles thrown out after consumer use is recycled. The rest may be incinerated or may comprise solid wastes causing greater environmental concerns.

As pointed out in Chapter 3, the HDPE granulates production step is underspecified to see the variation in life cycle impact assessment. The results of underspecification for all the scenarios are shown in Table 15.

Consider the case with 30% recycling rate. For the production of one HDPE container, 0.0544 kg of HDPE granules is used. The production of these granules contributed about 0.104 kg CO_2 eq (49.52%) to the overall GWP impact of 0.21 kg CO_2 eq. Therefore, when this step is underspecified to level 3, the relative impacts of using 0.0544 kg of "polyethylene" were manually calculated. From the average impact values for the production of 1 kg of polyethylene at L3 (refer Table 8); the GWP of producing 0.0544 kg of "polyethylene" granules was estimated using a direct relation. LCA being a linear additive process, these values could now be substituted in place of "HDPE granulates" impacts, maintaining the overall mass balance. Similar calculations were done for L3 (thermoplastics) and L1 (polymers) levels for the fossil depletion impact categories.

From the results, it can be seen that underspecification of HDPE introduces progressively large errors in the GWP impact assessment. For instance, for the first scenario, the GWP evaluated at L3 is off by almost 30% from the correct value evaluated at L4. The drastic increase in error from L4 to L3 is due to the sudden drop in specification of the materials.

Tables 15

Underspecification of HDPE

30% recycling rate, 51% recycling efficiency				
Level of specificity	**GWP (kg CO_2 eq)**	**Fossil Depletion (kg oil eq)**	**|% Difference| in GWP**	**|% Difference| in Fossil Depletion**
L4 (HDPE)	0.21	0.122	-	-
L3 (Polyethylene)	0.1512	0.0688	28	43.606
L2 (Thermoplastic)	0.311	0.1124	48.09	7.86
L1 (Polymers)	0.278	0.1056	32.380	13.393
100% recycling rate, 85% recycling efficiency				
Level of specificity	**GWP (kg CO_2 eq)**	**Fossil Depletion (kg oil eq)**	**|% Difference| in GWP**	**|% Difference| in Fossil Depletion**
L4 (HDPE)	0.153	0.0512	-	-
L3 (Polyethylene)	0.143746	0.04281	6.048	16.386
L2 (Thermoplastic)	0.16902	0.0507	10.470	0.97
L1 (Polymers)	0.16388	0.0486	7.058	5
No recycling				
Level of specificity	**GWP (kg CO_2 eq)**	**Fossil Depletion (kg oil eq)**	**|% Difference| in GWP**	**|% Difference| in Fossil Depletion**
L4 (HDPE)	0.222	0.137	-	-
L3 (Polyethylene)	0.1525	0.0735	31.30	46.35
L2 (Thermoplastic)	0.34178	0.1326	53.95	3.21
L1 (Polymers)	0.30314	0.11716	36.54	14.48

In other words, the information about the characteristics of the material are over-simplified leading to results arising out of a range of values distributed across different material categories in place of specific ones. Similarly, for the fossil depletion impact category, it can be seen that jumping from L4 to L3 introduces 43% error in impact assessment. Furthermore, it can be seen that the difference in errors arising out of underspecification between L2 and L1 is not very large. This substantiates our earlier argument about the decline in errors being relatively minor among the lower levels itself. This may be a function of the way the materials are classified. Variations in these patterns could be expected when a different type of classification system is adopted.

One interesting observation here is that beyond L3, underspecification does not have a significant effect on the fossil depletion impacts. Fossil depletion is representative of the amount of non-renewable resources exhausted for the manufacture of a particular product. In the present case, crude oil is extracted and refined for the manufacture of HDPE. However, the process of extraction of crude oil itself is an upstream process common to all the subsequent systems in the supply chain. That is, the relative amounts of crude oil extracted may not be significantly influenced by (underspecifying) the characteristics of the product itself. However, this is not the case with GWP. Greenhouse gases may be emitted at every step of the manufacturing process because of varying process conditions thereby making it sensitive to changes in the material grades. By looking at the raw data for these two environmental impact categories, it can be seen that the values for GWP change with different polymer grades (and thus different process conditions) unlike the values for fossil depletion that do not vary all that much. Quantitatively, the magnitude of variance across different levels for the GWP impact

category is higher than the same for fossil depletion (Figure 20). This shows that underspecification affects GWP estimates much more severely than fossil depletion. In other words, different impact categories are affected differently by underspecification. This has to be taken in to account when making life cycle impact assessments.

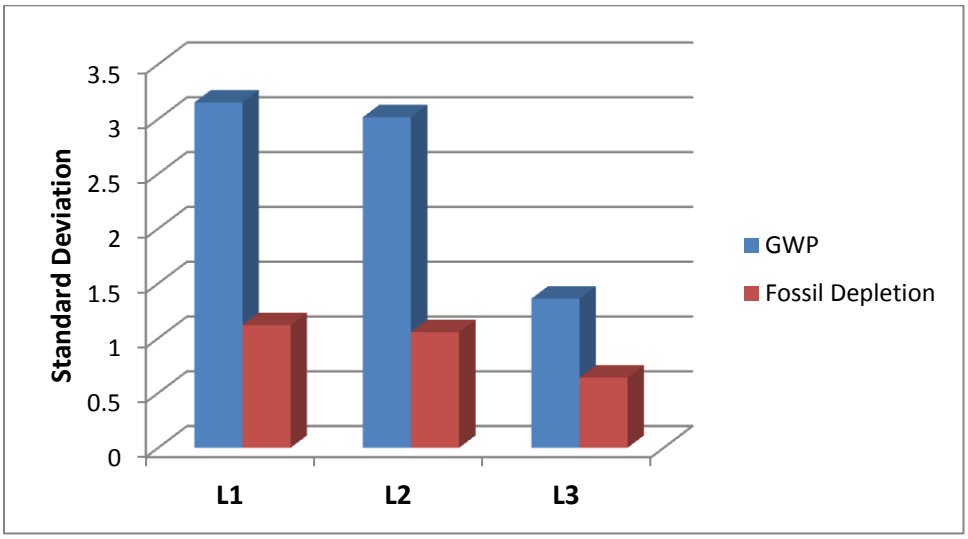


Figure 20. Variance of GWP vs. Fossil Depletion

The process flow diagrams with HDPE mis-specified as LDPE and LLDPE for the model with 30% recycling rate are shown in Figure 21. Table 16 below shows the variation in impacts due to mis-specification for all the scenarios. Consider the first scenario in Table 16. When HDPE is mis-specified as LDPE, there is a 4.28% error in the GWP. When HDPE is mis-specified as LLDPE, there is only a 1.90% error in GWP. This is because of the similarity in process conditions for the manufacture of HDPE and LLDPE. Both HDPE and LLDPE are either produced in gas phase processes in a fluidized bed reactor or in the solution process. In fact, the gas phase processes designed for LLDPE production are also used for the production of HDPE (PlasticsEurope, 2014). These are low pressure technologies and yield polymers with low or very short branches.

Moreover, the density of LLDPE (0.92-0.94 g/cm^3) and HDPE (0.94-0.96g/cm^3) are comparable. In contrast, the polymerization of LDPE takes place at high pressures and temperatures. Highly branched chains are produced at 1000-3000 bar and 100-300^{o}C by free radical polymerization (Lepoutre, 2008; PlasticsEurope, 2014).

Table 16

Mis-specification of HDPE

30% recycling rate, 51% recycling efficiency				
Type of Polymer	**GWP (kg CO_2 eq)**	**Fossil Depletion (kg oil eq)**	**|% Difference| in GWP**	**|% Difference| in Fossil Depletion**
HDPE	0.21	0.122	-	-
LDPE	0.219	0.121	4.28	0.819
LLDPE	0.206	0.121	1.90	0.819
100% recycling rate, 85% recycling efficiency				
Level of specificity	**GWP (kg CO_2 eq)**	**Fossil Depletion (kg oil eq)**	**|% Difference| in GWP**	**|% Difference| in Fossil Depletion**
HDPE	0.153	0.0512	-	-
LDPE	0.155	0.0511	1.307	0.19
LLDPE	0.152	0.051	0.6535	0.39
No recycling				
Level of specificity	**GWP (kg CO_2 eq)**	**Fossil Depletion (kg oil eq)**	**|% Difference| in GWP**	**|% Difference| in Fossil Depletion**
HDPE	0.222	0.137	-	-
LDPE	0.233	0.136	4.95	0.729
LLDPE	0.214	0.136	2.252	0.729

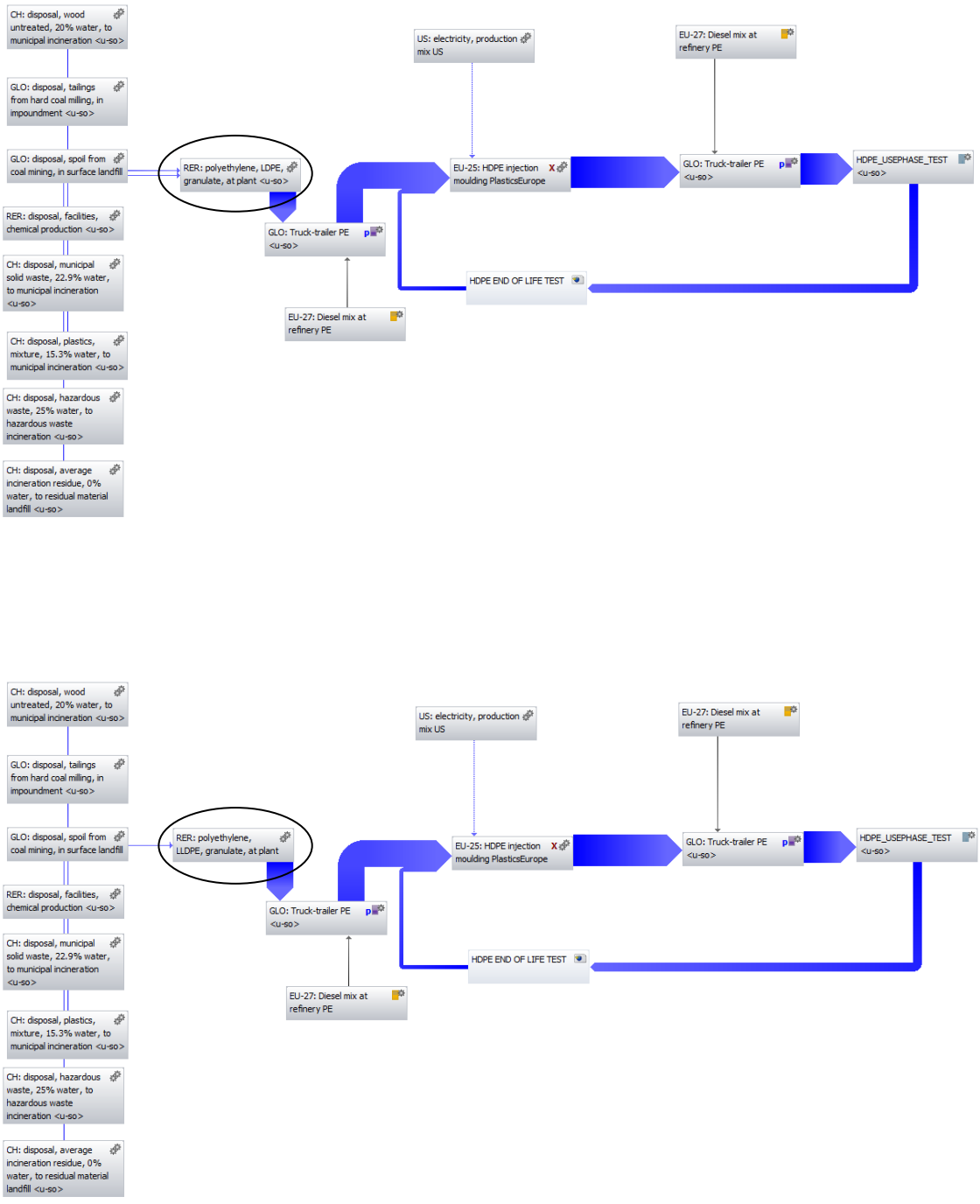


Figure 21. Mis-specification of HDPE

Therefore, as explained before, GWP is sensitive to process conditions. Thus wrongly specifying HDPE as LLDPE leads to a relatively smaller penalty compared to mis-specifying HDPE as LDPE. Interestingly enough, fossil depletion is not affected by mis-specification all that much. Again, this may be due to the fact that extraction of non-renewable fossil resources for the manufacture of these polymers is a step common to all these processes/polymer grades. Incorrect specification of the type of polymer has little or no effect on the impacts caused due to depletion of fossil resources. Judging by the raw data collected from Ecoinvent database, it can be seen that the difference in GWP values between HDPE and LLDPE is smaller than the same between HDPE and LDPE. Also, the values for fossil depletion are similar for all the three polymers (Table 17).

Table 17

GWP vs. Fossil Depletion of Polymers

Type of Polymer	GWP (kg CO2 eq/kg of polymer)	Fossil Depletion (kg oil eq/kg of polymer)
HDPE	1.91	1.70
LDPE	2.08	1.68
LLDPE	1.83	1.68

4.6.2 Life Cycle of Aerosol Air Freshener Cans

The life cycle of aerosol air freshener cans is shown in Figure 22 below. This model has been adapted from the life cycle impact study of aerosol air fresheners developed by The Sustainability Consortium.

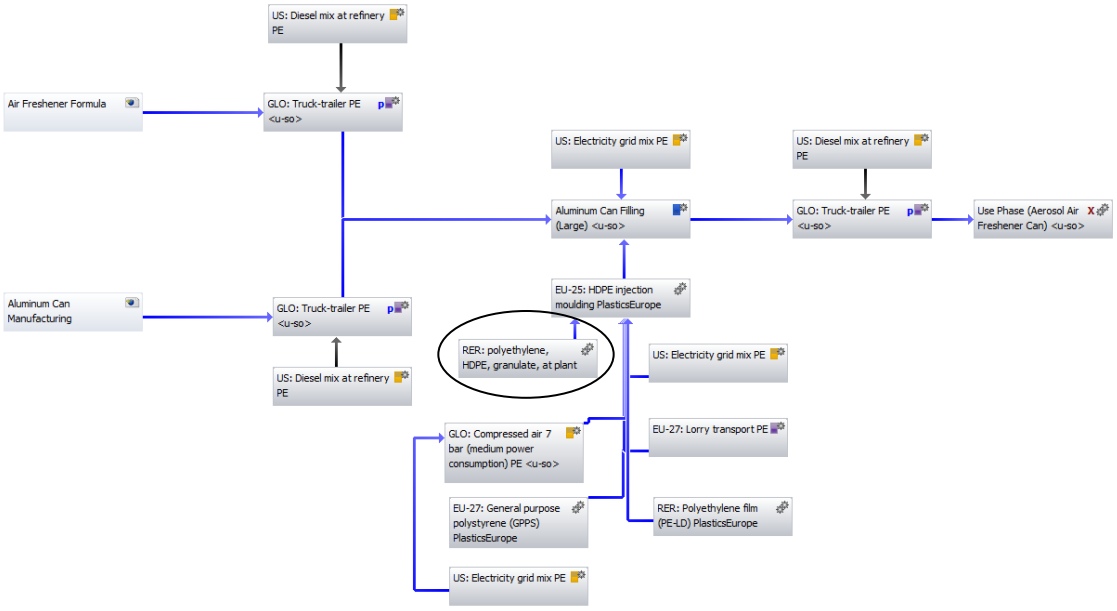


Figure 22. Life Cycle of Aerosol Air Freshener Cans (TSC, 2013)

The model was scoped to be from raw material extraction to retail. The functional unit for this model was one canister. This model was studied to see how underspecification of a component of a product affected the overall results of the analysis. Thus, in this case, the HDPE cap/trigger component in the canister was underspecified as well as mis-specified. The HDPE component analyzed in this model is marked in the figure above. The canister weighed about 0.362 kg of which HDPE cap and trigger comprise about 0.0232 kg (6.4% by weight). The overall GWP of the aerosol air freshener cans was 1.45 kg CO_2 eq. The HDPE granulate production process for this case contributed about 0.0438 kg CO_2 eq (3.02%).

The results of underspecifying and mis-specifying HDPE in this case are shown in Table 18 and 19 respectively. As can be seen, underspecification causes increasingly large errors in GWP impact assessment. Variations in the fossil depletion impacts remain

negligible beyond L3. These patterns are similar to the case of HDPE bottles discussed previously. The reasoning behind these patterns may be the same as discussed before. The variations in GWP are caused due to varying process conditions for the manufacture of different types of polymers. However, fossil depletion impacts are not significantly affected by underspecification and may only be affected by the amounts of non-renewable resources depleted for the manufacture of the polymer as part of common upstream processes.

However, note that the sheer magnitude of errors caused by underspecifying the same polymer, HDPE, in this case is very low as compared to the previous case study. For instance, in the case of HDPE bottles (without recycling), the jump from L4 to L3 caused a 30% difference in the GWP impact results and a 45% difference in fossil depletion impacts. In this case, the corresponding values are just about 1.7% and 3%. Moreover, the differences between the % errors in impacts across all the levels are very small (1.7 %, 2.9 % and 1.9 %). This may be because of the differences in relative contributions of the same process to the overall impact of the product. In the case of HDPE bottle production (no recycling), the granulate production process accounted for almost 50% of the total GWP impact of the life cycle of the bottle. In this case, the same process accounts for just about 3% of the impact of the canister over its entire life cycle. The mass of HDPE granulates produced for the manufacture of one bottle was 0.0644kg whereas the mass of HDPE granulates produced for the manufacture of one cap/trigger assembly is 0.0232 kg. This indicates that underspecification may be sensitive to variations in the contributions of the components under study to the overall impact of the entire process. Within the bounds of this study, it could be concluded that, for very little

difference in masses of the products, underspecification has a relatively smaller impact in terms of introducing errors in the LCA when the contribution of the process involved is less than 10% to the total impact of the whole system. However, this conclusion might not be entirely valid for all the systems and therefore additional case studies have to be explored to assess the validity of this claim.

Table 18

Underspecification of HDPE Cap/Trigger Assembly

Level of specificity	**GWP (kg CO_2 eq)**	**Fossil Depletion (kg oil eq)**	**|% Difference| in GWP**	**|% Difference| in Fossil Depletion**
L4 (HDPE)	1.45	0.733	-	-
L3 (Polyethylene)	1.4252	0.71055	1.710	3.06
L2 (Thermoplastic)	1.49253	0.731556	2.931	0.196
L1 (Polymers)	1.4787	0.72606	1.97	0.946

The results of mis-specification are given below.

Table 19

Mis-specification of HDPE Cap/Trigger Assembly

Type of Polymer	**GWP (kg CO_2 eq)**	**Fossil Depletion (kg oil eq)**	**|% Difference| in GWP**	**|% Difference| in Fossil Depletion**
HDPE	1.45	0.733	-	-
LDPE	1.46	0.732	0.689	0.136
LLDPE	1.45	0.732	0	0.136

Due to the similarity of HDPE and LLDPE process conditions and properties, incorrect specification of the polymer type does not affect the results of the LCA severely. However, mis-specification of HDPE as LDPE introduces a relatively larger error due to the differences in their processing methodologies. In this case too, fossil depletion being a common upstream process is not sensitive to variations in polymeric grades. Also, for reasons discussed above, the magnitude of these errors might be small themselves.

CHAPTER 5

CONCLUSIONS AND RECOMMENDATIONS

The prohibitive costs associated with collecting and specifying exact materials and processes for conducting a comprehensive LCA has limited its extensive application. To reduce the effort and costs of conducting an LCA, several streamlining methodologies have been proposed over the years. This thesis explored one such method called probabilistic underspecification, which uses a structured data classification system that enables an LCA modeler to specify the materials and processes in a less precise manner, thus saving time and cost. Extensive statistical analysis was done to quantify the uncertainty associated with underspecification and mis-specification by assessing the variation in impact estimates incurred by underspecifying material impact data for streamlined LCA.

5.1 Discussion

By applying the concept of probabilistic underspecification, common products from petrochemical refineries and polymer manufacturing plants were categorized into a structured hierarchical system that established materials specificity and the effort needed to retrieve environmental impact data at each level of specificity. Standard deviation computed at each of those levels was used to characterize the error in impact estimates arising out of underspecifying the materials. For the purpose of this thesis, environmental impact data for 10 products from refineries in Switzerland and Europe were collected from the Ecoinvent database. Impact data for eight different polymers from European

polymer manufacturing plants were also compiled. A total of 11 environmental impact categories were studied.

Major conclusions from this study can be summarized as follows:

- Magnitude of error in the impact estimates of refinery products and polymers decreases as the specificity of the materials increases
- The patterns of variance in the impact estimates in moving from one level to another suggest that most of the variability is caused due to the location from which the environmental impact data was collected. The effects of categorizing the materials into other (lower) levels of distinction are relatively small
- Precision of estimates of only certain environmental impacts namely GWP, freshwater eutrophication, freshwater ecotoxicity, human toxicity and terrestrial ecotoxicity are affected by changes in location. The evaluation of other impacts are relatively robust to geographic variations
- Product categories within each level of specificity that have similar chemical and physical properties have similar effects on the magnitude of variance in impact estimates

The variation in impact estimates between upstream (petroleum refineries) and downstream (polymer manufacturing) processes were also compared. As expected, at the least specific level, the results indicate that

- The environmental impacts of the upstream processes are captured while evaluating the impacts of downstream processes

- The variation in the estimation of environmental performance of polymers is higher than that of refinery products for most environmental impact categories studied

To test the effectiveness of structured underspecification and mis-specification at the level of product footprint, two case studies of HDPE bottles/containers and aerosol air fresheners were studied. The two largest impacts of global warming and fossil depletion were observed for these two studies. In each of the product cases studied, the HDPE component was underspecified as polyethylene at L3, thermoplastic at L2 and polymer at L1. The LCA of HDPE bottles and aerosol air fresheners was performed with HDPE specified at each of these levels and the impacts were recalculated to gauge the effectiveness of underspecification. Further, HDPE was also incorrectly specified as LDPE and LLDPE and LCA simulations were re-run to see the effects of mis-specification on the impact estimates. The results from these studies could be summarized as follows:

- For both products studied the error in the estimation of GWP increases progressively as the specificity of HDPE decreases. However, fossil depletion estimates remain relatively immune to underspecification of HDPE beyond L3
- The precision of estimation of GWP and fossil depletion impacts are not significantly affected by mis-specification of HDPE

5.2 Conclusions and Contributions

The developed statistical analysis methodology has proved to be promising for the characterization of variability in LCA results arising out of probabilistic underspecification as well as mis-specification. From the studies conducted herein, it could be concluded that underspecification and mis-specification rely heavily on the types of product systems examined and the methodology of classifying them. That is, a different scheme of categorizing the materials into different levels may lead to totally different conclusions. Further, within the bounds of this project, it could be declared that underspecification has different effects on the precision of estimates of environmental performance of products. In other words, environmental impact categories are unique and have to be treated on a case by case basis when comparing the effects of underspecification on LCA results. Although underspecification aids in lessening the burden of collecting information for conducting LCA, it adds another level of ambiguity in addition to other sources of uncertainty.

This study contributes to our knowledge of what the impact of probabilistic underspecification on the overall model uncertainty is. The study is also provides LCA modelers with valuable information on the repercussions of making the wrong selection (mis-specification) of process or materials while performing LCA modeling. Previous research on this topic has been extended by performing LCA of additional case studies of different product systems namely petrochemicals and polymers. Moreover, the available research on this topic only revolves around the effects of underspecification on cumulative energy demand estimates of products. This study has added value to the

existing body of research by estimating the effects of underspecification as well as mis-specification on a wider spectrum of impact categories for the particular cases studied.

5.3 Limitations and Future Work

This project only explored the case of petroleum refinery products and polymers. In order to gain confidence in this statistical methodology, more case studies covering a broad spectrum of products have to be performed. Future work could revolve around applying this methodology for different materials such as metals, glasses, specialty chemicals and so forth. Further, only a component of the life cycle has been underspecified/mis-specified in the case studies analyzed as part of this project. In the future, the complete life cycle of a product could be underspecified/mis-specified and their effects analyzed. Finally, a different scheme of classifying and resolving information could be adopted and statistical analyses could be performed to see how it affects the results of LCA. It would be interesting to see how this methodology could be extended to processes categorized based on different processing conditions. For example, the effects of underspecifying a particular process operating at different levels of temperature and pressure could be estimated and compared. Such a procedure would give the modeler an idea of the sensitivity of underspecification to varying process conditions.

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APPENDIX A

ENVIRONMENTAL IMPACT DATA FOR REFINERY PRODUCTS

L4	Terrestrial Acidification (kg SO2 Eq)	Freshwater Eutrophication (kg P Eq)	Freshwater Ecotoxicity (kg 1,4 DB Eq)	Human Toxicity (kg 1,4 DB Eq)	Marine Ecotoxicity (kg 1,4 DB Eq)
Diesel, at refinery/CH U	2.67E-05	2.16E-07	4.03E-05	4.04E-04	5.48E-06
Diesel, at refinery/RER U	1.80E-04	9.50E-08	1.89E-05	2.42E-04	1.58E-05
Diesel, low-sulphur, at refinery/CH U	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Diesel, low-sulphur, at refinery/RER U	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Heavy fuel oil, at refinery/CH U	1.87E-05	2.16E-07	4.05E-05	4.16E-04	5.78E-06
Heavy fuel oil, at refinery/RER U	1.03E-01	9.46E-08	1.95E-05	2.49E-04	1.61E-05
Light fuel oil, at refinery/CH U	2.67E-05	2.16E-07	4.02E-05	4.03E-04	5.48E-06
Light fuel oil, at refinery/RER U	1.80E-04	9.47E-08	1.89E-05	2.41E-04	1.57E-05
Kerosene, at refinery/CH U	2.67E-05	2.16E-07	3.99E-05	3.90E-04	5.18E-06
Kerosene, at refinery/RER U	1.79E-04	9.46E-08	1.87E-05	2.33E-04	1.53E-03
Naphtha, at refinery/CH U	1.59E-05	2.17E-07	4.03E-05	4.04E-04	5.48E-06
Naphtha, at refinery/RER U	1.08E-04	9.46E-08	1.88E-05	2.41E-04	1.57E-05
Petrol, low-sulphur, at refinery/CH U	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Petrol, low-sulphur, at refinery/RER U	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Petrol, unleaded, at refinery/CH U	4.80E-05	2.16E-07	4.03E-05	4.04E-04	5.49E-06
Petrol, unleaded, at refinery/RER U	3.23E-04	9.45E-08	1.88E-05	2.41E-04	1.57E-05
Electricity, at refinery/CH U	3.94E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Electricity, at refinery/RER U	3.22E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Propane/ butane, at refinery/CH U	4.00E-05	2.16E-07	4.03E-05	4.04E-04	5.49E-06
Propane/ butane, at refinery/RER U	2.69E-04	9.45E-08	1.88E-05	2.41E-04	1.57E-05
Refinery gas, at refinery/CH U	4.00E-05	2.16E-07	4.03E-05	4.04E-04	5.48E-06
Refinery gas, at refinery/RER U	2.70E-04	9.48E-08	1.89E-05	2.41E-04	1.58E-05
Secondary sulphur, at refinery/CH U	0.0225	2.28E-07	4.25E-05	3.64E-04	5.78E-06
Secondary sulphur, at refinery/RER U	0.0303	9.48E-08	1.89E-05	1.88E-04	1.57E-05

L4	Marine Eutrophication (kg N Eq)	Metal Depletion (kg Fe Eq)	Photo-chemical Oxidant Formation (NMVOC)	Terrestrial Ecotoxicity (kg 1,4 DB Eq)	Water Depletion (m3)
Diesel, at refinery/CH U	1.29E-05	2.73E-08	1.80E-04	4.04E-07	4.54E-03
Diesel, at refinery/RER U	1.15E-05	2.94E-08	1.81E-04	2.14E-07	4.51E-03
Diesel, low-sulphur, at refinery/CH U	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Diesel, low-sulphur, at refinery/RER U	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Heavy fuel oil, at refinery/CH U	1.76E-05	0.00E+00	1.75E-04	4.03E-07	4.53E-03
Heavy fuel oil, at refinery/RER U	1.15E-05	0.00E+00	1.69E-04	2.13E-07	4.49E-03
Light fuel oil, at refinery/CH U	1.29E-05	2.73E-08	1.80E-04	4.03E-07	4.53E-03
Light fuel oil, at refinery/RER U	1.14E-05	2.93E-08	1.80E-04	2.13E-07	4.50E-03
Kerosene, at refinery/CH U	1.99E-05	0.00E+00	1.80E-04	4.04E-07	4.50E-03
Kerosene, at refinery/RER U	1.43E-05	0.00E+00	1.80E-04	2.13E-07	4.49E-03
Naphtha, at refinery/CH U	1.85E-05	0.00E+00	1.70E-04	4.05E-07	4.50E-03
Naphtha, at refinery/RER U	1.13E-05	0.00E+00	1.66E-04	2.13E-07	4.49E-03
Petrol, low-sulphur, at refinery/CH U	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Petrol, low-sulphur, at refinery/RER U	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Petrol, unleaded, at refinery/CH U	2.60E-05	0.00E+00	1.94E-04	4.04E-07	4.50E-03
Petrol, unleaded, at refinery/RER U	2.16E-05	0.00E+00	2.08E-04	2.13E-07	4.49E-03
Electricity, at refinery/CH U	2.73E-05	0.00E+00	7.03E-05	0.00E+00	0.00E+00
Electricity, at refinery/RER U	2.23E-05	0.00E+00	5.74E-05	0.00E+00	0.00E+00
Propane/ butane, at refinery/CH U	2.41E-05	0.00E+00	1.89E-04	4.04E-07	4.57E-03
Propane/ butane, at refinery/RER U	1.90E-05	0.00E+00	1.98E-04	2.13E-07	4.48E-03
Refinery gas, at refinery/CH U	2.41E-05	0.00E+00	1.89E-04	4.03E-07	4.53E-03
Refinery gas, at refinery/RER U	1.91E-05	0.00E+00	1.98E-04	2.13E-07	4.50E-03
Secondary sulphur, at refinery/CH U	1.45E-05	0.00E+00	1.85E-03	4.23E-07	4.78E-03
Secondary sulphur, at refinery/RER U	1.49E-05	0.00E+00	2.49E-03	2.12E-07	4.50E-03

APPENDIX B

ENVIRONMENTAL IMPACT DATA FOR POLYMERS

L4	Terrestrial Acidification (kg SO2 Eq.)	Freshwater Eutrophicati-on (kg P Eq.)	Freshwater Ecotoxicity (kg 1,4- DB Eq.)	Human Toxicity (kg 1,4-DB Eq.)	Marine Ecotoxicity (kg 1,4-DB Eq.)	Fossil Depletion (kg Oil Eq.)
Nylon 6, at plant/RER U	2.74E-02	1.04E-04	1.18E-02	9.21E-03	1.08E-03	2.69E+00
Nylon 6, glass-filled, at plant/RER U	2.57E-02	7.37E-05	8.65E-03	7.06E-03	1.02E-03	2.27E+00
Nylon 66, at plant/RER U	2.71E-02	3.39E-04	3.84E-02	7.67E-03	3.32E-03	2.89E+00
Nylon 66, glass-filled, at plant/RER U	2.26E-02	2.66E-05	4.20E-03	7.21E-03	1.42E-03	2.35E+00
Polymethyl methacrylate, beads, at plant/RER U	3.58E-02	3.88E-04	4.28E-02	1.21E-02	2.62E-03	2.85E+00
Polymethyl methacrylate, sheet, at plant/RER U	3.74E-02	2.20E-04	2.42E-02	0.0153	1.50E-03	3.12E+00
Polyethylene, HDPE, granulate, at plant/RER U	5.89E-03	1.77E-07	2.06E-05	1.75E-03	2.03E-06	1.70E+00
Polyethylene, LDPE, granulate, at plant/RER U	7.15E-03	2.28E-07	2.71E-05	2.68E-03	3.07E-06	1.68E+00
Polyethylene, LLDPE, granulate, at plant/RER U	5.18E-03	6.07E-08	7.54E-06	1.59E-03	1.88E-06	1.68E+00
Fleece, polyethylene, at plant/RER U	0.00E+00	0.00E+00	0.00E+0	0.00E+0	0.00E+00	0.00E+00
Polyethylene terephthalate, granulate, amorphous, at plant/RER U	0.00E+00	0.00E+00	0.00E+0	0.00E+0	0.00E+00	0.00E+00
Polyethylene terephthalate, granulate, bottle grade, at plant/RER U	0.00E+00	0.00E+00	0.00E+0	0.00E+0	0.00E+00	0.00E+00
Polyester resin, unsaturated, at plant/RER U	0.00E+00	0.00E+00	0.00E+0	0.00E+0	0.00E+00	0.00E+00
Polystyrene, expandable, at plant/RER U	9.71E-03	6.29E-05	6.95E-03	9.21E-03	4.49E-04	2.03E+00
Polystyrene, general purpose, GPPS, at plant/RER U	1.03E-02	1.48E-06	3.25E-04	7.93E-03	1.68E-04	2.00E+00
Polystyrene, high impact, HIPS, at plant/RER U	1.10E-02	1.69E-06	3.72E-04	8.08E-03	1.92E-04	2.01E+00
Polyvinylchloride, emulsion polymerised, at plant/RER U	6.38E-03	5.98E-06	8.00E-04	2.28E-01	1.39E-04	1.30E+00
Polyvinylchloride, suspension polymerised, at plant/RER U	4.74E-03	5.48E-06	7.30E-04	1.28E-01	1.29E-04	1.11E+00
Polyvinylidenchloride, granulate, at plant/RER U	2.35E-02	1.86E-06	3.70E-04	1.06E+0	4.43E-03	1.49E+00
Epoxy resin, liquid, at plant/RER U	3.86E-02	3.19E-05	5.71E-04	5.55E-01	1.56E-04	2.88E+00
Epoxy resin, liquid, disaggregated data, at plant/RER U	3.22E-03	7.26E-05	1.59E-04	3.00E-01	6.03E-05	1.01E+00
Melamine formaldehyde resin, at plant/RER U	0.00E+00	0.00E+00	1.59E-05	1.14E-01	4.20E-06	0.00E+00
Urea formaldehyde resin, at plant/RER U	0.00E+00	0.00E+00	1.59E-05	1.14E-01	4.20E-06	0.00E+00
Polyurethane, flexible foam, at plant/RER U	0.00E+00	0.00E+00	0.00E+0	0.00E+0	0.00E+00	0.00E+00
Polyurethane, rigid foam, at plant/RER U	0.00E+00	0.00E+00	2.50E-08	0.00E+0	6.81E-07	0.00E+00

L4	Marine Eutrophication (kg N-Eq.)	Metal Depletion (kg Fe Eq.)	Photochemical Oxidant Formation (kg NMVOC)	Terrestrial Ecotoxicity (kg 1,4- DB Eq.)	Water Depletion (m3)
Nylon 6, at plant/RER U	9.95E-03	2.04E-03	2.82E-02	2.09E-04	1.85E-02
Nylon 6, glass-filled, at plant/RER U	8.78E-03	1.69E-03	2.34E-02	1.44E-04	3.13E-01
Nylon 66, at plant/RER U	1.37E-02	8.67E-04	2.04E-02	6.27E-04	6.63E-01
Nylon 66, glass-filled, at plant/RER U	1.02E-02	8.47E-04	1.66E-02	5.80E-05	5.25E-01
Polymethyl methacrylate, beads, at plant/RER U	5.69E-03	7.30E-04	2.94E-02	7.15E-04	7.61E-02
Polymethyl methacrylate, sheet, at plant/RER U	7.37E-03	1.12E-03	3.33E-02	4.13E-04	9.55E-02
Polyethylene, HDPE, granulate, at plant/RER U	1.26E-03	2.27E-04	8.57E-03	5.68E-07	3.23E-02
Polyethylene, LDPE, granulate, at plant/RER U	1.48E-03	1.00E-03	9.28E-03	8.69E-07	4.72E-02
Polyethylene, LLDPE, granulate, at plant/RER U	1.15E-03	8.67E-04	6.48E-03	3.24E-07	1.17E-01
Fleece, polyethylene, at plant/RER U	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.40E-02
Polyethylene terephthalate, granulate, amorphous, at plant/RER U	0.00E+00	0.00E+00	9.00E-05	0.00E+00	6.56E-03
Polyethylene terephthalate, granulate, bottle grade, at plant/RER U	0.00E+00	0.00E+00	1.00E-06	0.00E+00	4.85E-03
Polyester resin, unsaturated, at plant/RER U	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.00E-02
Polystyrene, expandable, at plant/RER U	1.91E-03	8.87E-03	1.11E-02	1.44E-04	1.71E-01
Polystyrene, general purpose, GPPS, at plant/RER U	2.08E-03	9.64E-03	9.58E-03	2.15E-05	1.41E-01
Polystyrene, high impact, HIPS, at plant/RER U	2.20E-03	9.31E-03	1.03E-02	2.66E-05	1.40E-01
Polyvinylchloride, emulsion polymerised, at plant/RER U	1.92E-03	4.45E-05	1.13E-02	7.21E-05	6.09E-01
Polyvinylchloride, suspension polymerised, at plant/RER U	1.59E-03	1.26E-04	9.23E-03	5.08E-05	4.65E-01
Polyvinylidenchloride, granulate, at plant/RER U	3.61E-03	2.94E-03	1.61E-02	5.26E-04	1.55E-01
Epoxy resin, liquid, at plant/RER U	1.36E-02	2.76E-03	4.26E-02	1.14E-04	4.03E-01
Epoxy resin, liquid, disaggregated data, at plant/RER U	1.06E-03	0.00E+00	3.40E-03	5.18E-05	3.91E-01
Melamine formaldehyde resin, at plant/RER U	0.00E+00	0.00E+00	8.77E-04	5.10E-05	0.00E+00
Urea formaldehyde resin, at plant/RER U	0.00E+00	0.00E+00	8.77E-04	5.10E-05	0.00E+00
Polyurethane, flexible foam, at plant/RER U	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.10E-02
Polyurethane, rigid foam, at plant/RER U	0.00E+00	0.00E+00	2.00E-03	5.73E-08	0.00E+00

APPENDIX C

ERROR CHARACTERIZATION OF REFINERY PRODUCT IMPACTS

Impact Category	Std Dev at L0	Std Dev at L1	Std Dev at L2	Std Dev at L3	Std Dev at L4
Global Warming Potential	0.00046948	0.000465444	0.000456736	0.000497714	0.000348743
Terrestrial Acidification	0.02179101	0.021385958	0.021776815	0.022969706	0.021000023
Freshwater Eutrophication	8.786E-08	8.87423E-08	8.85067E-08	8.45758E-08	7.52132E-08
Freshwater Ecotoxicity	1.6255E-05	1.64073E-05	1.63373E-05	1.35541E-05	1.32347E-05
Human Toxicity	0.00015856	0.000161678	0.000159937	0.000148231	0.000100473
Marine Ecotoxicity	0.00031081	0.000317231	0.000323133	0.00027847	0.000311308
Marine Eutrophication	8.2624E-06	8.44804E-06	8.0244E-06	7.44363E-06	3.02868E-06
Metal Depletion	1.0792E-08	1.09335E-08	1.09115E-08	1.03564E-08	5.9196E-10
Photochemical Oxidant Formation	0.0005856	0.000121966	0.000122066	0.00013617	0.000130732
Terrestrial Ecotoxicity	1.6133E-07	1.62753E-07	1.61585E-07	1.54546E-07	1.18186E-07
Water Depletion	0.00200199	0.002008962	0.001967084	0.001647758	6.18587E-05

APPENDIX D

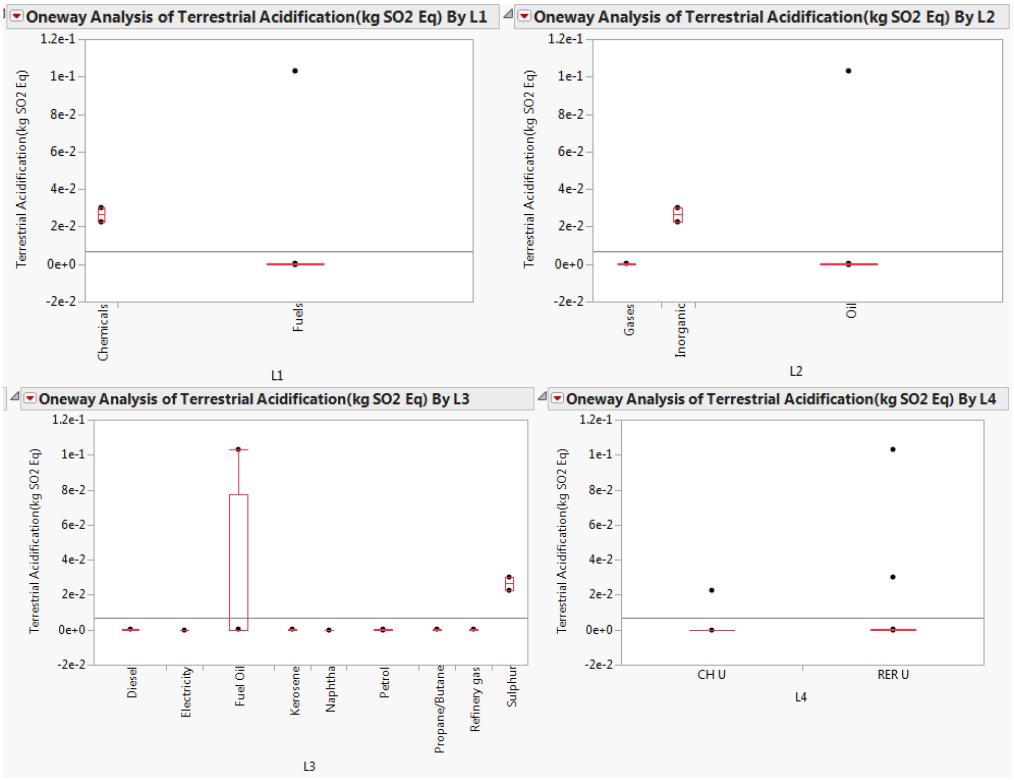
ERROR CHARACTERIZATION OF POLYMER IMPACTS

Impact Category	Std Dev at L1	Std Dev at L2	Std Dev at L3
Global Warming Potential	3.151633911	3.01723107	1.360545837
Terrestrial Acidification	0.0133016290	0.013255541	0.007370755
Freshwater Eutrophication	0.000106023	0.000106228	6.66595E-05
Fossil Depletion	1.119986161	1.055333825	0.641152892
Freshwater Ecotoxicity	0.011876636	0.011698002	0.007335102
Human Toxicity	0.237062176	0.237927485	0.180871273
Marine Ecotoxicity	0.001175458	0.001142524	0.000986178
Marine Eutrophication	0.004430759	0.004483355	0.002411472
Metal Depletion	0.002974956	0.002947456	0.000835747
Photochemical Oxidant Formation	0.011899592	0.011988161	0.007640125
Terrestrial Ecotoxicity	0.000208216	0.00020658	0.000152004
Water Depletion	0.209240272	0.212310794	0.144250668

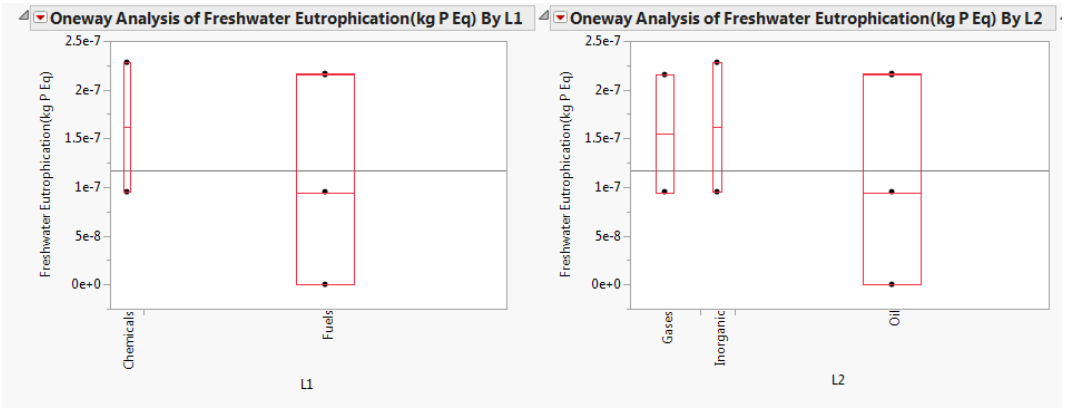
APPENDIX E

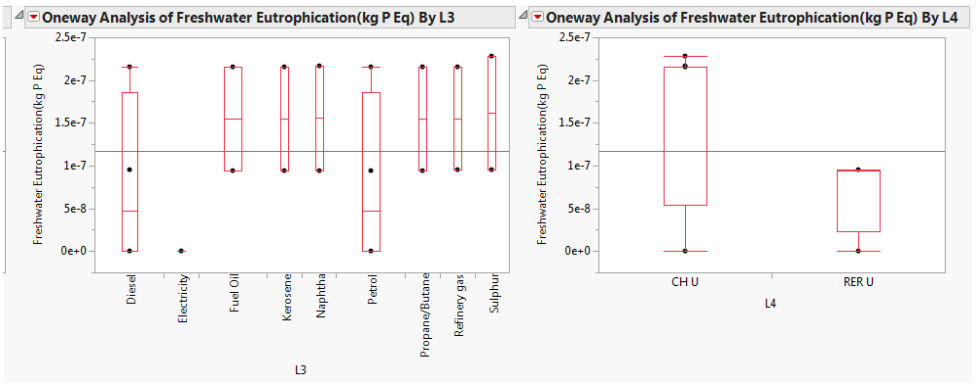
BOX PLOTS OF ENVIRONMENTAL IMPACT CATEGORIES

Terrestrial Acidification

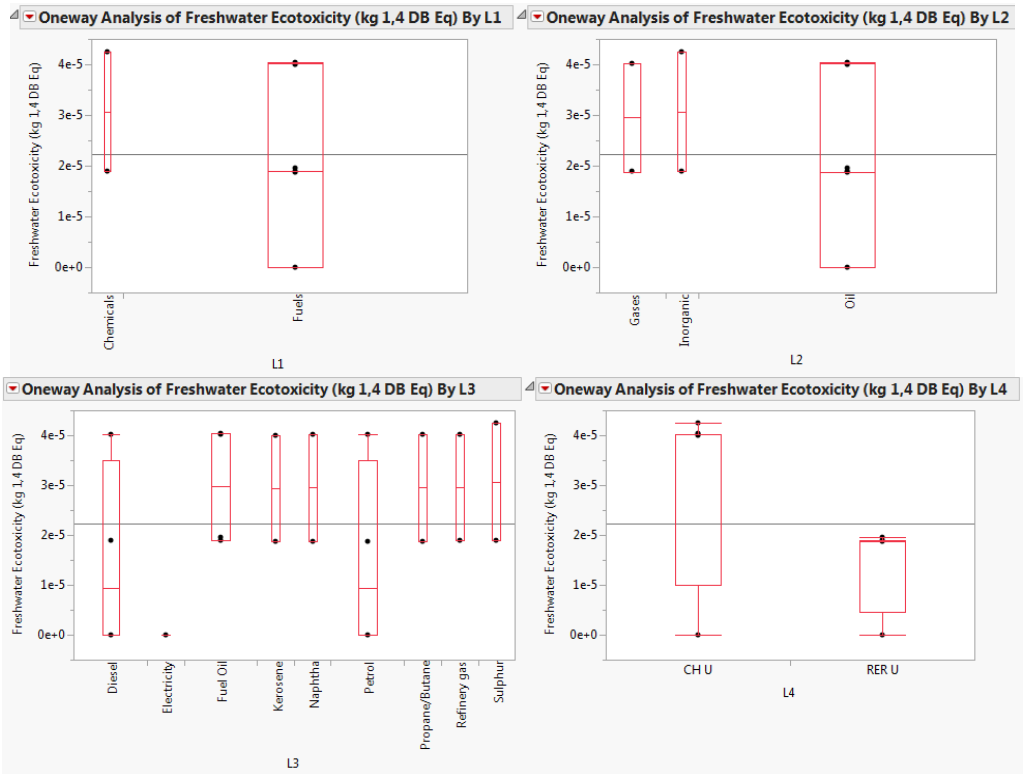


Freshwater Eutrophication

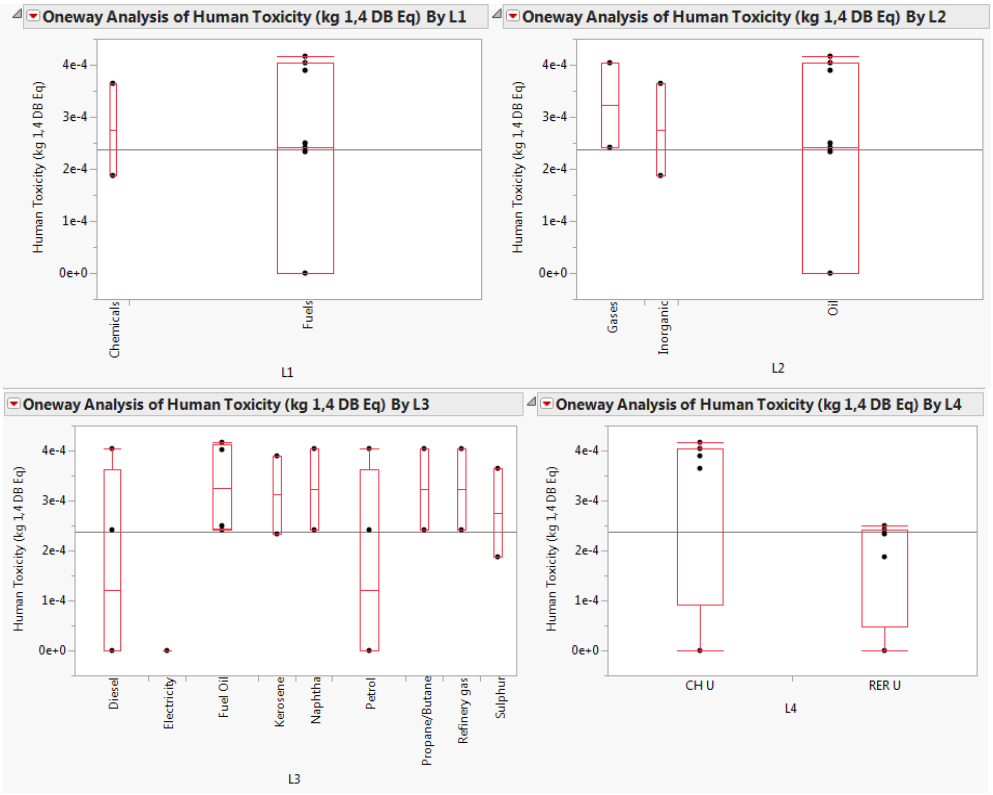




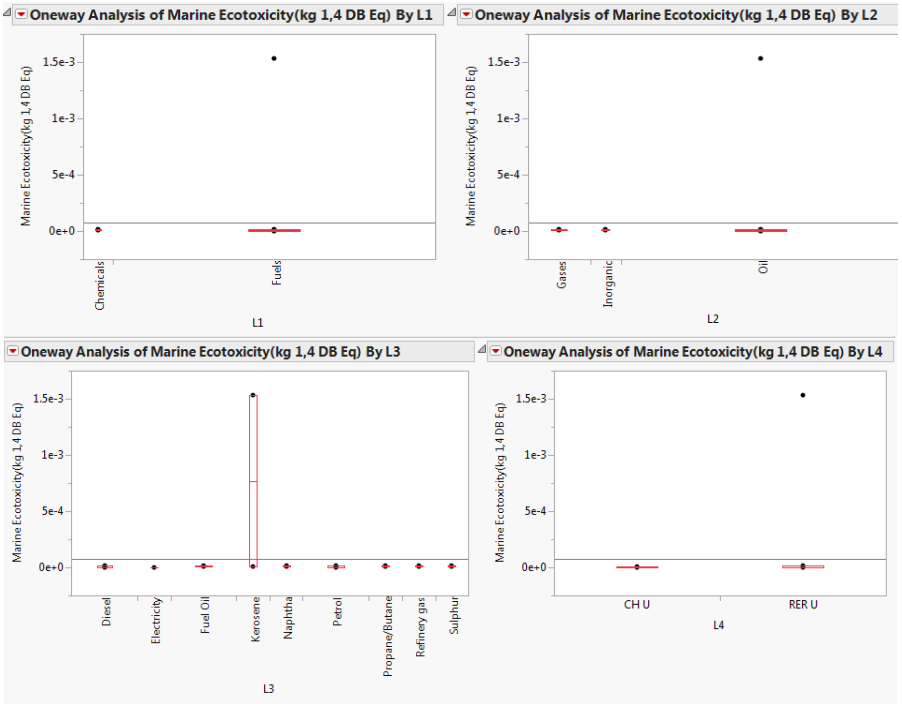
Freshwater Ecotoxicity



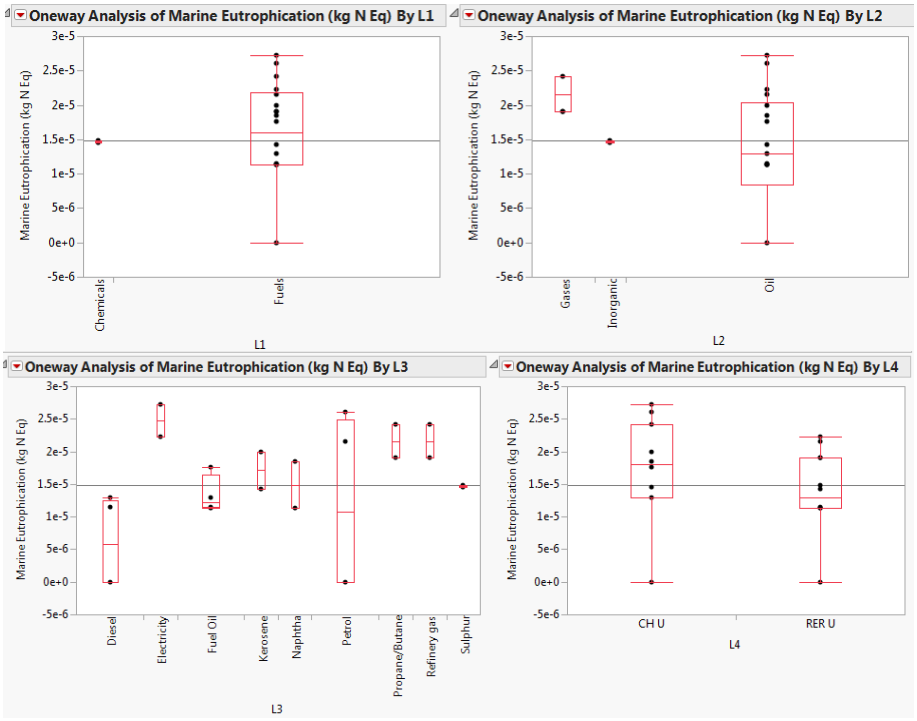
Human Toxicity



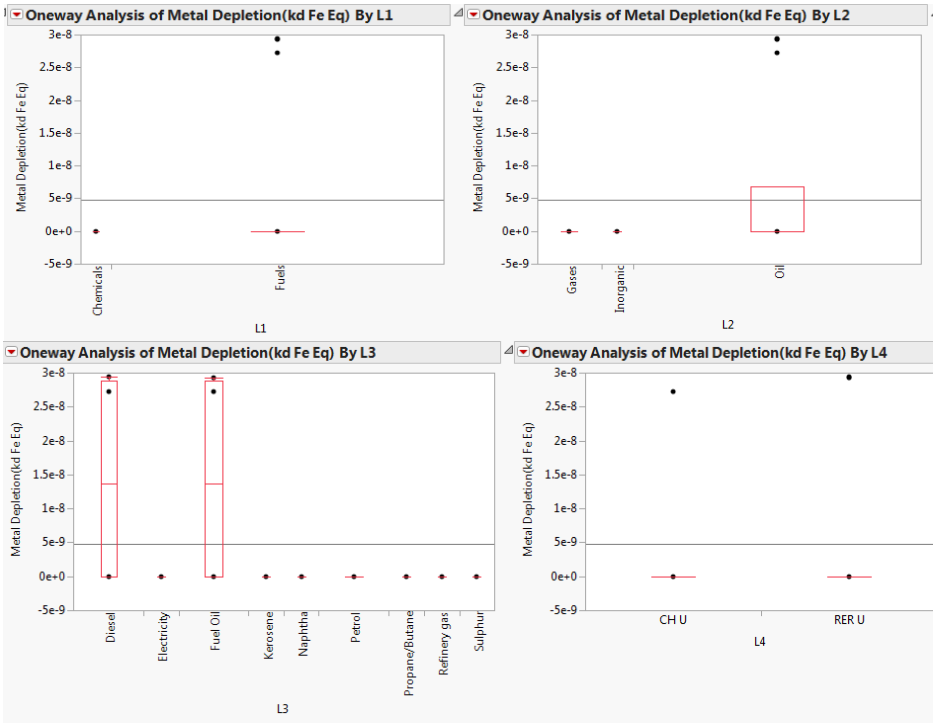
Marine Ecotoxicity



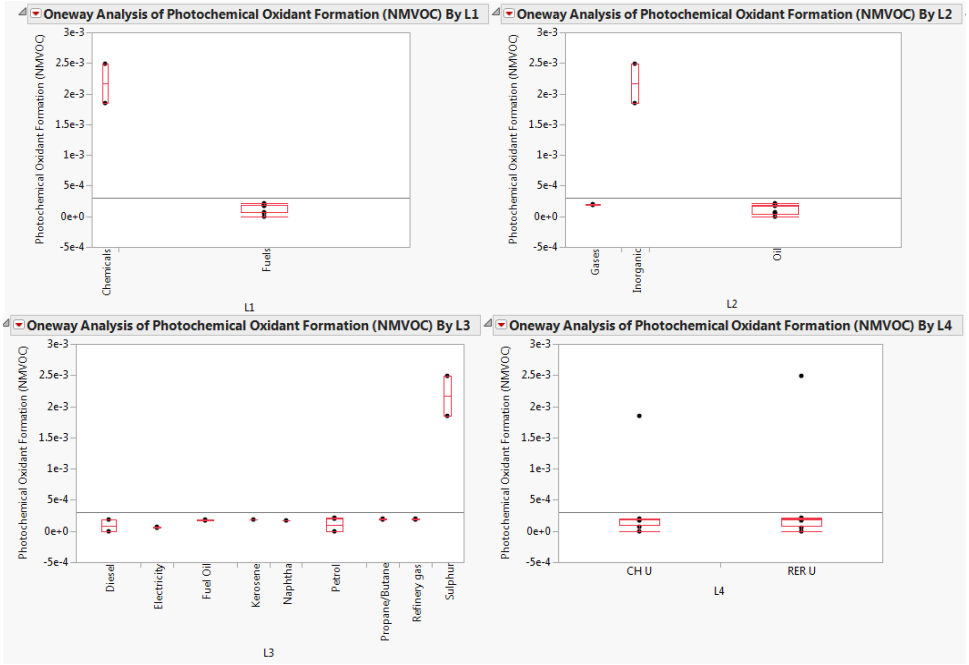
Marine Eutrophication



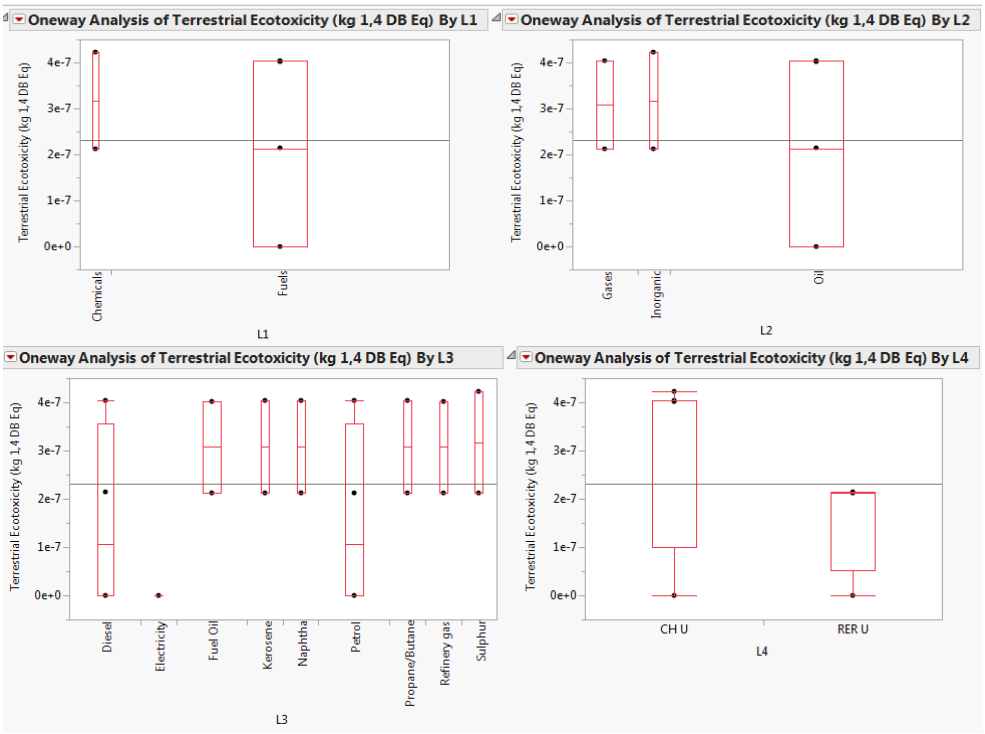
Metal Depletion



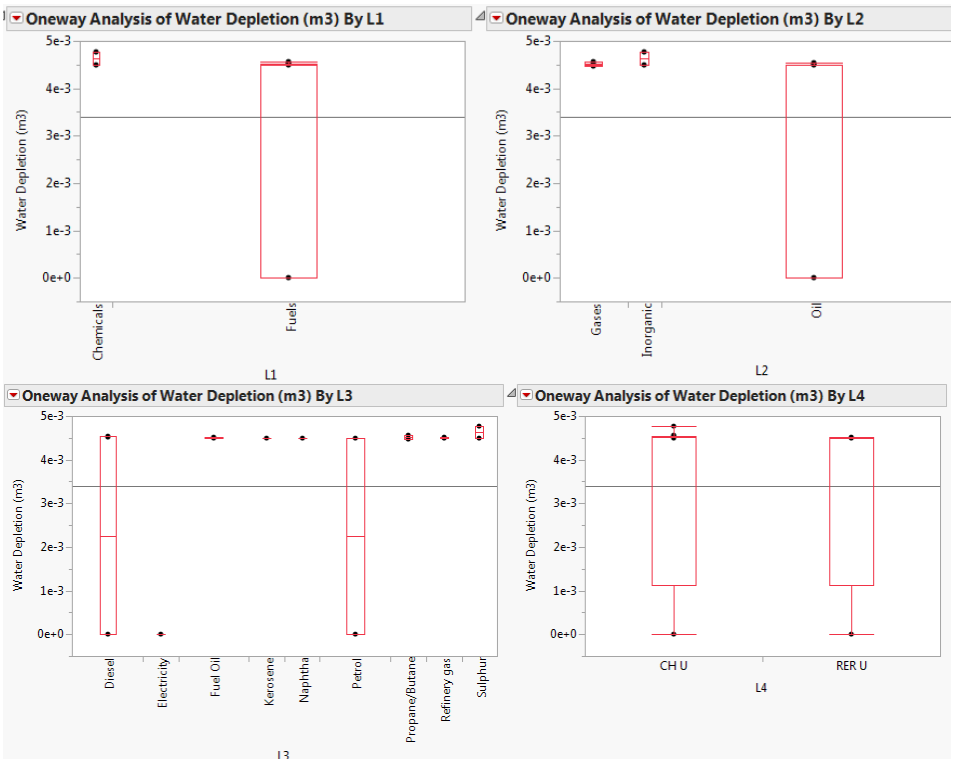
Photochemical Oxidant Formation



Terrestrial Ecotoxicity



Water Depletion



APPENDIX F

SAMPLE CALCULATIONS FOR CASE STUDIES

Life cycle analysis of 1 HDPE bottle with 30% recycling rate, 50% recycling efficiency

Functional Unit = 1 Bottle = 0.065 kg

Total GWP from the life cycle of 1 bottle = 0.21 kg CO_2 eq.

Mass of HDPE granules used per bottle = 0.0544 kg

GWP of HDPE granulate production process = 0.104 kg CO_2 eq.

% contribution of HDPE granulate production process to the total GWP = 49.52

Underspecification

@ L3, substituting HDPE granules with "polyethylene" granules

GWP of 1 kg of polyethylene = 0.831 kg CO_2 eq. (see Appendix A for impact data)

↳ Average of GWP impacts of polyethylene category at L3

∴ GWP of 0.0544 kg of polyethylene = 0.0544*0.831 kg CO_2 eq. = 0.0452 kg CO_2 eq.

Now, total GWP from the life cycle of 1 bottle with HDPE underspecified as polyethylene = (0.21 – 0.104) + 0.0452 kg CO_2 eq. = 0.1512 kg CO_2 eq.

@ L2, substituting HDPE granules with "thermoplastic" granules

GWP of 1 kg of thermoplastic = 3.77 kg CO_2 eq. (see Appendix A for impact data)

↳ Average of GWP impacts of thermoplastics category at L2

∴ GWP of 0.0544 kg of thermoplastic = 0.0544*3.77 kg CO_2 eq. = 0.205 kg CO_2 eq.

Now, total GWP from the life cycle of 1 bottle with HDPE underspecified as thermoplastic = (0.21 – 0.104) + 0.205 kg CO_2 eq. = 0.311 kg CO_2 eq.

@ L1, substituting HDPE granules with "polymer" granules

GWP of 1 kg of polymer = 3.17 kg CO_2 eq. (see Appendix A for impact data)

↳ Average of GWP impacts of polymers category at L1

$\therefore$ GWP of 0.0544 kg of polymer = 0.0544*3.17 kg CO_2 eq. = 0.172 kg CO_2 eq.

Now, total GWP from the life cycle of 1 bottle with HDPE underspecified as polymer = (0.21 – 0.104) + 0.172 kg CO_2 eq. = 0.278 kg CO_2 eq.

% error incurred in underspecifying HDPE as polyethylene = |(0.21-0.1512)/0.21| = 28

% error incurred in underspecifying HDPE as thermoplastic = |(0.21-0.311)/0.21| = 48.09

% error incurred in underspecifying HDPE as polymer = |(0.21-0.278)/0.21| = 32.380

Mis-specification

Total GWP from the life cycle of 1 bottle with HDPE mis-specified as

- LDPE = 0.219 kg CO_2 eq.
- LLDPE = 0.206 kg CO_2 eq.

→ Obtained from GaBi simulations

% error incurred in mis-specifying HDPE as LDPE = |(0.21-0.219)/0.21| = 4.28

% error incurred in mis-specifying HDPE as LLDPE = |(0.21-0.206)/0.21| = 1.90

Similar calculations are repeated for the fossil depletion impact category and for all the other cases.