

**ENVIRONMENTAL EVALUATION OF NON-ALCOHOLIC SINGLE-SERVE PET
BEVERAGE BOTTLES IN THE STATE OF CALIFORNIA USING LIFE CYCLE
ASSESSMENT AND SYSTEM DYNAMICS**

By

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ABSTRACT

ENVIRONMENTAL EVALUATION OF NON-ALCOHOLIC SINGLE-SERVE PET BEVERAGE BOTTLES IN THE STATE OF CALIFORNIA USING LIFE CYCLE ASSESSMENT AND SYSTEM DYNAMICS

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An integrated environmental evaluation of non-alcoholic single-serve PET beverage bottles was conducted using life cycle assessment (LCA) and system dynamics. The life cycle of PET bottles was divided into 4 main phases: upstream, downstream, transportation and environmental benefit. The upstream phase included the production of PET resin, the manufacture of the PET bottles, the process of beverage filling and the production of secondary packaging. The downstream phase depicted the material recovery process of post-consumer PET bottles (PCB), recycling and landfill. The transportation phase was composed of the transportation during the PET bottle delivery and the PCB collection. The environmental benefit phase included the energy recovery from incineration, and the benefits from two different recycling routes, open loop and closed loop recycling.

First, an LCA model of PET bottles in the state of California was developed. The contribution analysis showed that most of the life cycle impacts were contributed by the production of the PET bottles. Moreover, sensitivity analysis was performed to evaluate the effect of the increase of PET recycled resin in the system by reducing either waste during PCB collection or yield loss in the recycling. The results implied that larger potential environmental benefit could be achieved by increasing yield efficiency in the recycling process than by improving the PCB collection system.

Secondly, a meta-analysis was performed to review the LCA literature on the PET bottle system using a harmonization process and statistical assessment. The goals were to evaluate the

variation of the environmental impact in each life cycle stage of the PET bottle system, and to identify the source of variation by using global warming potential (GWP) and energy consumption (EC) impact indicators. Based on the statistical assessment results, the largest contribution to GWP and EC indicators was found from bottle grade PET resin production. The largest variation of GWP and EC indicators was for incineration of plastic waste due to a large variation in electricity efficiency for energy recovery from the incineration facility. This implied that the environmental performance of the PET bottle could be improved by optimizing the electricity recovery efficiency.

Lastly, a system dynamics and LCA approach was preliminarily employed to conduct a dynamic environmental assessment of the GWP of PET bottles in the state of California. The goals were to conduct a contribution analysis of the historical LCA of the PET beverage bottle system and to evaluate the impact of recycled PET (RPET) content and crude oil price over time on the PET beverage bottle in terms of CO₂ tax (\$/ton) and GWP. Approximately 67% of total GWP was contributed by the upstream phase of the PET beverage bottle system from 1988 to 2013. The effect of RPET content was more significant than the effect of crude oil price on the CO₂ tax (\$/ton) and GWP. By increasing from 20% to 60% and 60% to 100% of RPET content in the PET bottle, the expected CO₂ tax (\$/ton) saving was an average of 3.24 and 1.98 million dollars and 0.81 and 0.5 billion kg CO₂ eq., respectively.

Overall, this dissertation presented a methodology to construct a dynamic LCA model of PET bottles in California and the U.S., and can be used as a model to inform future studies of packaging systems.

Dedicated to my family

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KEY TO ABBREVIATIONS

aLCA	Attributional life cycle assessment
cLCA	Consequential life cycle assessment
CO ₂	Carbon dioxide
CRV	California refund value or California redemption value
EC	Energy consumption
GWP	Global warming potential
ISO	International organization for standardization
LCA	Life cycle assessment
LCI	Life cycle inventory analysis
LCIA	Life cycle impact assessment
MFA	Material flow analysis
MRF	Material recovery facility
MSW	Municipal solid waste
PCB	Post-consumer PET beverage bottle
PDCA	Plan-Do-Check-Act
PET	Polyethylene terephthalate
PP	Polypropylene
RPET	Recycled polyethylene terephthalate
VPET	Virgin polyethylene terephthalate

Chapter 1. INTRODUCTION

1.1 Motivation

Since 1970s, the awareness of sustainability has gradually increased due to population growth and natural resource depletion. The United Nation's population report predicted that 11 billion people will be on earth in the year 2100 – assuming fertility in all countries converges eventually toward a level of 1.85 children per woman (UN 2013). In the report, *The Limits to Growth: A Report to The Club of Rome* (Meadows *et al.* 1972), if the growth trends of the time in world population, industrialization, pollution, food production, and resource depletion continued unchanged, the limits to growth and sustain population on this planet would be reached sometimes between 2010 and 2050 (Figure 1-1). Although outdated and despite criticism for its lack of real world reflection, it produced enough awareness to rethink our life style on this planet and the use of resources.

Crude oil supplied approximately 40% of the US energy need in 2012. In 2012, the US consumed 18.9 millions of barrels of petroleum products and direct combustion of crude oil and represents the number one country for petroleum consumption in the world (US EIA 2013).¹

¹ A 42-US gallon barrel of crude oil is equal to about 45 gallons of petroleum products, such as gasoline, heating oil and diesel fuel, petrochemical feedstock and jet fuel in 19%, 12%, 7% and 4%, respectively US EIA (2013). International Energy Statistics. Independent Statistics & Analysis. Energy Information Administration.

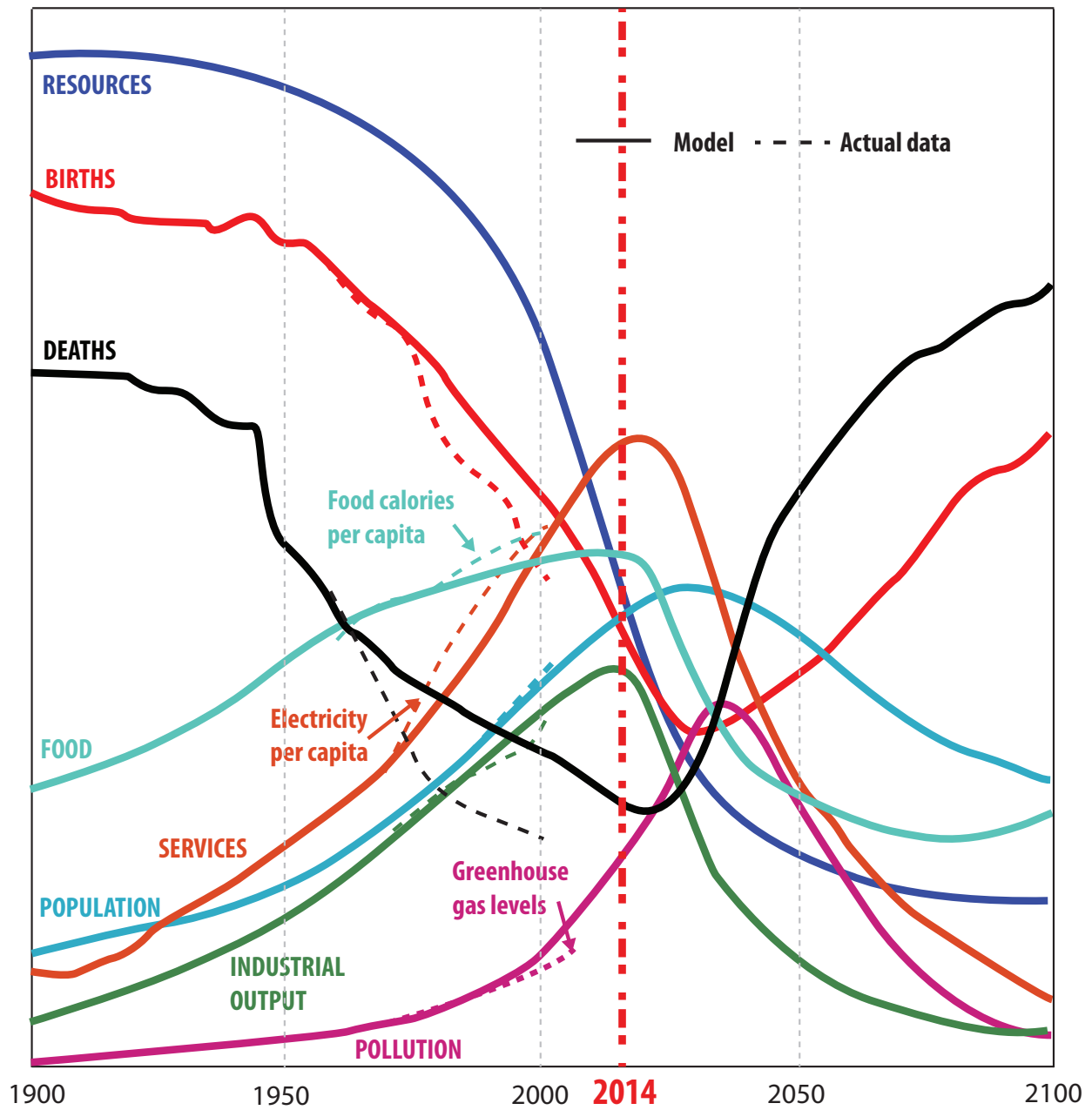


Figure 1-1. World 3 model simulation (Meadows *et al.* 2004)

One of the important applications of crude oil is petrochemical feedstock, especially for plastics. Polyethylene terephthalate (PET) is the number one plastic used in beverage packaging. In 2013, approximately 29% of total global beverage packaging is expected to be made of PET (Euromonitor International 2009). In 2012 in the US, 5.5 billion pounds of PET bottles were used with a 30% gross recycling rate (NAPCOR 2012). Because of its large share in the beverage market, it also generates a lot of municipal solid waste. About 30% of municipal solid waste (MSW) is made by containers and packaging, and 4% belonged to PET bottles and jars in 2011 in the US (US EPA 2013).

Among the fifty US states, California generated the largest amount of MSW in 2008, reporting approximately 40 million tons (Cascadia Consulting Group 2009; Haaren *et al.* 2010). Thus, the state of California has a large motivation to reduce the amount of plastics, specially PET, that is sent to landfill. Furthermore, the state of California consumes and recycles the largest numbers of bottles and cans in the US (CalRecycle 2013). With 2,400 certified recycling centers, hundreds of curbside recycling programs and the initiative of the California Beverage Container Recycling Litter Reduction Act, 70 percent of PET beverage bottles were recycled out of approximately 9 billion units sold in 2012 (CalRecycle 2013). So, the geographical boundary of this study is the state of California.

In this study, the environmental burdens of the life cycle of PET beverage bottles in the state of California was modeled and evaluated by different techniques. The following structure is established for this study. In chapter 2, a detailed literature survey summarizes sustainability, industrial ecology, market dynamics of PET beverage bottles and life cycle assessment (LCA). In chapter 3, LCA is used to evaluate the environmental burden of non-alcoholic single serve PET beverage bottles (PET bottles) in California. In chapter 4, a meta-analysis is presented using

a harmonization process and statistical assessment to evaluate the variation of the environmental impact in each life cycle stage of the PET bottle system. In chapter 5, system dynamics and LCA approaches were preliminarily employed to evaluate the GWP of PET bottles in the state of California and to evaluate the effect of RPET content in PET bottles and crude oil price over time on CO₂ tax (\$/ton) and GWP.

1.2 Objectives

The objectives of this dissertation are:

1. To evaluate the environmental burden of PET bottles in the state of California, and to seek options to improve the environmental performance of PET bottles (Chapter 3).
2. To review the LCA literature for PET bottles, and to evaluate the variation of the environmental burden for each life cycle stage of PET bottles (Chapter 4).
3. To construct a dynamic environmental assessment of PET bottles using system dynamics and LCA approaches, and to assess the effect of RPET content in PET bottles and crude oil price over time on CO₂ tax (\$/ton) and GWP (Chapter 5)

1.3 Structure of dissertation

Figure 1-2 shows the structure of this study, which consists of 3 parts. Chapter 3 is an LCA of the non-alcoholic single serve PET beverage bottle system in California. The results of the first study provided an LCA model of the environmental profile of PET bottles in 2010 in California, which is then used for chapter 5. Chapter 4 collects and classifies the existing LCA studies for the PET beverage bottle system using meta-analysis. The results of this second study, global warming potential estimates and probability distribution of each life cycle stage, is then used in chapter 5. Chapter 5 combines system dynamics and LCA approaches to construct a dynamic model of the GWP of PET bottles over time in California.

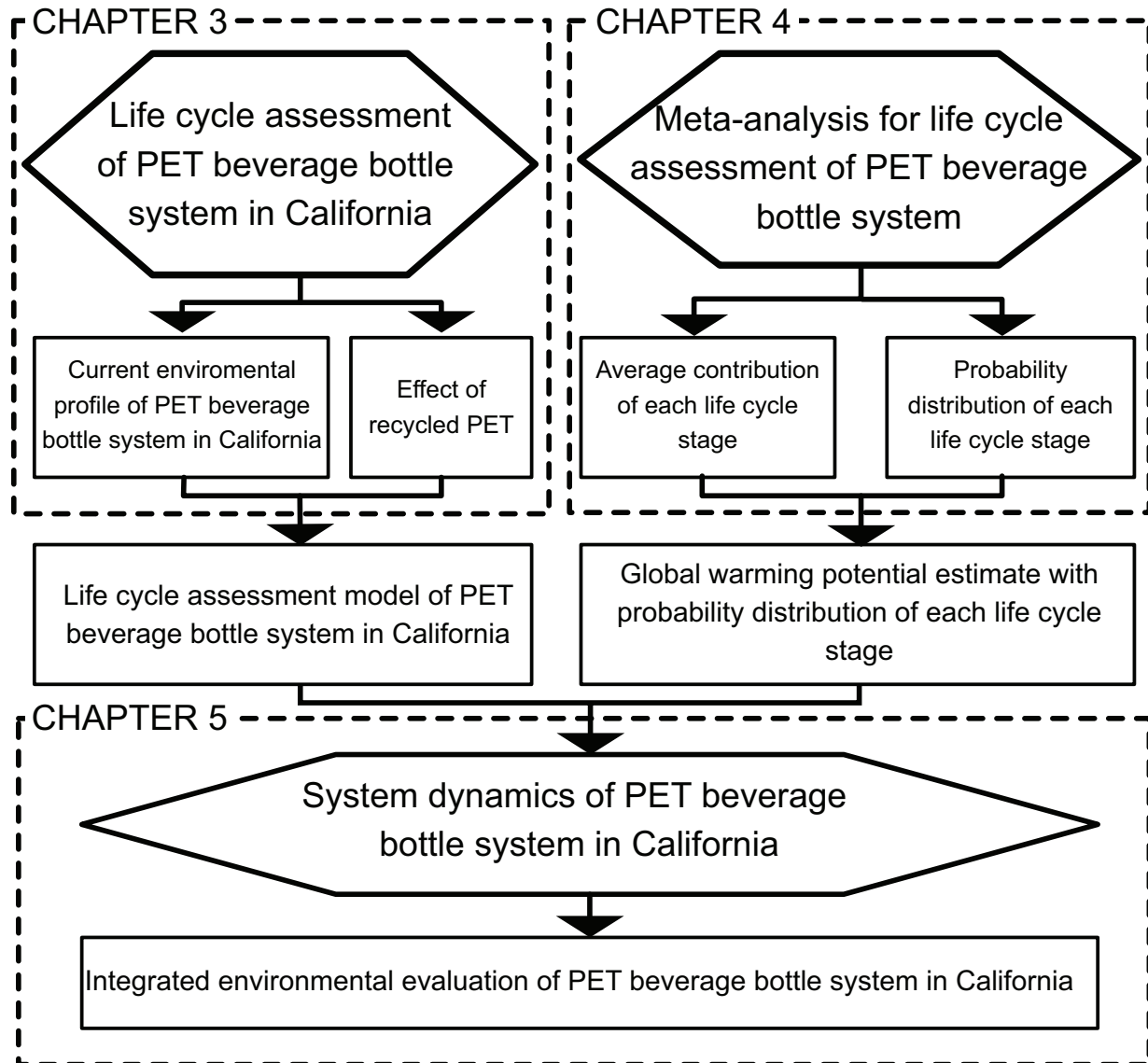


Figure 1-2. Structure of this stud

Chapter 2. LITERATURE REVIEW ²

2.1 Sustainability

Notwithstanding its importance, sustainability has been called one of the least meaningful and most overused words in the English language (Owen 2011). The concept of sustainability has evolved since 1972, when the international community first explored the connection between quality of life and environmental quality at the United Nations Conference on the Human Environment in Stockholm (Sohn 1973).

Over the course of nearly three decades, sustainability has been established on the three pillars of Society, Ecology, and Economy, also known as the “triple bottom line” (Thiele 2013). As illustrated in Figure 2-1, the concept of sustainability attempts to balance ecological health, economic welfare, and social empowerment. Balancing these three ideals does not mean that they all can be optimized at the same time. In order to pursue them in tandem, compromise among them is inevitable.

² Part of chapter 2 was submitted as a chapter titled “Sustainable Food Packaging” in the book “Introduction to Food Packaging” and currently is under review and resubmit.

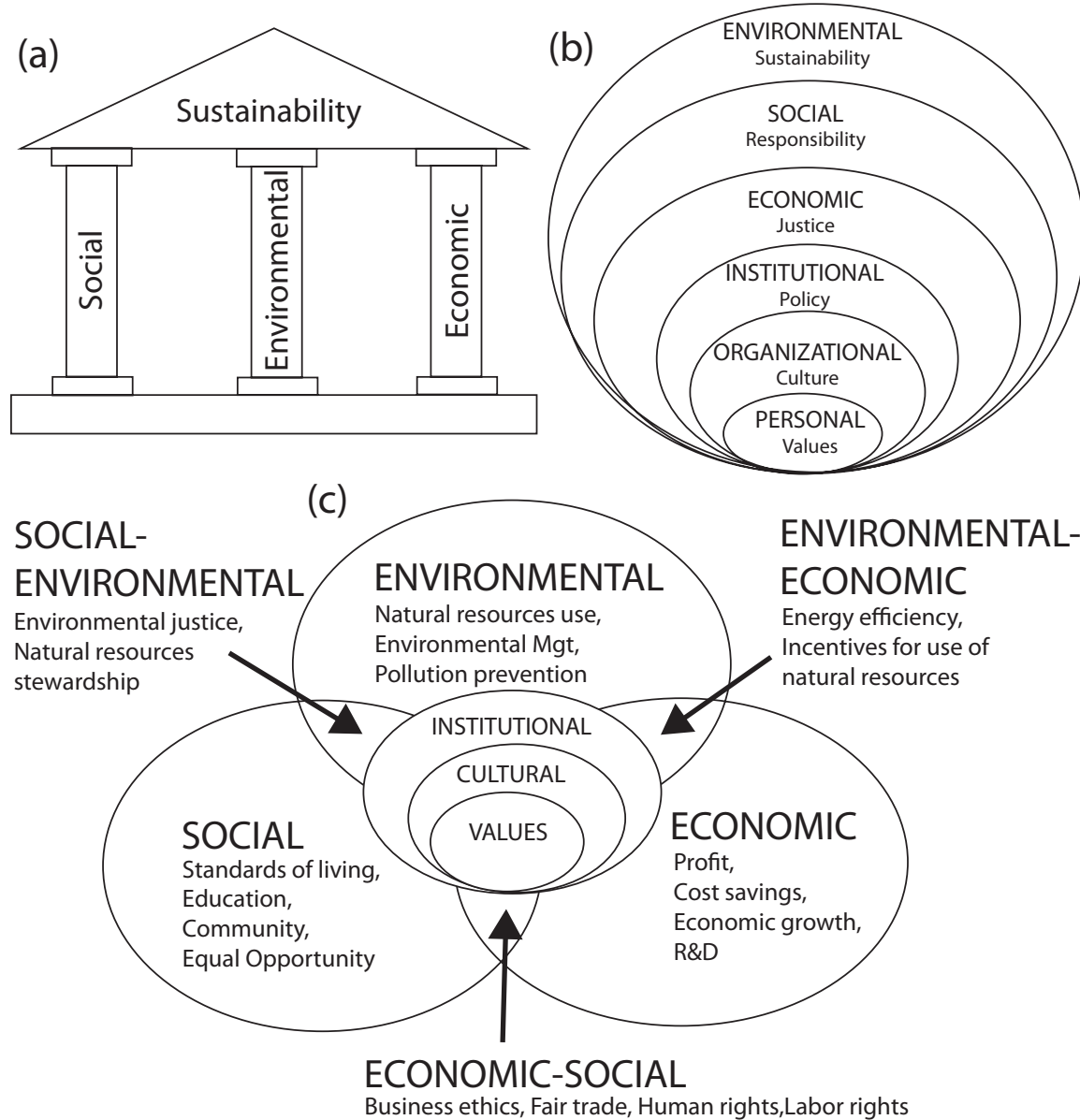


Figure 2-1. Schematic diagram of sustainability a) Three pillars of sustainability (Wilford 2013)
 b) Concentric sustainability framework (Tavanti 2010a) c) Three spheres of sustainability (Tavanti 2010b)

2.1.1 Brief history of Sustainability

The term sustainability has been widely used around the world over several decades. It has been transformed from a desirable concept to “the triple bottom line”. The concept of sustainability is rooted in the debates and events that shaped the environmental movement. The earliest environmental studies dealt with management of natural resources sustainably. In the sixteenth century, human populations began to cause significant impacts on ecological systems due to the economic exploitation of natural resources (Weddell 2002). During the sixteenth and seventeenth centuries of colonization and settlement of new lands, natural resource depletion increased to keep up with growing populations, agricultural needs, and industrial development, which led to a growing awareness of intentional management of natural resources.

Two core ideological perspectives of natural resource management are conservation and preservation. Conservation denotes the use of natural resources, while it simultaneously considers the biological limits of a resource. From the sustainability perspective, sustainable yield is a term closely tied to conservation. The concept was developed due to the concern over deforestation of Germany in the 1700s (Table 2-1). At that time, this term was outlined in a book of forest management in the limited sense for natural habitat and forest conservation. Unlike exploitation, conservation includes both a consumption aspect and a protection quality. That is, conservation is concerned with how much of a resource may be used for human consumption without eliminating the resource itself (Farley *et al.* 2013).

Preservation, on the other hand, focuses on saving the resource rather than using it. It is defined as the non-use or the non-consumption use of a resource (McManus *et al.* 2000). It emphasizes the potential inherent value of the resource. That is, preservation saves certain

resources for aesthetic and/or biodiversity reasons that go beyond the consumptive value of the resource.

Then, the transcendentalist movement of the 1800s emphasized the connection between humans and nature. As Emerson stated, “*The Transcendentalist adopts the whole connection of spiritual doctrine. He believes in miracle, in the perpetual openness of the human mind to new influx of light and power; he believes in inspiration, and in ecstasy.*”(Edwards 2005).

The preservation, conservation and transcendentalist movement acted as precursors for the modern sustainability concept. In the early twentieth century, preservation and conservation were the primary approaches to natural resource management. During this time, articles and books by Gifford Pinchot and John Muir were published such as *Our National Parks* (Muir 1901), *The Yosemite* (Muir 1912) and *The Fight for Conservation* (Pinchot 1910). The publication of those books and articles were watershed events, giving rise to conservation and preservation ideologies.

Several decades later, in 1972, the concept of sustainability was expanded from isolated practices to the global system as expressed in the book, *The Limits to Growth* (Meadows *et al.* 1972). The authors examined the impact of increasing human populations on pollution and natural resource consumption. This book has been the best-selling environmental book ever written, with 30 million copies distributed. Also, in 1972, a landmark event in the history of modern environmentalism was held in Stockholm, Sweden, at the 1972 United Nations Conference on the Human Environment. It was a catalytic event to establish the numerous national environmental protection agencies, as well as the United Nations Environmental Programme (UNEP).

In 1987, the prominence of sustainability and sustainable development began to emerge in earnest when the United Nations' World Commission on Environment and Development, chaired by former Norwegian prime minister Gro Harlem Brundtland, published its report *Our Common Future* (Brundtland 1987). To this day, the most popular definition of sustainability comes from the pages of this report.

In the century preceding the World Commission, the emergence of sustainability in its modern form was established. With the publication of the Brundtland report, sustainability found its linguistic basis and moved into the main stream of governmental and scholarly interest. In the early 1990s, sustainability had become the “dominant global discourse of ecological concern”(Dryzek 1997). It was a major topic of the 1992 United Nations Conference on Environment and Development, the so-called “Earth Summit” held in Rio de Janeiro, Brazil, and gained global awareness again in the 2002 World Summit on Sustainable Development in Johannesburg, South Africa, and at the “Rio +20” Earth Summit in 2012 in Rio de Janeiro.

The sustainability movement stems from the conservation and preservation movements from the 19th century and the environmental movement of the 20th century. Over the course of several centuries, the idea that the protection of nature is most effectively achieved when economic development and social empowerment are simultaneously pursued is seeded in the contemporary concept of sustainability.

Table 2-1. Development of sustainability concept over time

Century	Year	Authority	Major ideas/events	Era
17 th	1627	Francis Bacon	Describing the creation of a utopian land (Bacon 1915)	Scientific revolution
18 th	1713	Hans Carl von Carlowitz	Outlining the methods for the sustainable use of forests (Von Carlowitz 2000)	Industrial revolution, French revolution
	1798	Thomas Robert Malthus	Essay on Population (Malthus 2013)	
19 th	1800s	B. Alcott, M. Fuller, Ralph W. Emerson	Describing the natural world as a source of guidance and a mirror (Edwards 2005)	Transcendentalist movement
	late 1800s	Gifford Pinchot	Developed a conservation ethic - Conservationism	
20 th	1901	John Muir	<i>Our National Park</i> (Muir 1901)	Environmental movement
	1912		<i>The Yosemite</i> (Muir 1912)	
	1949	Aldo Leopold	Land ethic (Leopold 1970)	
	1962	Rachel Carson	Investigating the impact of pesticides and other industrial chemicals (Carson 2002)	
	1972	Donella Meadows	The impact of populations, pollution, and resource consumption (Meadows <i>et al.</i> 1972)	Contemporary Environmentalism
		United Nations	Conference on the Human Environment in Stockholm, Sweden	
	1980	IUCN ¹	World Conservation Strategy (IUCN 1980)	Sustainability revolution
	1982	United Nations	Environmental Conference in Stockholm, Sweden	
	1987	Gro Harlem Brundtland	<i>Our common future</i> (Brundtland 1987) in the WCED ²	
	1992	United Nations	Environmental Conference in Rio de Janeiro – Earth summit	
21 st	2002	United Nations	Environmental Conference in Johannesburg – World summit	
	2012	United Nations	Environmental Conference in Rio de Janeiro – “Rio+20” Earth summit	

¹ the International Union for the Conservation of Nature and Natural Resources

² the World Commission on Environment and Development

2.1.2 Sustainable Development

According to Rogers et al. in 2008 there were approximately 60 definitions of sustainable development (Table 2-2). Among them, the most popular definition of sustainable development was described in the Brundtland Commission Report, which defined sustainable development as development that “*meets the needs of the present without compromising the ability of future generations to meet their own needs*”(Brundtland 1987).

Table 2-2. Sustainable development: Definitions, Principles, Criteria, Conceptual Frameworks, and Indicators, adapted from Rogers *et al.* 2008.

Subject	Number
Definitions	57
Principles	19
Criteria	12
Conceptual frameworks	4
Indicators	28 sets

Due to the many definitions, confusion was created regarding a standard definition. Because of this, the effort has been made to bring some order to establish a clear definition of sustainable development. As part of these efforts, the report *Our Common Journey: A Transition toward Sustainability* clarifies the relationship between what advocates and analysts sought to sustain and what they sought to develop, and the time horizon of the future used for the definitions (Table 2-3).

Table 2-3. Definition of sustainable development, adapted from National Research Council 1999

Values	For how long?	What is to be sustained?	What is to be developed?
Freedom	5, 10, 20, 50, 100 years, forever, etc.	(S1) Nature	(D1) People
Equality		Earth	Child survival
Solidarity		Biodiversity	Life expectancy
Tolerance		Ecosystems	Education
Respect for nature			Equity, Equal opportunity
Shared responsibility		(S2) Life support	(D2) Economy
		Ecosystem services	Wealth
		Resources	Productive sectors
		Environment	Consumption
		(S3) Community	(D3) Society
		Peace	Institutions
		Cultures	Social capital
		Groups	States
		Places	Regions

Sustainable development has three dimensions: economic, environmental, and social. As described in Figure 2-1, these are the three pillars of sustainability. It is critical to give equal attention to each component to ensure a sustainable outcome.

2.2 Industrial Ecology

The concept of industrial ecology began to appear sporadically in the literature of the 1970s. In the early stage the concept was used only to describe the regional economic environment of companies or used as a green slogan by some industrial lobbies in reaction to the creation of the US Environmental Protection Agency (Hoffman 1971, Erkman 1997). During the 1990s, industrial ecology re-emerged in the discussion to establish the relationship among the size of a population, the level of industrial and economic activity of that population, and the environmental impact of its industrial and economic activities. Further discussions of this

relationship led to the equation IPAT ($I = P \times A \times T$), explaining environmental impact as a function of population, affluence and technology. Such discussions have played an important role in generating widespread awareness of sustainability, eco-efficiency and breakthrough innovations in technology and consumption (Schmidheiny 1992, Von Weizsacker *et al.* 1997).

Robert White, the former president of the US National Academy of Engineering, defined industrial ecology as “*the study of the flows of materials and energy in industrial and consumer activities, of the effects of these flows on the environment, and of the influences of economic, political, regulatory, and social factors on the flow, use and transformation of resources*” (Allenby 1994). Raymond Cote, at Dalhousie University, compiled a number of definitions from the early literature on industrial ecology (Cote 2007). Despite the slightly different expressions of the industrial ecology definition, all authors more or less agree on at least three key elements:

1. It is a systemic, comprehensive, integrated view of all the components of the industrial economy and their relations with the biosphere,
2. It emphasizes the biophysical substratum of human activities,
3. It considers technological dynamics, *i.e.*, the long-term evolution of clusters of key technologies as a crucial element for the transition from the actual unsustainable industrial system to a viable industrial ecosystem (Erkman 1997).

2.2.1 Systems perspective of industrial ecology

Industrial ecology targets to support sustainable development through two operational objectives: closing material cycles, and realizing a fundamental paradigm shift in the thinking concerning industry-ecology relations (O'Rourke *et al.* 1996). This nature of industrial ecology takes into account the systems perspective in environmental analysis and decision-making. The systems orientation is manifested in several different forms: use of a life cycle perspective, use of

materials and energy flow analysis, use of system modeling, and sympathy for multidisciplinary and interdisciplinary research and analysis.

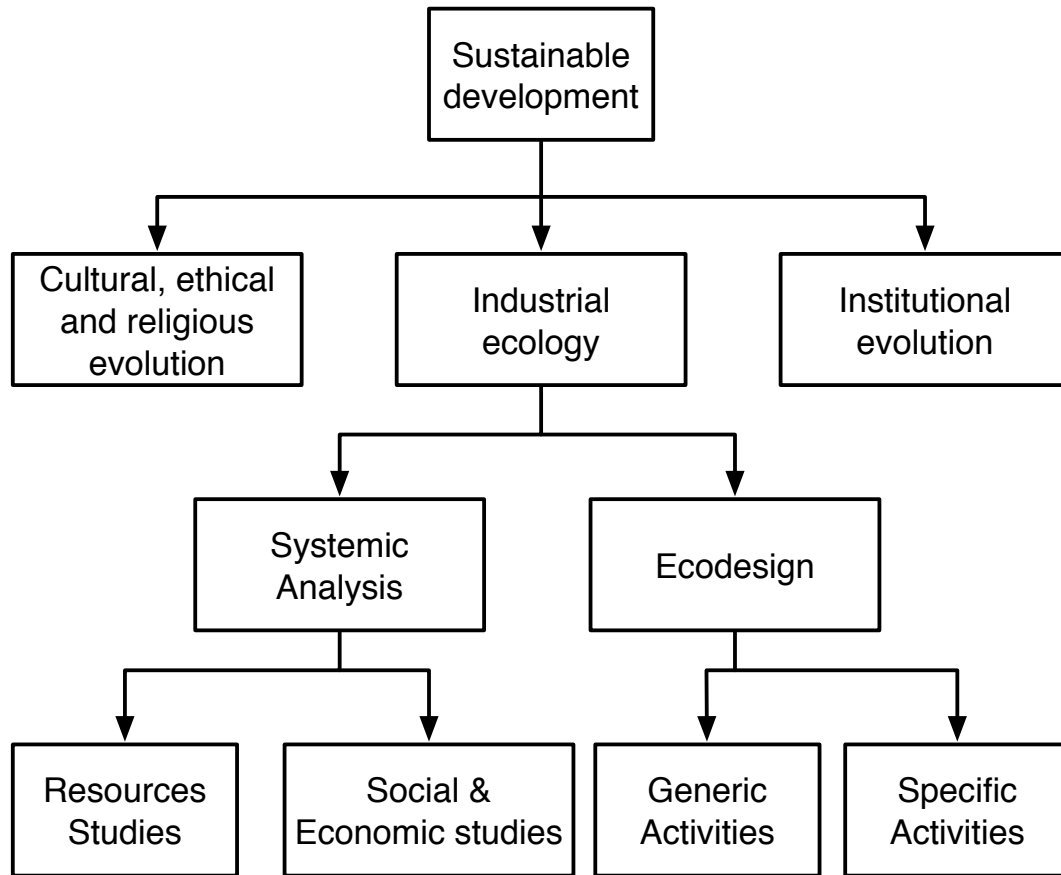


Figure 2-2. Industrial ecology conceptualized in terms of its system-oriented and application-oriented elements (Reid Lifset *et al.* 2003)

2.2.2 Material flow-related analysis

Material flow analysis (MFA) is defined as the analysis of the throughput of process chains including extraction or harvest, chemical transformation, manufacturing, consumption, recycling and disposal of materials (Bringezu *et al.* 2003). One of the basic strategies to describe the material flow analysis is detoxification. This refers to the mitigation of

the releases of critical substances to the environment by pollution reduction (Bringezu *et al.* 2003). It is converted to specific environmental impacts such as toxicity to human beings and other organisms, eutrophication, acidification, ozone depletion, global warming and so on. Another basic strategy considered is dematerialization. This refers to the absolute or relative reduction in the quantity of materials used and/or the quantity of waste generated in the production of a unit of economic output (Cleveland *et al.* 1998). Table 2-4 describes MFA as divided in two types based on their primary focus. The importance of the detoxification concepts seems highest in Ia and lowest in IIc. On the other hand, the importance of dematerialization is highest in IIc and lowest in Ia. Type I is conducted from a technical engineering perspective, whereas type II analyses are more related to socioeconomic relationships.

Table 2-4. Types of material flow-related analysis (Bringezu *et al.* 1997)

Type of analysis	I		
	a	b	c
Objects of primary interest	Specific environmental problems related to certain impacts per unit flow of:		
	Substances e.g. Cd, Cl, Pb, Zn, Hg, N, P, C, CFC	Materials e.g. wooden products, energy carriers, biomass, plastics	Products e.g. diapers, batteries, cars, bottles
	within certain firms, sectors, regions		
	II		
	a	b	c
	Problems of environmental concern related to the throughput of:		
	Firms e.g. single plants, medium and large companies	Sectors e.g. product sectors, chemical industry, construction	Regions e.g. total or main throughput, mass flow balance
	associated with substances, materials, products		

When the primary interest is to evaluate the environmental impact of certain products and processes as denoted in Ic, life cycle assessment (LCA) is the methodology to approach that interest.

In general, MFA has been considered as the analyses of types Ia, Ib, IIb and IIc. Type Ic has been fully defined by LCA. Type IIa is mainly related to environmental management. Despite their different primary interests, all of these analyses were designed to account for the material inputs and outputs of processes in a quantitative manner with a systems perspective (Bringezu *et al.* 2003).

2.3 Life Cycle Assessment (LCA)

Life Cycle Assessment (LCA) has continuously developed over the last three decades due to the increased demand for studying environmental impacts of consumer products and systems. Originally, LCA was developed to answer the comparative context (Product A is better than Product B). However, for many products, environmental impacts are mainly contributed by its production, transportation, or disposal, not by the use of products (Guinee *et al.* 2010). Gradually, the importance of evaluating the environmental impact of the life cycle of products became an issue in the 1980s and 1990s. Figure 2-3 shows that the number of articles using LCA has exponentially increased since 1992. The use of LCA is recommended as a core element in environmental policy or as a voluntary action in many countries such as the European Union, USA, Japan, Korea, Canada, Australia, India, and China (Guinee *et al.* 2010). With the popularity of LCA increasing, LCA has been applied in many areas: waste management, building materials, military systems, tourism, etc. LCA as a tool is still improving in many areas such as type of applications, breadth and depth.

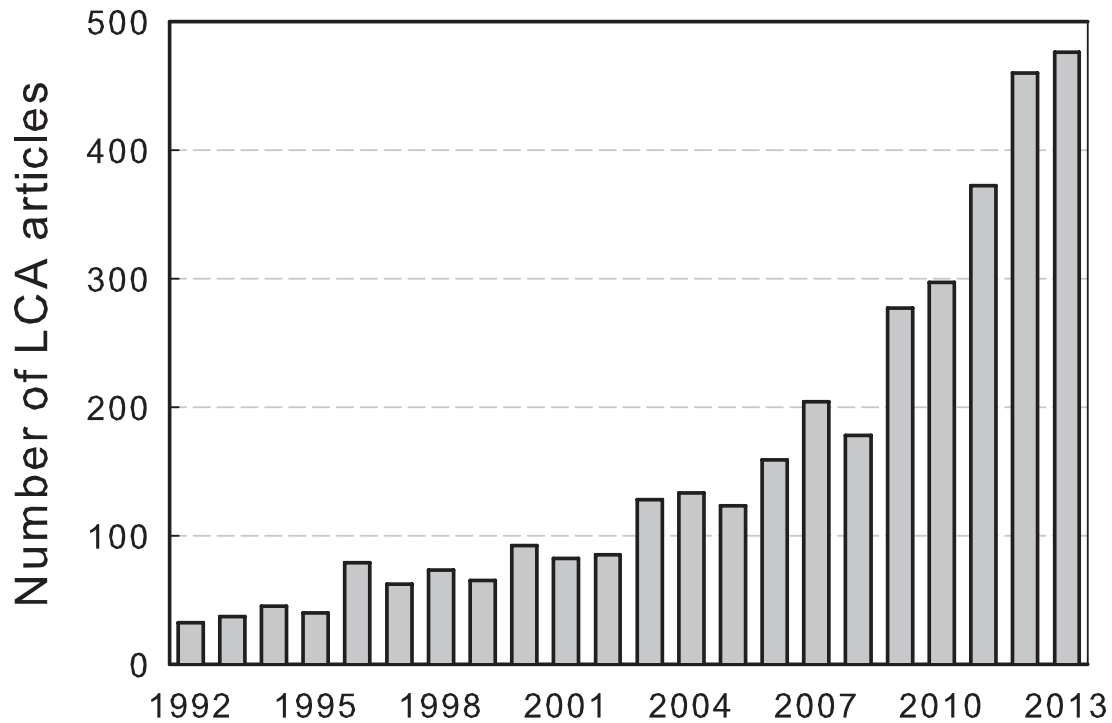


Figure 2-3. Histogram of the number of articles mentioning life cycle assessment from 1991 to 2013 (search on Web of Science on key word “life cycle assessment”, accessed January 10, 2014)

2.3.1 Structure of LCA

The International Organization for Standardization (ISO) has developed standards that help organizations to take a proactive approach to managing environmental issues: the ISO 14000 family of environmental managements standards which can be implemented in any type of organization in either public or private sectors (ISO 2010a). The ISO 1400 family is designed for a Plan-Do-Check-Act (PDCA) cycle, as illustrated in Figure 2-4. Although the ISO 14000 standards are designed to be mutually supportive, they can be also used independently of each other to achieve environmental goals (ISO 2010a). Life cycle assessment is implemented in the “Do” step of the PDCA cycle, as a tool to evaluate the environmental impacts of products or systems.

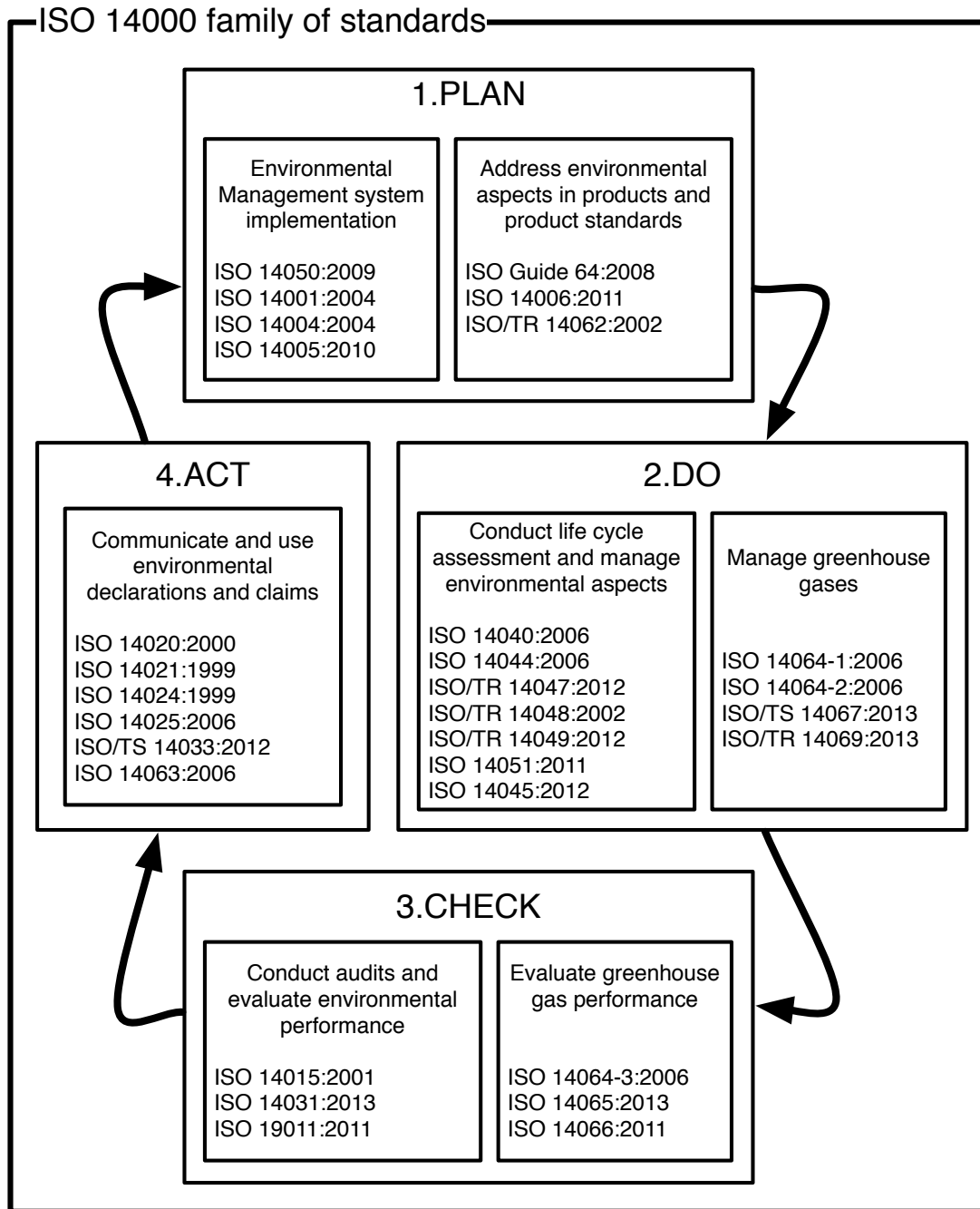


Figure 2-4. The ISO 14000 family and the Plan-Do-Check-Act (PDCA) cycle (ISO 1999a; b; 2000; 2001; 2002a; b; 2004; 2006a; b; c; d; e; f; g; 2008; 2009; 2010a; b; 2011a; b; c; d; 2012a; b; c; d; 2013a; b; c; d); DIS (Draft International Standard); TR (Technical Report); TS (Technical Specification); AWI (Approved Work item); WD (Working Draft); CD (Committee Draft)

Life Cycle Assessment (LCA) refers to the methodology to compile and evaluate the inputs, outputs and the potential environmental impacts of a product system throughout its life cycle (ISO 2006b). The LCA framework is made of four phases: Goal and Scope definition, Life Cycle Inventory analysis (LCI), Life Cycle Impact Assessment (LCIA) and Interpretation (Figure 2-5). Generally, LCA starts by defining the goal and scope, then proceeds to the inventory analysis, then continues to the impact assessment, and ends with the interpretation. All four phases are interconnected and performed iteratively.

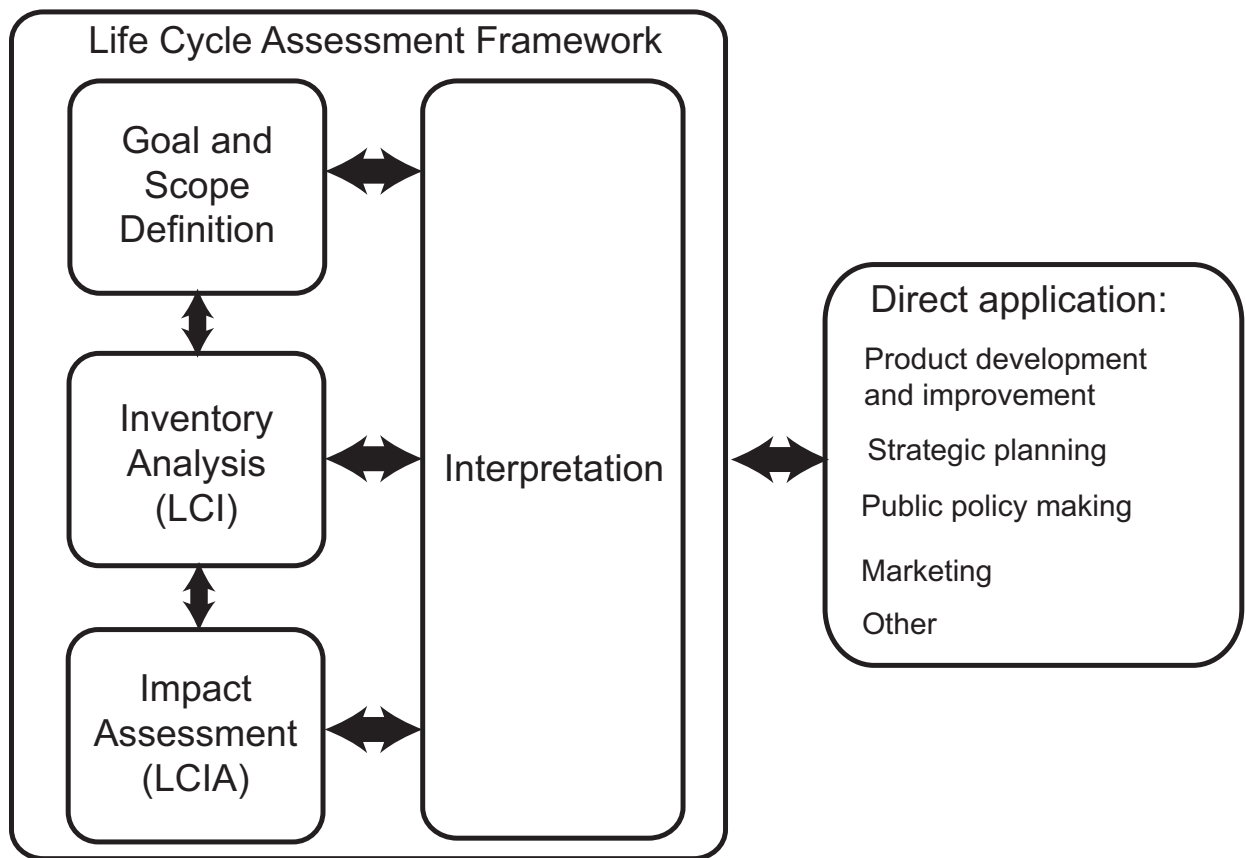


Figure 2-5. LCA framework (ISO 2006b)

2.3.1.1 Goal and Scope definition

The first step of a LCA study is the goal and scope definition. The goal of the LCA should contain the intended application, the reasons for carrying out the study, the intended audience, and whether the results are to be used in comparative assertions disclosed to the public (ISO 2006b). In the scope definition, the product system and its boundary are defined. The function of the product system delivered is also defined with the functional unit. The functional unit expresses the function of the products, and, thereby, offers a way to equalize differences in performance (Curran 2012). The scope definition further establishes the number of subjects that are discussed and further modified in more detail in the later phases. Those subjects are impact categories, treatment of uncertainty, assumptions, limitations, and data requirements (ISO 2006b).

2.3.1.2 Life Cycle Inventory analysis (LCI)

According to ISO, LCI is defined as the phase of the LCA involving the compilation and quantification of inputs and outputs for a product throughout its life cycle (ISO 2006b). The main concern of this step is the quantification regarding data collection and calculation. The unit process is the smallest element considered in the LCI, for which inputs and outputs are quantified (Curran 2012). That is, the sizes of the inflow and outflow need to be specified in the unit process. Two issues must be addressed to be able to process and simplify the unit process: cut-off and co-product allocation (Curran 2012). Cut-off is a solution to the problem that the system is theoretically infinitely large. Often, LCA studies can easily comprise several thousands of unit processes. For this reason, some inflows that are negligible contributions to mass or cost are cut-off based on criteria. Co-product allocation is a method to deal with some unit processes that produce not just one product but also several co-products. This is still a very controversial topic

in LCA theory. Many methods have been proposed to deal with this issue like system expansion or substitution. With proper cut-off and allocation steps, the final inventory results can be calculated. Table 2-5 describes some commercially and publically available databases for LCI.

Table 2-5. Some commercially and publically available databases

Database	Description
BUWAL 250	Inventory of packaging materials for the Swiss Packaging Institute, made by EMPA. The inventory includes emissions from raw material production, energy production, production of semi-manufactures and auxiliary materials, transport and the production process of the materials. (Pre Consultants 2004)
Ecoinvent 3.0	The Swiss centre for Life Cycle Inventories has combined and extended different LCI databases. The data are mainly investigated for Swiss and Western European conditions. The Ecoinvent database contains about 4100 datasets of products and services from the energy, transport, building materials, chemicals, pulp and paper, waste treatment and agricultural sectors. Updated version of Ecoinvent 2.2. The inventory is separated into the product names and activity (process) names. (Weidema <i>et al.</i> 2013)
US-EI 2.2	The US Life-Cycle Inventory (LCI) database contains data modules that quantify the material and energy flows into and out of the environment for common unit processes. This dataset was created to bridge the current gap in US LCI data. The US LCI database has some serious gaps in both the existing processes and in the broader context of typical raw materials and processing occurring in the US. To overcome those limitations, Ecoinvent data has been modified, replacing Swiss and general European electricity with US electricity as appropriate. In addition, the formerly empty processes have been filled with the appropriate proxy data from Ecoinvent. (Sylvatica 2009)

2.3.1.3 Life Cycle Impact Assessment (LCIA)

LCIA is the phase of life cycle assessment aimed at understanding and evaluating the magnitude and significance of the potential environmental impacts for a product system throughout the life cycle of the product (ISO 2006b). It stems from two issues: 1. The final result of the inventory analysis is too long, 2. The inventory table contains many items that require expert knowledge. At the LCIA phase, the LCI results are converted to common units, and an aggregation of the converted results are reported within the same impact category. This conversion process follows several phases, depending on the level of detail required in the study. Those phases are classification, characterization, normalization, grouping and weighting. Generally, classification and characterization are the core LCIA phases contained in ready-made impact assessment methods, such as IMPACT 2002+, TRACI, CML, ReCiPe, etc. (Table 2-6). All these methods comprise a recommended set of impact categories with a category indicator and set of characterization factors. Table 2-6 describes an overview of some often-used impact categories and category indicators.

In the classification phase, the LCI results are sorted and assigned to the various impact categories. After classification of the LCI results, the sizes of the environmental impacts are calculated per category using characterization factors defined while modeling the cause-effect chains (Baumann *et al.* 2004). The definition of characterization methods with suitable characterization factors is in principle based on the physico-chemical mechanisms of how different substances contribute to the different impact categories (Baumann *et al.* 2004).

Table 2-6. Commonly used impact categories (Curran 2012)

Impact Category	Midpoint Category	Endpoint Category
Climate change	Infra-red radiative forcing	loss of life years, fraction of disappeared species
Ozone layer depletion	change in tropospheric ozone concentration	loss of life years
Acidification	H ⁺ concentration	fraction of disappeared species
Eutrophication	biomass potential	fraction of disappeared species
Human toxicity	time-integrated exposure	loss of life years
Ecotoxicity	time-integrated exposure	fraction of disappeared species
Depletion of energy carriers	primary energy requirement	decreased availability
Depletion of material resources	amount of material used	decreased availability
Land use impacts	amount of land occupied	fraction of disappeared species
Water use impacts	amount of water used	decreased availability

Figure 2-6 illustrates the characterization phase. After the classification phase for each emission is generated from each inventory process, the emissions are multiplied by a suitable characterization factor and converted to an amount of a common reference substance that contributes to the same impact category. Each of the emission impacts after the conversion is summed up to the impact indicator category.

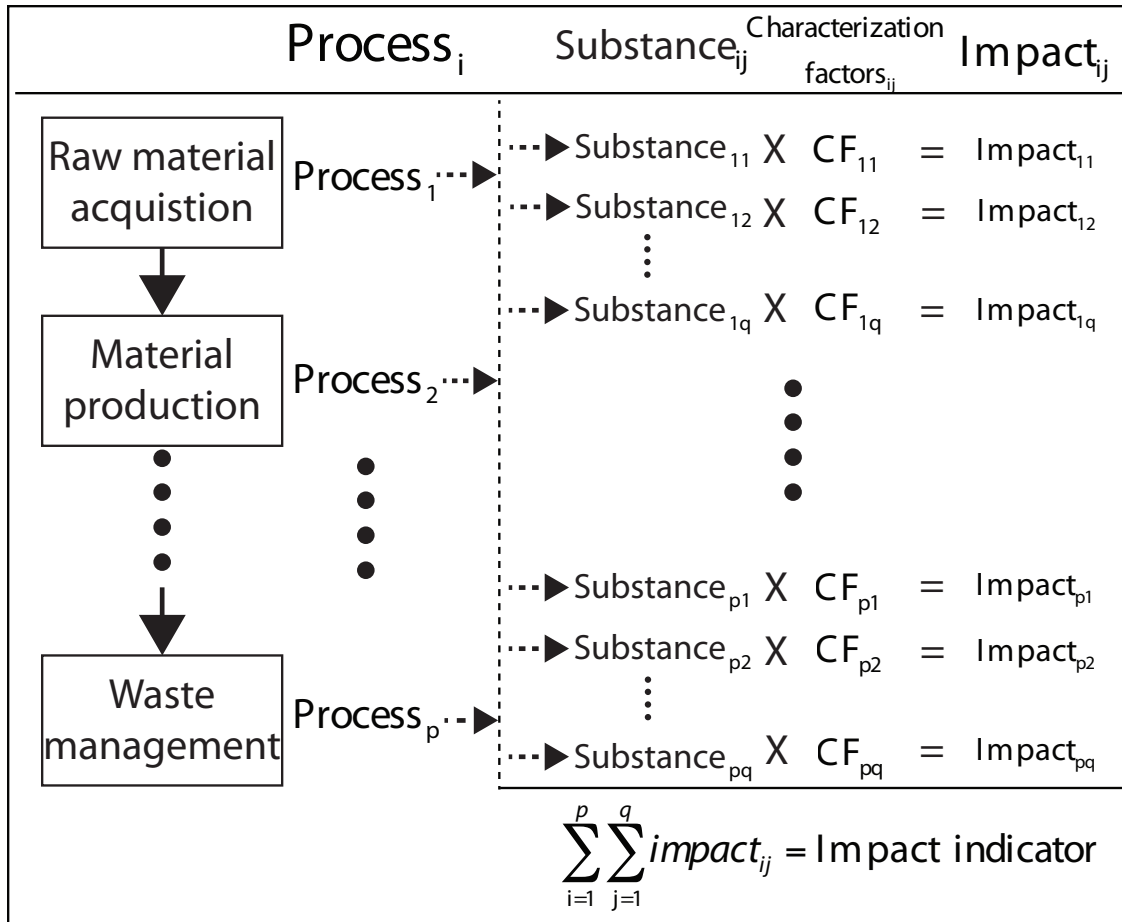


Figure 2-6. Example of LCI to LCIA conversion

2.3.1.4 Interpretation

According to ISO, interpretation is defined as the phase of life cycle assessment in which the findings of either the inventory analysis or the impact assessment, or both, are evaluated in relation to the defined goal and scope in order to reach conclusions and recommendations (ISO 2006b). According to Heijungs and Kleijn (2001), they introduced a distinction between the procedural and numerical approaches of interpretation. The procedural approaches include all types of analysis that deal with the data and results in relation to other sources of information, whereas numerical approaches use algorithms to produce indications of reliability, key issues,

discernibility, robustness, and so on. Table 2-7 provides an overview of five numerical approaches to life cycle interpretation.

Table 2-7. Numerical approaches to life cycle interpretation (Heijungs *et al.* 2001)

	One product alternative	More than one product alternative
Without uncertainty estimate	Contribution analysis Perturbation analysis	Comparative analysis
With uncertainty estimate	Uncertainty analysis	Discernibility analysis

Contribution analysis, also known as dominance analysis, decomposes the aggregated results of inventory analysis, characterization, normalization or weighting into a number of constituent elements (Heijungs *et al.* 2001). For example, the PET beverage bottle system can be decomposed into material production, bottle production, transportation, collection and waste management to identify the dominant life cycle stages in the PET beverage bottle system.

Perturbation analysis, also similar to a sensitivity analysis, explores the sensitivity of a calculation result (Heijungs 1994). The main aspect of this analysis is that small perturbations of the input parameters propagate as smaller or larger deviations of the resulting output, which will provide knowledge about what specific parameters lead to large deviations or small deviations. For example, in the PET beverage bottle system, the recycling amount for post-consumer PET beverage bottles may be perturbed to see if it is a significant parameter.

As the name implies, comparative analysis lists the LCA results for different product alternatives simultaneously. The environmental burden comparison of PET beverage bottles and aluminum cans is an example of comparative analysis.

Generally, an LCA study is composed of several thousand input parameters, which have uncertainty in nature. Uncertainty analysis analyzes the uncertainty of those input parameters. That is, it is a systematic study of the propagation of input uncertainties into output uncertainties (Heijungs *et al.* 2001). To assess the variation and the uncertainty of those parameters, Monte Carlo simulation is generally applied. Monte Carlo simulation is a method that replaces point estimates with random variables drawn from probability density functions (LaGrega *et al.* 2010). Generally, the probability distribution function of point estimates is determined by a pedigree matrix in LCA (Bo 1998).

The discernibility analysis stems from the desire to combine the comparative analysis and the uncertainty analysis, which need a Monte Carlo simulation. By using this analysis, statistical comparisons can be made such as ‘product A has a 95% chance of being better than product B’. In other words, rather than evaluating the uncertainty of certain input parameters, discernibility analysis estimates the difference between two products or two scenarios with respect to the selected item, such as an impact indicator or emission.

2.3.2 Attributional (aLCA) and consequential LCA (cLCA)

In the context of LCA, multi-functional processes are included in the analyzed system. Eventually, a choice of how to handle co-products is inevitably connected with performing an LCA. Thus, two main principles are frequently applied in parallel: the attributional LCA and the consequential LCA. The term consequential was first used in a workshop in 2001 (Curran *et al.* 2005), inspired by the suggestion of Frischknecht (Frischknecht 1998) and Tillman (Tillman 2000) that two very distinct perspectives of LCA exist: attributional LCA (aLCA) and consequential LCA (cLCA). The distinction between aLCA and cLCA was developed in the

process of resolving the methodological debates over allocation problems and the choice of data (Thomassen *et al.* 2008). Attributional modeling, also known as accounting, book-keeping, retrospective or descriptive, depicts its actual or forecasted specific or average supply-chain with its use and end-of-life value chain (Joint Research Centre 2010). That is, aLCA includes the potential environmental impacts that can be attributed to a system over its life cycle (Joint Research Centre 2010). On the other hand, consequential modeling, also called change-oriented, effect-oriented, decision-based or market-based, models the analyzed system around consequences (Joint Research Centre 2010). In other words, the cLCA is not based on the actual specific or average supply-chain, but on a hypothetical generic supply-chain that is forecasted along market mechanisms, political interactions and consumer behavior changes (Joint Research Centre 2010). Another way to describe the cLCA is that it represents the convergence of LCA and economic modeling methods (Earles *et al.* 2011). Because economic modeling affects national policy-making and strategic environmental planning, incorporating LCA with economic models is of growing importance (Earles *et al.* 2011). Figure 2-7 illustrates the system boundary of PET beverage bottles in aLCA and cLCA.

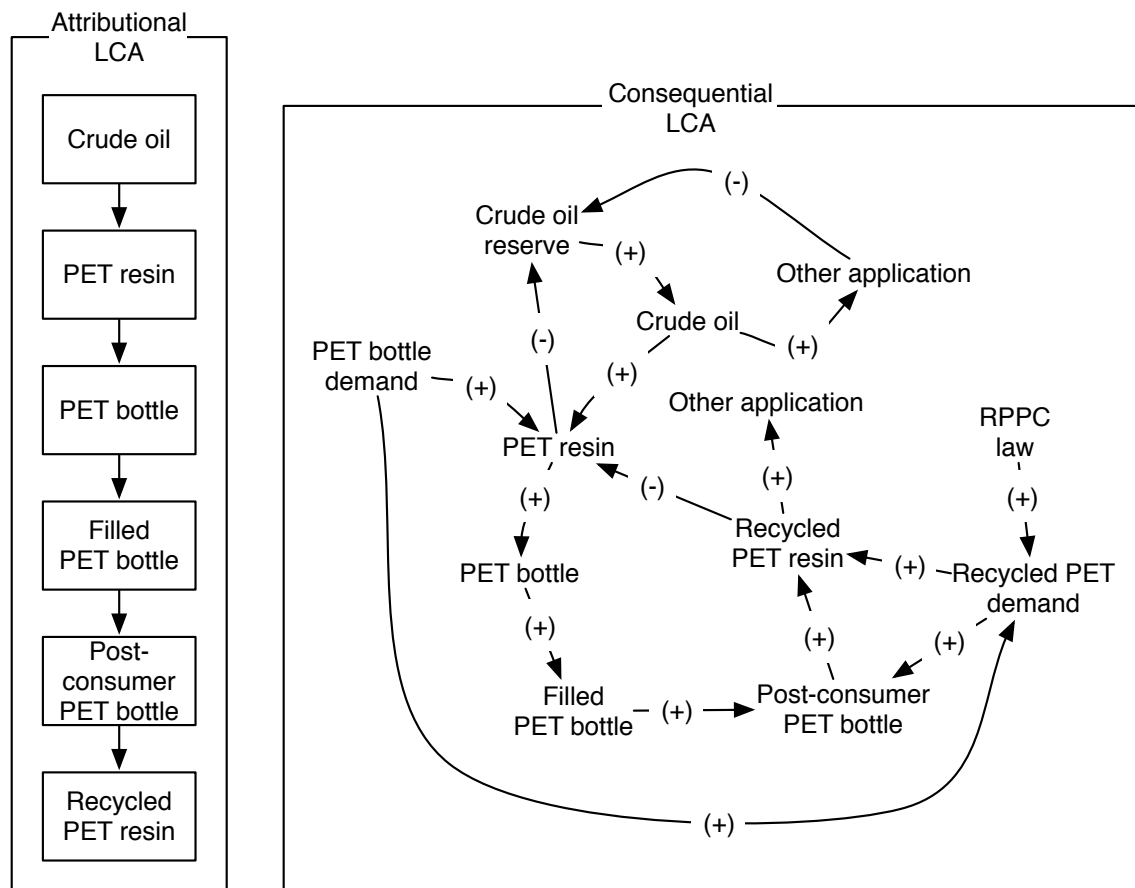


Figure 2-7. Example of aLCA vs cLCA

2.4 Beverage bottle markets

Packaging has four basic functions: containment, protection, communication and utility. One of the definitions of packaging is “A form that is intended to contain, protect/preserve, aid in safe and efficient transport and distribution, and finally act to inform and motivate a purchase decision on the part of a consumer.” (Soroka 2009). According to the Euromonitor International market database (Euromonitor International 2013d), 4144 billion units of packaging were sold in 2013 in the categories of beauty and personal care, beverages, dog and cat food, food, home care, tissues and hygiene and tobacco goods. Based on Figure 2-8, global packaging decreased between 2012 and 2013 due to the decrease of tobacco packaging units. On the other hand, beverage packaging has gradually increased with an average 3.1% growth rate.

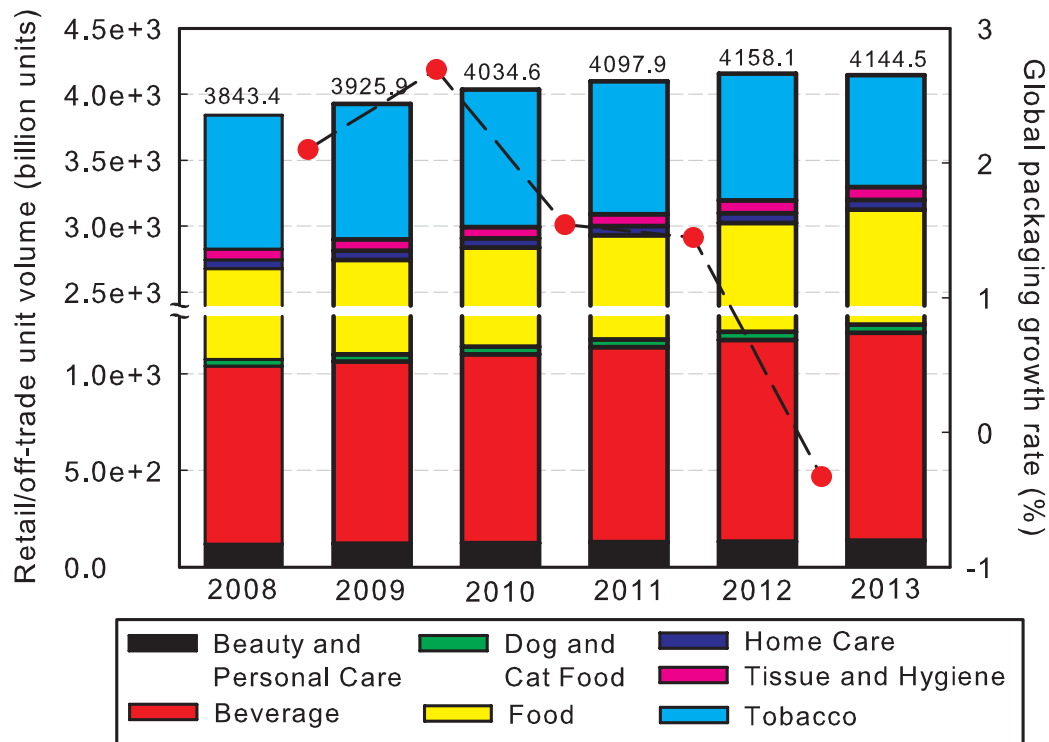


Figure 2-8. Global packaging breakdown from 2008 to 2013 (Euromonitor International 2013d)

2.4.1 Global beverage market

The second largest packaging market is beverage packaging, after food packaging. According to the Euromonitor International market database (Euromonitor International 2013c), 214 billion units were used for beverage packaging in 2013. As shown in Figure 2-9, beverage packaging can be categorized based on beverage and package type. PET beverage bottles are mainly used for soft drinks and are the most popular plastic for the beverage industry.

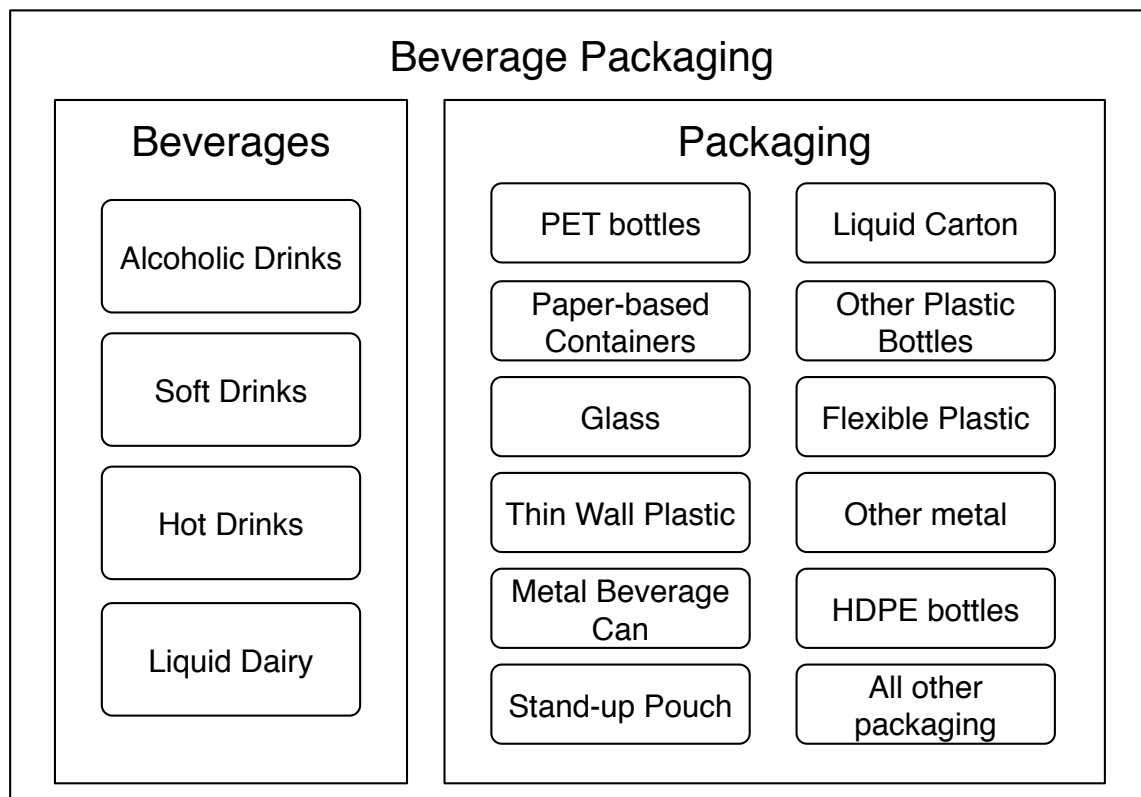


Figure 2-9. Beverage packaging category

Figure 2-10 illustrates the retail beverage packaging market by region. The numbers on top of the bars indicate the number of billion units of beverage packaging sold. Asia consumed the largest amount of beverage packages in the world, which can be expected due to their population density. The second largest market was North America. Globally, metal beverage cans are the largest portion of the market, especially in North America, representing over 40% of the total beverage container market. PET beverage bottles were reported as the second largest type of beverage package in most regions, except Australasia, the Middle East and Africa.

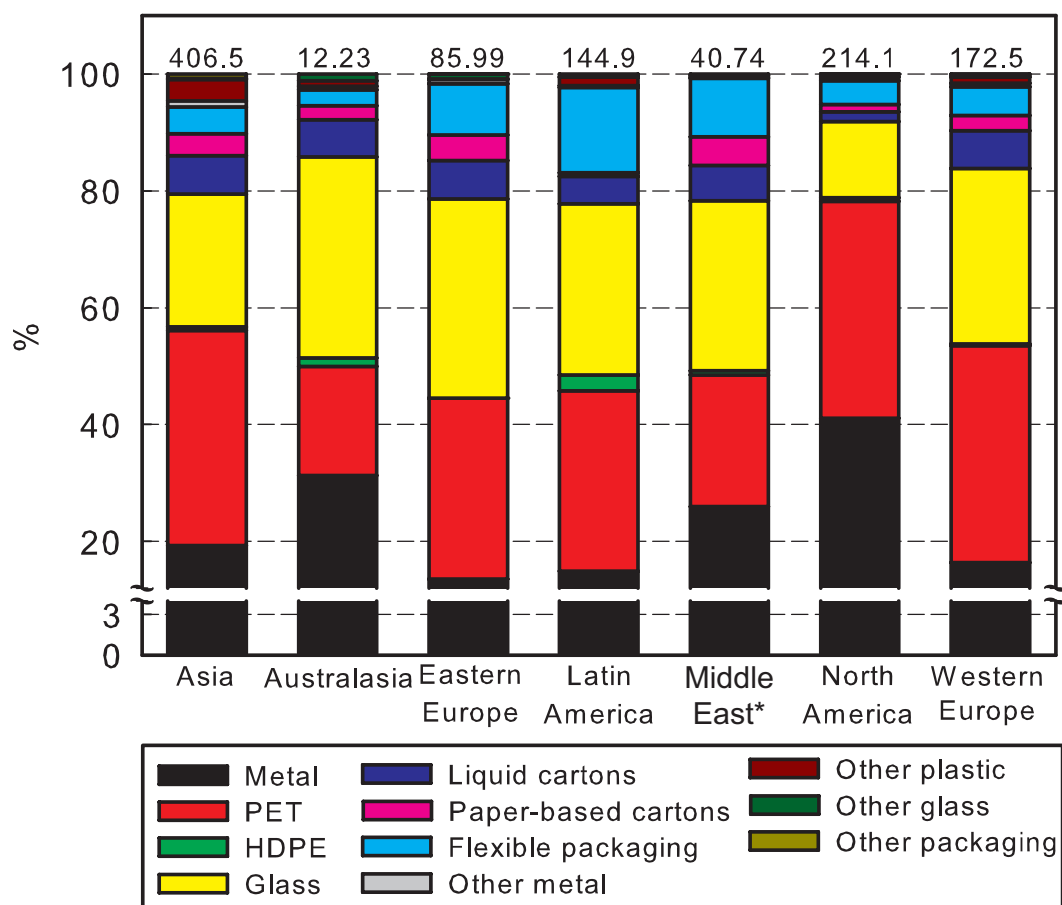


Figure 2-10. Beverage packaging market breakdown by region: % volume 2013 (Euromonitor International 2013a) *Middle East includes Africa

As illustrated in Figure 2-11, the highest percent growth in the beverage packaging market was observed in Asia. This is attributed to the emerging economies that are key to both current and forecast growth as consumer-spending power strengthens, retail infrastructure develops and subsequent consumption of packaged beverages rises. On the other hand, North America, Eastern Europe, Western Europe and Australasia were saturated market for beverage packaging due to the global financial crisis and lack of strong consumption growth opportunities.

2.4.2 Beverage market in North America

The beverage market in North America has been relatively unchanged since 2008 due to the decreased sales of carbonated drinks (Euromonitor International 2010). As shown in Figure 2-12, North American beverage packaging sales amounted to 214.1 billion units in 2013, slightly up from 2012. Metal beverage cans suffered the most from the falling consumption of carbonated drinks, especially in the US, with the metal beverage can share of total retail beverage packaging sales falling from 44% in 2008 to 41% in 2013 (Euromonitor International 2010). Liquid carton volumes also declined due to the decrease of liquid dairy sales. In contrast, PET beverage packaging continued to grow, especially for bottled water, functional drinks and Ready-To-Drink (RTD) tea (Euromonitor International 2010). It is expected that the demand for beverage packaging in North America will be static because of the changing market in carbonated drink consumption and the weak US economy (Euromonitor International 2010).

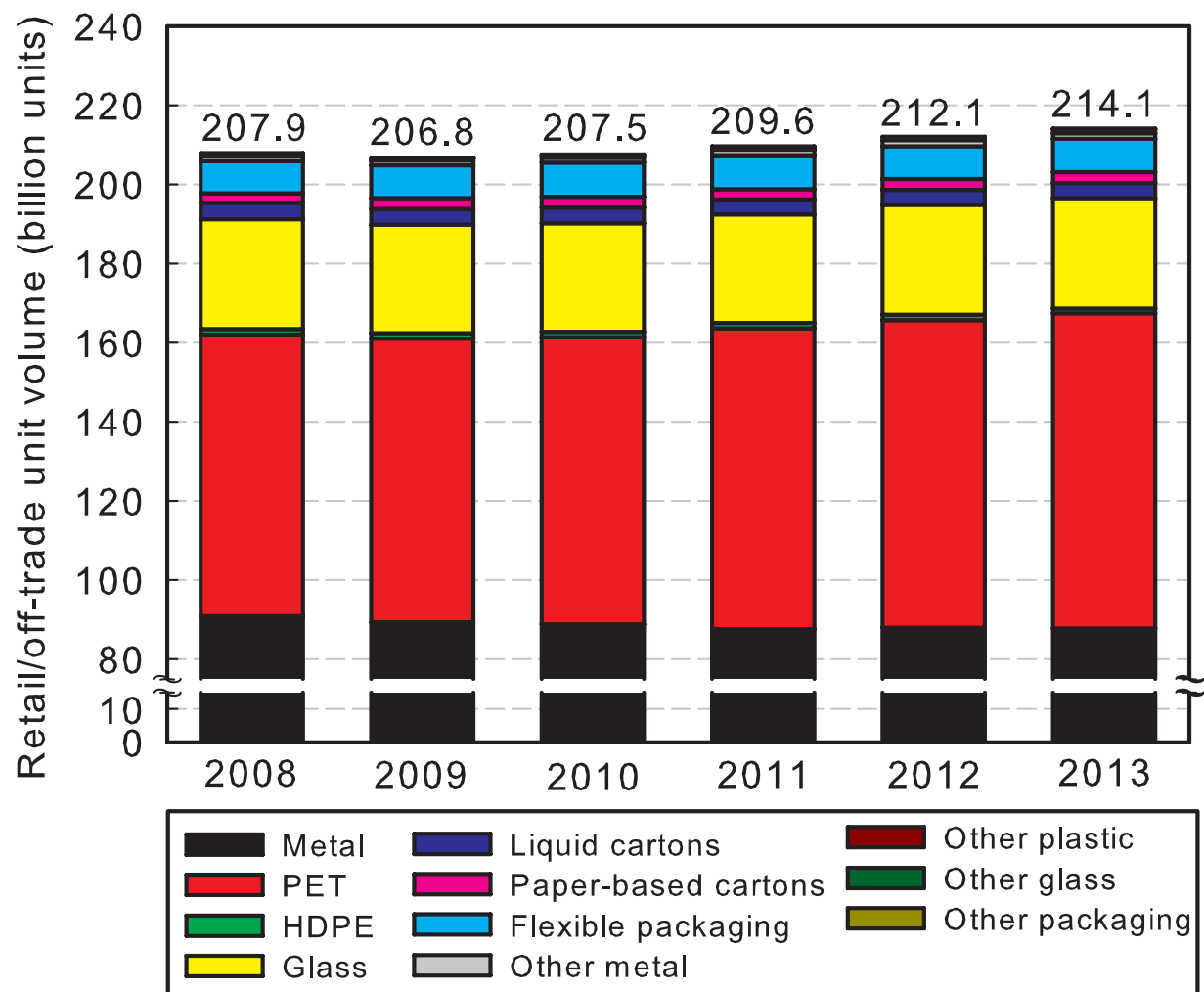


Figure 2-12. Beverage packaging market breakdown for North America, from 2008 to 2013

(Euromonitor International 2013a)

2.4.3 Beverage market in the US

US beverage packaging sales amounted to 195 billion units in 2013, and soft drink sales were reported as US \$ 176 billion in 2012, which makes the US the number one nation for beverage packaging sales (Figure 2-13 and Table 2-8) (Euromonitor International 2013b; e).

Table 2-8. Soft drinks sales in different countries (Euromonitor International 2013e)

Country	US\$ billion
USA	176.05
Japan	86.481
China	66.603
Brazil	42.722
Germany	37.303
Mexico	36.625
United Kingdom	20.517
Italy	19.916
Spain	19.377
France	19.290

The beverage market in the US, however, has been saturated for the same reason as North American 's beverage market suffered due to the decline in sales of packaged carbonates. Because of this trend, metal beverage packaging sales have dropped from 86 billion units in 2008 to 83 billion units in 2013. In contrast, PET beverage packaging increased from 67 billion units in 2008 to 85 billion units in 2013 due to the increasing demand for bottled water, functional drinks, RTD tea, and flavored milk drinks (Euromonitor International 2010).

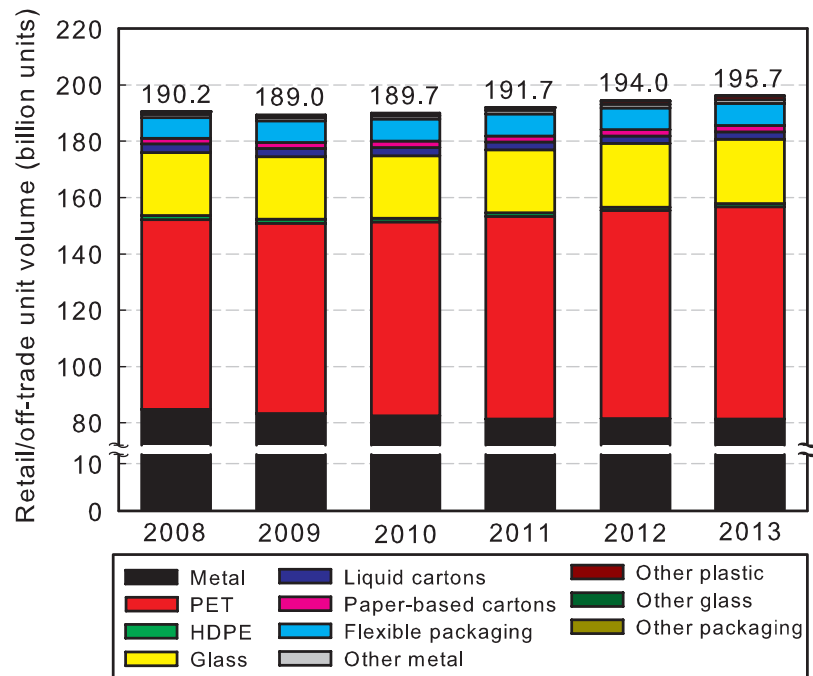


Figure 2-13. Beverage packaging market breakdown in US, from 2008 to 2013 (Euromonitor International 2013b)

Due to the increased demand for PET beverage bottles and rising crude oil prices, the price of PET resin increased since 2008. PET bales are the compressed PET flakes after post-consumer PET bottle are sorted and broken down. The PET bale price also increased.

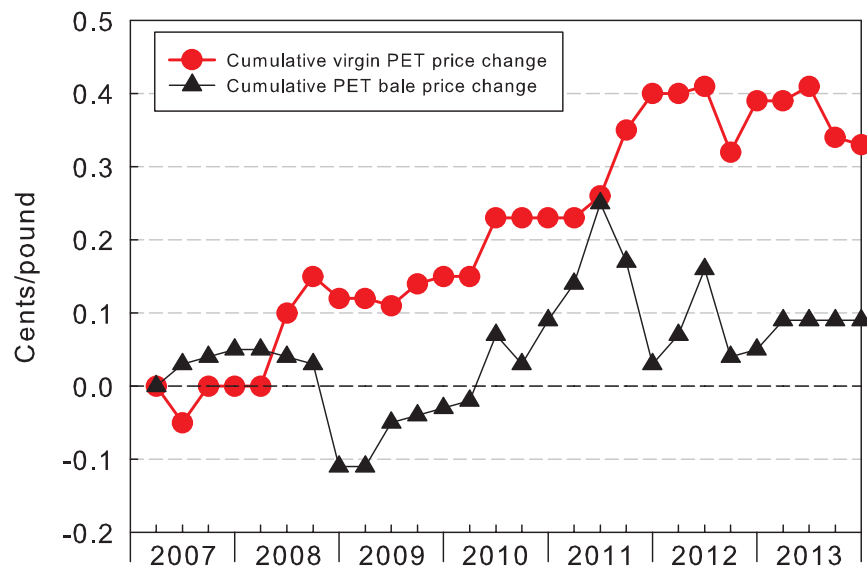


Figure 2-14. PET resin and bale price change, from 2007 to 2013 (Shinn *et al.* 2013)

2.4.4 Municipal Solid Waste (MSW) from beverage packaging in the US

The breakdown, by weight, of containers and packaging MSW from 2008 to 2011 is shown in Figure 2-15. Containers and packaging made up the largest portion of MSW generated, about 30 percent and 76 billion kg, while 51 percent (38 billion kg) of containers and packaging MSW was recovered in 2011 (US EPA 2013).

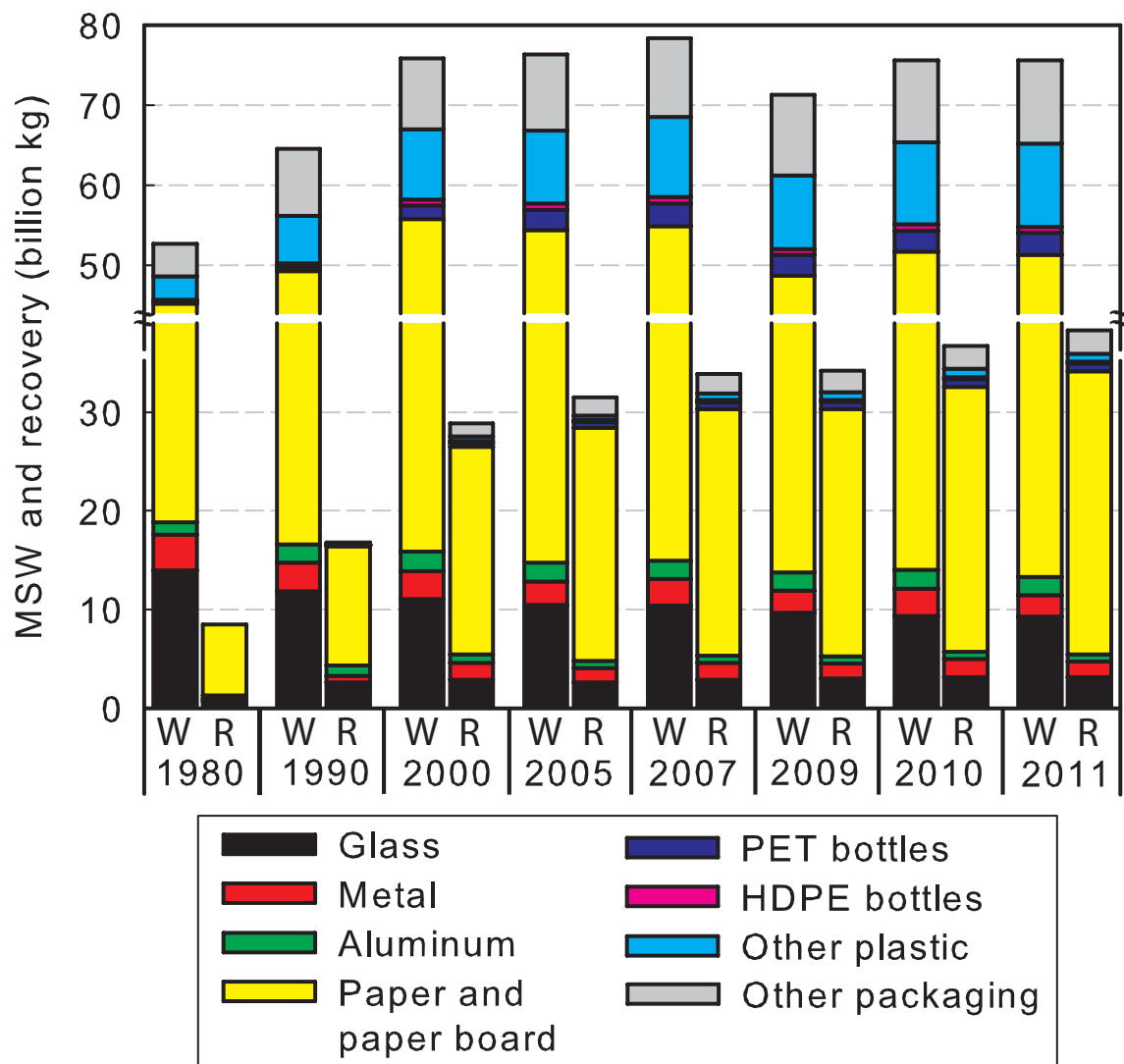


Figure 2-15. MSW and recovery of different product categories, from 1980 to 2011 (US EPA 2013) W: Waste, R: Recovery

In the container and packaging categories, paper products, metal, and aluminum were the most recycled materials by percentage in 2011; over 75 percent of paper and paperboard containers and packaging was recycled, while about 72 percent of metal packaging (mostly cans) was recycled (US EPA 2013). The recycling rate for aluminum packaging was about 39 percent including almost 55 percent of aluminum beverage cans (US EPA 2013). Over 34 percent of glass containers were recycled, while about 13 percent of plastic containers and packaging were recycled, mostly from soft drink, milk, and water bottles (US EPA 2013). PET bottles and jars contributed 2.7 billion kg of MSW in 2011 (US EPA 2013). It was found that PET bottles and jars were recovered amounted to about 0.8 billion kg in 2011 (US EPA 2013). MSW for PET bottles and jars has continuously increased between 2009 and 2011, 3.5 percent annually, while the recovery rate has increased annually by about 3~8 percent (US EPA 2013).

2.4.5 Municipal Solid Waste of PET beverage bottle in US

According to the report prepared by the Waste & Resources Action Programme (WRAP) (Michaud *et al.* 2010), mechanical recycling is the best waste management option for plastics with respect to the climate change potential, depletion of natural resources and energy demand impacts. The benefits of recycling are mainly achieved by avoiding production of virgin plastics.

In 2012 in the US, post consumer PET bottles collected for recycling and sold were 1718 million pounds (NAPCOR 2013). This number represents a 114 million pound increase in total mass of bottles collected over 2011, for a 30.8% PET bottle recycling rate (NAPCOR 2013). Despite the increase of PET bottles, the PET utilization rate, which is determined by adding the amount of clean flake produced by US reclaimers to the amount of clean flake exported divided by the total US bottles available for recycling, was a slight rebound from 2011, representing 21.1%

in 2012 (NAPCOR 2013). In 2012 recycled PET (RPET) was used in fiber, sheet & film, strapping, food & beverage bottles and non-food bottles at percentages of 40%, 23%, 10%, 21% and 6%, respectively (NAPCOR 2013).

2.5 LCA studies for beverage bottles

Over the past decades, numerous LCA studies on the environmental impacts of beverage packaging systems have been conducted. Many of the studies were conducted as comparative approaches to compare different beverage packaging options (Kristian Jelse *et al.* 2009; von Falkenstein *et al.* 2010; Gironi *et al.* 2011; Amienyo *et al.* 2013), whereas some other studies focused on supporting decision-making for waste management, such as recycling, landfill or incineration (Song 1999; Song *et al.* 1999; Perugini *et al.* 2005; Foolmaun *et al.* 2008; Romero-Hernández *et al.* 2009; Chilton *et al.* 2010; Li *et al.* 2010; Michaud *et al.* 2010).

Gironi, F. *et al* compared the environmental burden of polylactic acid (PLA) and polyethylene terephthalate (PET) water bottles. This paper highlighted the result that the environmental benefit of PLA bottles compared to PET bottles stems from the use of renewable resources, but this benefit is offset in environmental terms due to the use of pesticides, consumption of land and consumption of water for the production of raw materials (Gironi *et al.* 2011). Eva von Falkenstein and colleagues conducted a meta-analysis of LCA studies on beverage cartons and alternative packaging (von Falkenstein *et al.* 2010). The results indicated that the beverage carton has the lowest environmental burden compared to other types of beverage packaging, such as PET, HDPE, PVC and glass. On the other hand, Amienyo *et al.* (2013) concluded that PET bottles are the most sustainable option for most impact indicators compared to glass bottles and aluminum cans.

Jean-Charles Michaud and his colleagues (2010) evaluated the environmental impact of various waste managements options (recycling, landfilling or incineration) for different types of materials (paper and cardboard, plastics, biopolymers and food & garden waste). In the plastics sector, the results confirm that mechanical recycling is the best waste management option with respect to the climate change potential, depletion of natural resources and energy demand impact. Li et al. (2010) established an LCA model of PET beverage bottles and compared the environmental impacts of open loop recycling with multiple recycling trips in different scenarios. The results showed that multiple recycling trips can maximally reduce the impacts by 26% but additional savings are negligible after three recycling trips. In addition to these, there are many more studies reporting the LCA of PET recycling. Despite the different goals of these studies, all of them concluded that recycling of PET is the most favorable waste management option.

Chapter 3. LIFE CYCLE ASSESSMENT OF NON-ALCOHOLIC SINGLE-SERVE PET BEVERAGE BOTTLES IN THE STATE OF CALIFORNIA ³

3.1 Abstract

In this study, a life cycle assessment (LCA) was performed to evaluate the environmental performance of non-alcoholic single serve size PET beverage bottle (PET bottle) systems in the state of California. The LCA model was designed with five sections; 1. Material production, 2. PET bottle production, 3. Waste management, 4. Environmental benefit, and 5. Transportation. The scope of this study is cradle-to-grave with a representative functional unit as the amount of PET necessary to deliver 1,000 L of beverage, specifically in carbonated soda, water and tea. Several scenarios were also established to evaluate the effect of recyclable PET increase by reducing two different PET waste sources: post-consumer PET bottle (PCB) collection waste (Scenario ‘c’) and yield loss of reclamation process (Scenario ‘r’). The results indicate that the PET bottle production section was the highest environmental burden source in most of the impact indicator results. It was also found that scenario ‘r’ has higher environmental benefit than scenario ‘c’ in every impact indicator result. Despite the lack of consideration regarding the difficulty level of technology development, it may be proposed that increasing efficiency of the reclamation process will have priority over improving the PCB collection system in terms of environmental management for PET bottles in the state of California.

³ Chapter 3 was submitted as DongHo Kang, Rafael Auras, Jay Singh. 2014. *Life Cycle Assessment of Non-Alcoholic Single-Serve PET Beverage Bottles in the State of California*. Under review.

3.2 Introduction

In 2012, a total of 193 billion beverage packaging units were sold in the US., representing 176 billion US Dollars (Euromonitor International 2013b). The state of California consumed about 11 % of these total beverage-packaging units sold (CalRecycle 2013). Figure 3-1 shows that polyethylene terephthalate (PET) is the number one plastic, making up to 38 and 42 percent of the total 194.0 and 21.2 billion units of beverage packaging in 2012 in the US and the state of California, respectively (CalRecycle 2013; Euromonitor International 2013a). Despite the high volume of beverage packaging unit sales, the US market has been saturated due to the decline in sales of carbonated soft drinks (CSD), reporting only a 0.6 percent average growth rate (Euromonitor International 2010). This trend resulted in a decrease of metal beverage packaging sales in the US, dropping from 86 billion units in 2008 to 83 billion units in 2013 (Euromonitor International 2013a). In contrast, US PET beverage packaging sales increased from 67 billion units in 2008 to 85 billion units in 2013 due to the increasing demand for bottled water, functional drinks, ready-to-drink tea, and flavored milk drinks delivered in PET containers (Euromonitor International 2010).

The state of California consumes and recycles the largest numbers of bottles and cans in the US. (CalRecycle 2013). With 2,400 certified recycling centers, hundreds of curbside recycling programs, the California Beverage Container Recycling Litter Reduction Act and the California bottle bills, 70 percent of PET beverage bottles were recycled in California in 2012. As shown in Figure 3-1, the average recycling rate of PET beverage bottle in California is twice that of the US average.

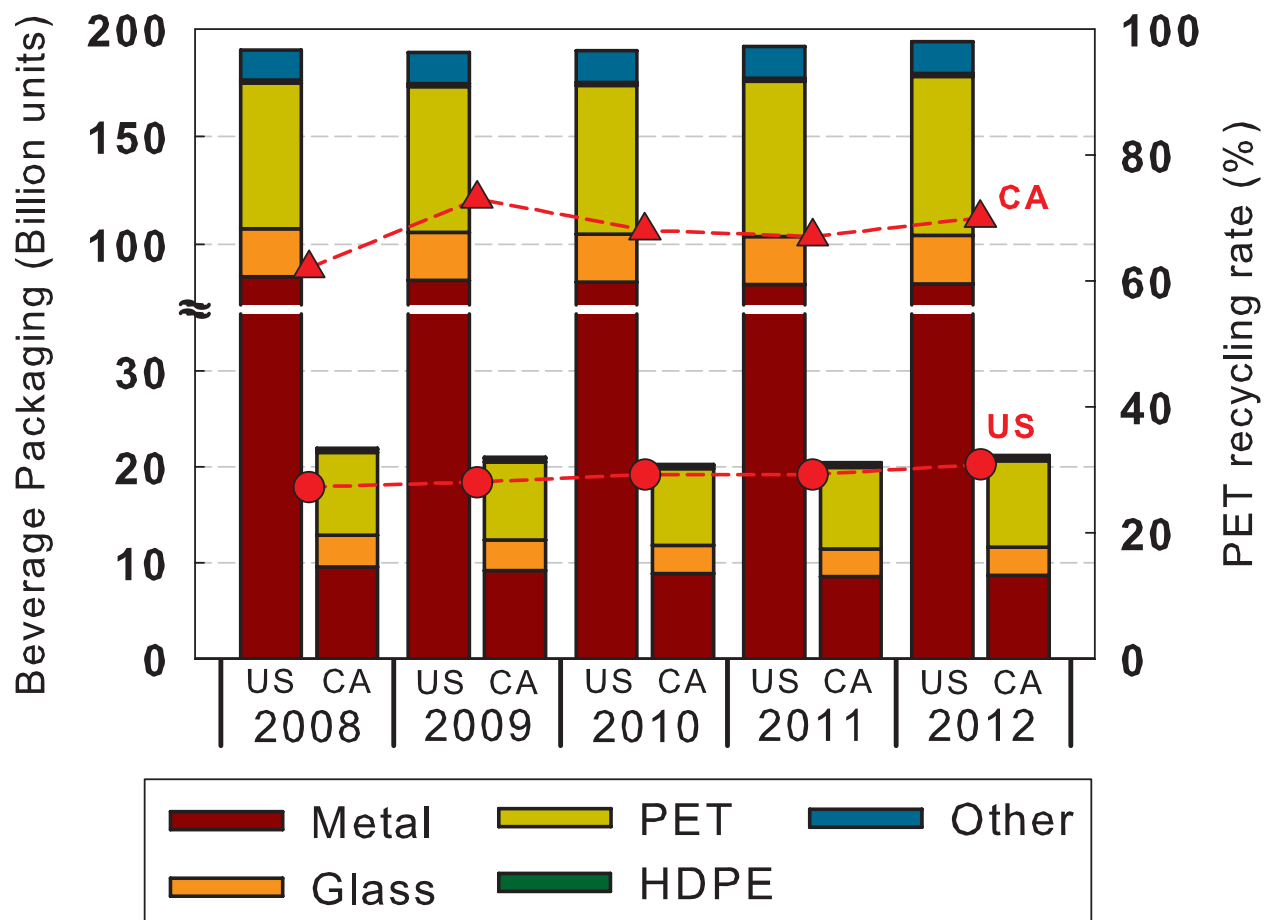


Figure 3-1. Beverage packaging market in the US and the state of California; red triangle indicates the recycling rate of PET in the state of California, whereas red round circle indicates the PET recycling rate in the US, data obtained from Ref. (CalRecycle 2013; Euromonitor International 2013a; US EPA 2014)

Life cycle assessment (LCA) is a useful technique for analyzing the environmental footprint of products like PET beverage bottles at all stages in their life cycle – from the extraction of resources, through the production of materials, parts, and the product itself, the use of the product and its disposal, either by reuse, recycling, or landfilling with or without energy recovery (*i.e.*, “from the cradle to the grave”) (Guinée 2001). LCA is composed of four steps:

goal and scope, inventory analysis, impact assessment, and interpretation of results. These steps are extensively described in the ISO 14040 and 14044 standards (ISO 2006b; c).

LCA of beverage packaging, especially PET, has been extensively conducted (Song 1999; Song *et al.* 1999; IFEU 2004; Franklin Associates 2007; Foolmaun *et al.* 2008; Franklin Associates 2009; Romero-Hernández *et al.* 2009; Chilton *et al.* 2010; Franklin Associates 2010; Li *et al.* 2010; Nakatani *et al.* 2010; Gironi *et al.* 2011). Based on these studies and a report (Michaud *et al.* 2010), mechanical recycling was found to be the best waste management option for plastic waste. The environmental benefit of mechanical recycling is mainly from the avoided production of virgin plastics. Plastic waste can be recovered in two ways: closed and open loop recycling. In closed loop recycling, the end-of-life of products is recycling for producing the same application as the initial product, whereas in open loop recycling the end-of-life of products is “down-cycling” (*i.e.*, products are recycled to be used in lower grade applications). In LCA studies, closed loop recycling is handled by replacing the virgin material with recycled material, whereas in open loop recycling an increasing trend is to manage by the systems expansion method, which extends the system boundary hypothetically to include the environmental benefit of the recycled product. However, no LCA studies of PET beverage bottle systems look at the trade offs of managing both closed and open loop recycling. Even though much research indicates that mechanical recycling brings the maximum environmental benefit for plastic waste, no LCA studies identify which steps can be modified to increase the amount of recycled content to improve the environmental performance of the final PET beverage bottle system.

In an attempt to provide an enhanced understanding of the environmental consequences of the non-alcoholic single serving size PET beverage bottle system in the state of California, this study tried to provide insights into the following two objectives:

- (1) The full life cycle impacts of the non-alcoholic single serve size PET beverage bottle system using LCA.
- (2) The potential improvement of the environmental performance of the system by minimizing the rejected fraction of post-consumer beverage bottles or maximizing the yield efficiency of the recycling process to increase the total recyclable PET resin in the system.

3.3 Experimental methods

3.3.1 LCA Scope and Functional Unit Definition

The functional unit was defined as the amount of PET necessary to deliver 1000 L of beverage, specifically carbonated soft drink (CSD), water and tea, accounting for 66.2 percent of total US non-alcoholic beverages consumed (Beverage World 2006). Ten bottles of each volume and each type of beverage were purchased at local retailers (in Lansing, Michigan). The functional unit selected is a representative mix of the market in terms of volumes and types of beverages. Since the weight of single serving size PET beverage bottle varies depending on the type of beverage and their volume, equation (3-1) was applied to calculate the appropriate functional unit for this study. Size and weight of single serving size PET beverage bottles are similar across the US, so it was assumed that there were no statistically significant differences in weight and size of PET bottles used in Michigan and California. The beverage type considered in this study was carbonated soft drink (CSD), water and tea. Using the percentage of sales amount of each type of beverage in the Pacific region of the US as a weighting factor (α_i) (Beverage World 2006), the functional unit of this study was calculated for each component: PET body (34212.2 g/1000 L) and polypropylene (PP) cap and PP label (8362.7 g/1000 L).

$$F_j = \sum_{i=1}^3 \sum_{k=1}^2 \alpha_i \frac{b_{ij}}{m_k} \quad (3-1)$$

$$i = \begin{cases} 1 : \text{Carbonated Soda} \\ 2 : \text{Water} \\ 3 : \text{Tea} \end{cases}, j = \begin{cases} 1 : \text{Body} \\ 2 : \text{Cap} \\ 3 : \text{Label} \end{cases}, k = \begin{cases} 1 : 591 \text{ mL volume} \\ 2 : 500 \text{ mL volume} \end{cases}$$

b_{ij} = weight of beverage packaging component in i th beverage in j th component (kg)

m_k = k th volume of beverage packaging (liter)

α_i = i th beverage weighting factor

F_j = Functional unit of j th beverage packaging component (kg/1000L)

The system boundary of this study is cradle-to-grave, and it is discretionally divided into 5 main sections; 1. Material production, 2. PET bottle production, 3. Waste management 4. Environmental benefit and 5. Transportation. These five main sections were established based on the general PET bottle production process (Lim *et al.* 2008). In the material production section, the inventory processes include extraction of natural resources, such as crude oil and natural gas, used for PET and PP resin production. PET bottle production includes injection stretch blow molding (ISBM) of the PET bottle, and extrusion and injection molding for the PP label and cap, respectively. Waste management represents the environmental impact of waste landfill, incineration and recycling processes. Environmental benefit accounts for the energy recovery generated by combustion of waste and recycled PET made through closed and open loop recycling. Transportation consists of transport of packaging material (PET and PP), post-consumer PET bottles (PCB) to the collection facility, collected PCB to the material recovery facility (MRF), and PET bales to the reclamation facility. Detailed descriptions of the inventory processes and stocks for each section are provided in Table 3-1.

Table 3-1. Phases of non-alcohol single serving size PET beverage bottles, including processes and stocks for each phase

Phase	Process	Stock
Material production	Extraction of natural resources	Crude oil and natural gas
	PET resin production	Amorphous PET
	PP resin production	PP
PET bottle production	Injection stretch blow molding	PET bottle
	Film extrusion	PP label
	Injection molding	PP cap
Waste management	Landfill of plastic waste	PET and PP waste
	Combustion of plastic waste	
	Material recovery process	PET bale
	Reclamation	Clean PET flake
	Solid state polymerization	PET bottle grade resin
Environmental benefit	Open loop recycling	Recycled fiber, recycled strap, recycled sheet & film, and others
	Closed loop recycling	Recycled PET bottle
	Energy recovery	Electricity from combustion of plastic waste
Transportation	Distribution of filled bottle	Diesel powered truck
	PCB collection	
	PCB to material recovery facility	
	PET bale to reclamation facility	

3.3.2 Key Assumptions

The following assumptions were made to close the gap between the LCA models and the actual life cycle of the PET beverage bottle. Because some of the inventory data is not available, several assumptions and limitations were taken into consideration.

- The majority of the processes of the life cycle of PET beverage bottles were assumed that it is performed in the US. The depreciation and environmental impact of existing infrastructures was assumed as negligible.
- The secondary and tertiary packaging of the PET beverage bottle were assumed to be negligible. The environmental impact of the ink on the PP label and cap was also considered negligible.
- The beverage production was excluded.
- All the PET and PP waste, except that handled by recycling, was assumed to be managed through incineration with energy recovery and landfill at a 20% and 80% ratio, respectively (Van Haaren *et al.* 2010).
- To consider the energy recovery from incineration of PET and PP waste, the heating value of PET bottles and PP caps/labels was estimated as 21,825 and 43,894 BTU/kg, respectively (Franklin Associates 2009).
- Surfactant and wetting agent used for the material recovery process were treated as detergents, and modeled as sodium tripolyphosphate.
- Trucks were assumed to be fully loaded coming into the facility and returned empty or with empty containers.
- PET preforms and bottles were made at the same location.

- Most of the LCI data were obtained from US-EI v2.2, which established based on European data with US average electricity. Detailed information of the LCI data is provided in the Appendix A Table A-1 and A-2 provided online.

3.3.3 Life Cycle Inventory Analysis (LCI)

The data in this LCA were acquired from various literature sources and databases from SimaPro software, like Ecoinvent V2.2. Details of the data sources (Davis 2007; US Census Bureau 2007; NewPoint Group 2009; Sylvatica 2009; Franklin Associates 2010; NAPCOR 2010; US ITC 2010; American Chemistry Council 2012; US Census Bureau 2012; CalRecycle 2013) are provided in Appendix A Tables A-1 and A-2. Based on these data sources, a Sankey diagram of mass flow of PET beverage bottle in US and California was constructed (Figure 3-2). The thickness of the flow arrows is proportional to the mass flow magnitudes.

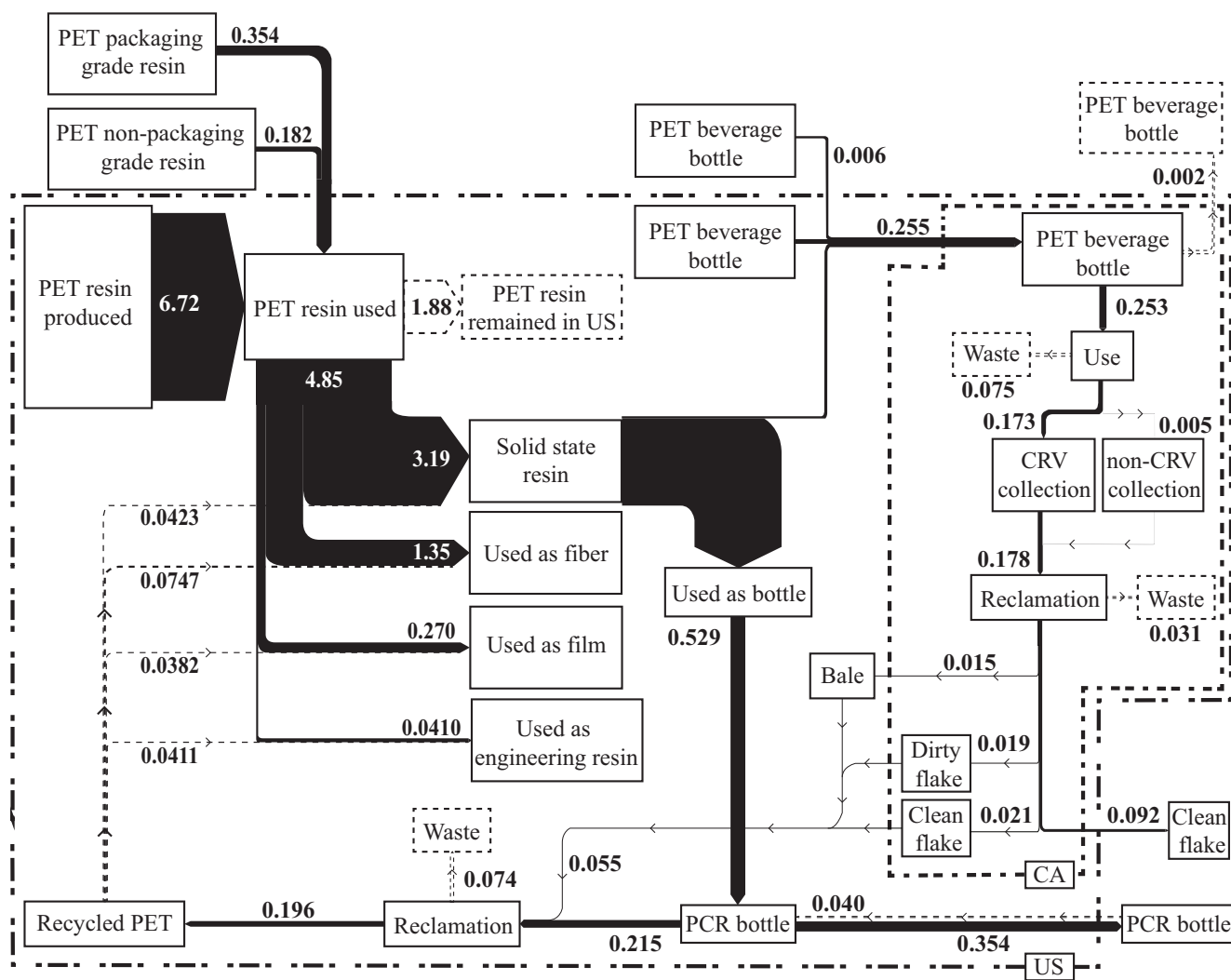


Figure 3-2. Sankey diagram of PET beverage bottle system for this study in 2010 (billion tons)

For the material production section, the database for PET bottle grade resin includes the production of ethylene glycol (EG), purified terephthalic acid (PTA), amorphous PET resin and solid-state polymerization. Also, energy inputs, wastes, and air and water emissions for each step were included. For the PP resin, Ecoinvent V2.2 provides aggregated data for all processes from raw material extraction until delivery at the plant.

ISBM, injection molding and extrusion molding were used to produce PET bottles, PP caps and PP labels, respectively. ISBM contains the auxiliaries and energy demand processes. Ecoinvent V2.2 indicates 2.2% of yield loss during ISBM, while 0.6% and 2.4% yield loss occur in injection and extrusion molding, respectively. The end of life of these yield losses are managed as 20% incineration and 80% landfill.

The waste management section contains material recovery, reclamation process and solid-state polymerization for recycled PET as well as combustion and landfill for PET and PP waste. The data for the material recovery and reclamation process was obtained from the report of Franklin Associates (Franklin Associates 2010). Due to the lack of reported data, the LCI of the solid-state polymerization process for closed loop recycling was obtained from a reference (Dogan 2008), which oversimplified the input of solid-state polymerization considering just the electricity (584-1260 kWh) and the cooling water (0.4-10 m³). There are two sources of PCB collection, California Refund Value (CRV) and non-CRV. During the PCB collection, uncollected or low quality PCB goes to waste (Weight is equal to 30% of initial PET resin), and this waste was one of the variables to evaluate the impact on the LCA results. Another variable in this study was the yield loss (Weight is equal to 12% of initial PET resin) during reclamation process. We assumed that these two variables were easy to be improved in a waste management perspective.

In the environmental benefit section, all the activities to reduce the environmental burden were included such as closed loop and open loop recycling and energy recovery from combustion of plastic waste. The amount of PET closed loop and open loop recycling was obtained from the report of the National Association for PET Container Resources (NAPCOR) (NAPCOR 2010). For energy recovered by incineration, 21,825 and 43,894 Btu/kg of calorific value were used for PET and PP, respectively (Franklin Associates 2009).

In order to evaluate the overall environmental burden of the transportation activities, the transportation section grouped the distribution of filled bottles, PCB collection through three different collection methods (drop off centers, curbside programs and recycling centers), and PCB transport to MRF and from MRF to reclamation facility. An average distance of 107 km (67 miles) was determined for filled PET beverage bottles from the 2007 commodity flow survey of the US Census Bureau (US Census Bureau 2007). The distance and amount of PCB collection by the three different collection methods was obtained from the report of Franklin Associates and the California Department of Resources, Recycling and Recovery (Franklin Associates 2010; CalRecycle 2011).

3.3.4 Scenario setup

In this study, two variables were selected to evaluate the impact on the LCA results. Table 3-2 describes these variables: recycling route and source of recyclable PET. There are two different recycling routes: closed loop and open loop recycling. For closed loop recycling ($= r_{j=1}$), recycled PET from PET beverage bottles goes to produce the PET beverage bottle. For open loop recycling ($= r_{j=2}$), also called down-cycling, recycled PET is used to produce products requiring lower quality PET resin, such as films and sheet rather than PET beverage bottle. Besides the recyclable PET (21% of functional unit) in the current PET beverage bottle system, hypothetical

scenarios were established to increase recyclable PET. Two sources were considered: PCB collection waste ($= r_{i=1}$) and yield loss of the recycling process ($= r_{i=2}$).

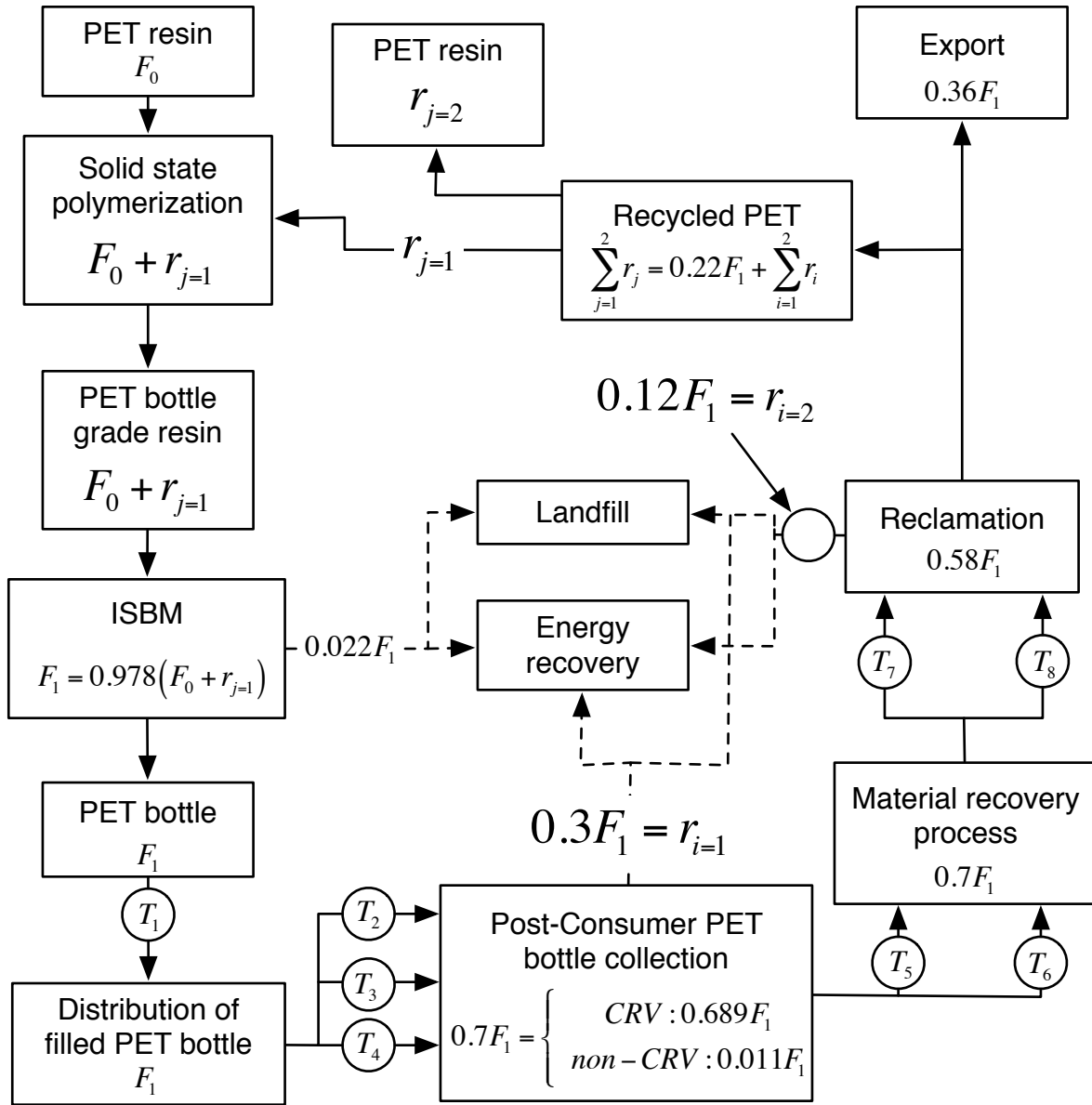
Table 3-2. Parameters used in this study for recyclable PET; Parameter i indicates the source of recyclable PET acquired from PCB collection waste ($i=1$) and yield loss of the recycling process ($i=2$). Parameter j represents closed loop recycling ($j=1$) and open loop recycling ($j=2$)

r_{ij} : Recyclable PET		Source of recyclable PET	
		$i = 1$	$i = 2$
Recycling route	$j = 1$	Waste from PCB collection waste recycled in closed loop ($= r_{11}$)	Yield loss of recycling process recycled in closed loop ($= r_{12}$)
	$j = 2$	Waste from PCB collection waste recycled in open loop ($= r_{11}$)	Yield loss of recycling process recycled in open loop ($= r_{12}$)

The comparison of open and closed loop recycling scenarios, however, was assumed to not be statistically significantly different. The main difference between open and closed loop recycling was the solid-state polymerization process, which presently is oversimplified due to lack of primary data for the process. For this reason, even though open and closed loop recycling was parameterized in this study, recycled PET from these two recycling routes was considered as equal.

Figure 3-3 describes the mass flow diagram of PET beverage bottles. The system starts with amorphous PET resin production ($= F_0$). During ISBM, 2.2% of yield loss is assumed to occur. After the ISBM process, 34.212 kg of PET beverage bottles ($= F_1$) are produced. The amount of 10.264 kg are not collected during PCB collection ($= 0.3F_1 = r_{i=1}$), while 4.105 kg are

lost during the reclamation process ($= 0.12F_1 = r_{i=2}$). F_1 (0.36) is exported to China, and the rest of it goes back to the life cycle of PET beverage bottles managed by closed loop or open loop recycling. To sum up, a total of 22% of F_1 is recycled and re-introduced to the PET beverage bottle system in California. This amount is hypothetically increased by reducing either the PCB collection waste ($= r_{i=1}$) or yield loss of the recycling process ($= r_{i=2}$). In conclusion, the total amount of recyclable PET is a sum of 22% of F_1 , and a reduction amount of PCB collection waste or yield loss of the recycling process $\left(= \sum_{j=1}^2 r_j = 0.22F_1 + \sum_{i=1}^2 r_i \right)$. The maximum increase of recyclable PET from PCB collection is 29.6% of F_1 , while 12.2% of F_1 is the maximum amount from the yield loss of recycling process.



- T_1 : Distribution of filled bottle (107.8 km) T_5 : Delivery to MRF by truck 1 (57.2 km)
 T_2 : Collected through recycling center (241.4 km) T_6 : Delivery to MRF by truck 2 (53.0 km)
 T_3 : Collected by curbside program (80.5 km) T_7 : Delivery to Reclamation facility by truck (703.9 km)
 T_4 : Collected by drop-off center (128.7 km) T_8 : Delivery to Reclamation facility by train (170.6 km)

Figure 3-3. Parameterized flow diagram of the life cycle of non-alcoholic single serving size PET beverage bottle

In order to analyze the effect of these variables, several scenarios were established as indicated in Table 3-3 and compared to evaluate the sensitivity of recyclable PET. Scenario ‘c’ is hypothetically increasing the total amount of recyclable PET by reducing PCB collection waste, whereas scenario ‘r’ is increasing the total amount by lowering the yield loss of the recycling process.

Table 3-3. Description of the scenario setup based on two different sources (scenario ‘c’ and scenario ‘r’) to increase the recyclable PET

Scenario	Scenario code	Variable	Recyclable PET
Base	S1		21.73% of F_1
Scenario ‘c’	S2	$r_{i=1}$	21.73% of F_1 + 10% of F_1 from $r_{i=1}$
	S3		21.73% of F_1 + 29.6% of F_1 from $r_{i=1}$
Scenario ‘r’	S4	$r_{i=2}$	21.73% of F_1 + 10% of F_1 from $r_{i=2}$
	S5		21.73% of F_1 + 12.2% of F_1 from $r_{i=1}$

3.3.5 Life Cycle Impact Assessment (LCIA)

The tool for the reduction and assessment of chemical and other environmental impacts (TRACI) was employed for calculating the life cycle impact assessment (Bare 2012). Especially, in this study, a recent version of TRACI, TRACI v2.1, is used. TRACI v2.1 was specifically designed for the US using input parameters consistent with US locations (Bare 2012). Moreover, TRACI v2.1 is consistent with existing policies and regulations in the US and provides high versatility in the US market (Bare 2012). Many of the impact assessment methodologies within TRACI v2.1 are based on “midpoint” characterization approaches (Bare *et al.* 2000). In the other words, the impact assessment models reflect the relative potency of the stressors at a common

midpoint within the cause-effect chain (Bare *et al.* 2000). One of the impact indicators in TRACI v2.1 is the global warming potential (GWP) referring to the potential change in the earth's climate caused by the buildup of chemicals, known as greenhouse gases, such as carbon dioxide (CO₂), methane (CH₄), and nitrous oxide (N₂O). While GWP is the most often quantified environmental impact with international agreements, TRACI v2.1 provides a wide range of environmental impact indicators, such as acidification, eutrophication, smog, ecotoxicity, respiratory effects, carcinogenics, and non-carcinogenics (Bare 2012).

3.3.6 Interpretation

By definition, interpretation in LCA is “the phase in which the findings of either the inventory analysis or the impact assessment, or both, are evaluated in relation to the defined goal and scope to reach conclusions and recommendations” (ISO 2006b). Heijungs and Kleijn (2001) have defined five numerical approaches to life cycle interpretation: contribution analysis, perturbation analysis, uncertainty analysis, comparative analysis and discernibility analysis.

Contribution analysis is used to find ‘hot spot’ by decomposing the aggregated results of the inventory analysis into a number of constituent elements. For this reason, the model in this study was designed with 5 sections (1. Material production, 2. PET bottle production, 3. Waste management 4. Environmental benefit and 5. Transportation). To assess the variation and the uncertainty of the results, uncertainty analysis was performed at the characterization level of impact assessment using Monte Carlo simulation. Monte Carlo simulation is often used in measuring the uncertainty of complex systems by replacing point estimates with random variables drawn from probability density functions (LaGrega *et al.* 2010). In this study, the standard deviation and probability density function for most of the input parameters was implemented by the data base provider for SimaPro software , and some of it was determined by

using a pedigree matrix (Weidema 1998). In order to apply the statistical comparison for scenario ‘c’ and ‘r’, a discernibility analysis was also conducted. This analysis stems from the desire to combine the comparative analysis and the uncertainty analysis, which requires a Monte Carlo simulation. Unlike uncertainty analysis, however, this analysis estimates the difference between two products or two scenarios with respect to the selected item, such as the results of an impact indicator or emission.

3.4 Results and discussion

3.4.1 Contribution and uncertainty analysis of the base scenario

Table 3-4 explains the uncertainty analysis result for the base scenario. Some of the indicators show high standard deviation, coefficient of variation (CV) and wide 95% confidence interval (CI), such as carcinogens, non-carcinogens, eutrophication and ecotoxicity. This is mainly because all these impact indicators reflect the disposal of various wastes, such as PET, hard coal ash and waste from coal mining, which have high uncertainty in the inventory data. Despite its high uncertainty, results of those impact indicators were considered to provide wider environmental insight of this system.

Table 3-4. Results of uncertainty analysis for S1 with coefficient of variance (CV), mean $\pm$ standard deviation and 95% confidence interval for each impact indicator

Impact category	Unit	CV (%)	Total	95% CI
Global warming	kg CO ₂ eq	15.2	187.4 $\pm$ 28.5	[141, 259]
Acidification	H ⁺ moles eq	22.4	46.80 $\pm$ 10.5	[30.6, 72.8]
Carcinogenics	kg benzene eq	109	0.3865 $\pm$ 0.421	[0.181, 0.880]
Non-carcinogenics	kg toluene eq $\times 10^3$	207	6.343 $\pm$ 13.1	[2.18, 15.2]
Respiratory effects	kg PM _{2.5} eq	33.1	0.215 $\pm$ 0.0711	[0.127, 0.396]
Eutrophication	kg N eq	67.8	0.6205 $\pm$ 0.421	[0.277, 1.71]
Ozone depletion	kg CFC-11 eq $\times 10^{-6}$	16.9	9.70 $\pm$ 1.64	[6.93, 13.3]
Ecotoxicity	kg 2,4-D eq	71.8	281.4 $\pm$ 202	[108, 685]
Smog	g NO _x eq	14.1	0.398 $\pm$ 0.0561	[0.309, 0.539]

Figure 3-4 describes the results of the contribution analysis for the base scenario, which includes 21.73% of F₁ as recyclable PET, equal to 7.434 kg of PET. PET bottle production is the largest contributing section in almost every impact indicator except GWP, eutrophication and smog. Material production, PET bottle production, waste management and transportation sections contributed to the environmental burden, whereas the environmental benefit section reduced the environmental burden as described by the negative percentage.

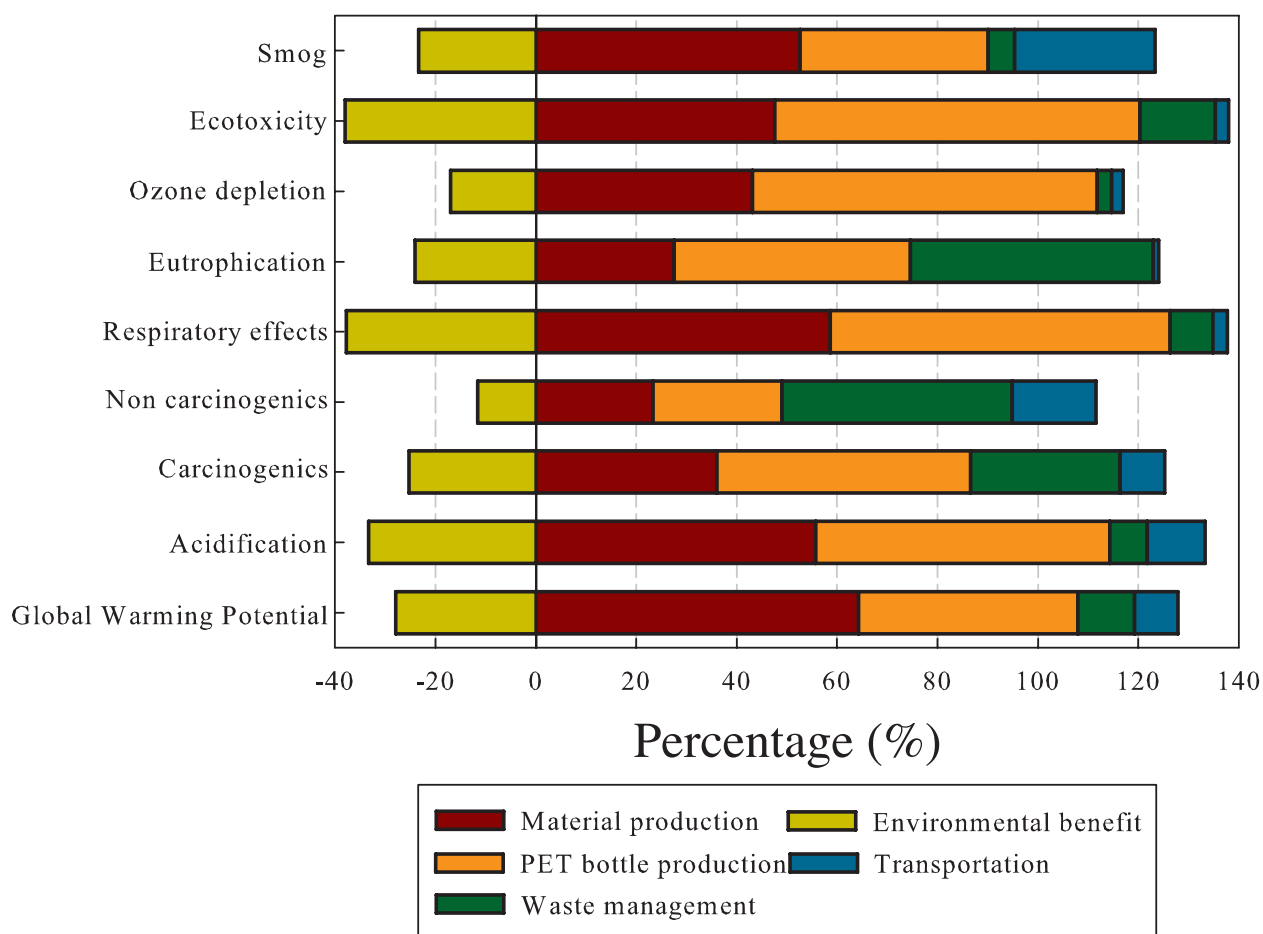


Figure 3-4. Results of contribution analysis for scenario S1; results are standardized in percentage value for each life cycle stages. Due to the negative value of environmental benefit, the total is presented in more than 100 percent

The highest GWP (120.4 kg CO₂ eq.) and smog (0.201 g NO_x eq) was recorded in the material production section. Specifically, production of xylene was the highest contributing inventory process. The second highest section was the PET bottle production (81.9 kg CO₂ eq and 0.149 g NO_x eq), and hard coal combustion for electricity generation was the largest GWP and smog generating inventory process. The recycling and energy recovery from combustion of waste allocated to the environmental benefit section saved 52.3 kg CO₂ eq and 0.0928 g NO_x eq.

PET bottle production (27.4 H⁺ moles eq) was the largest contributing section for acidification, specifically due to hard coal combustion during electricity generation. Because electricity generation is a significant inventory process in acidification, the largest environmental benefit was also found in the energy recovery from the incineration of plastic waste, to reducing the amount of hard coal (8.611 H⁺ moles eq.)

Carcinogen and non-carcinogen indicators are often significant indicators in terms of disposal of material. For carcinogen, PET bottle production (0.195 kg benzene eq) was the largest contributing section, and the disposal of uranium tailings and spoil from coal mining for electricity generation was the main inventory processes, whereas in non-carcinogens, plastic waste dominated the total environmental burden, possessing 66% of the total non-carcinogens impact indicator, specifically landfill of PP and PET. This trend was also found in the results of the ecotoxicity and eutrophication impact indicators.

Respiratory effects were mainly interpreted as the effect of air quality change (PM 2.5 level change) on human health. In other words, this indicator is mainly related to air emissions, which are mostly generated by combustion of hard coal for electricity generation in the PET bottle production process.

PET bottle production (6.65×10^{-6} kg CFC-11 eq) was the largest contributing section to ozone depletion. Specifically, the production of tetrachloroethylene and dichloromethane, used as the solvent for injection molding were the most significant inventory process.

3.4.2. Discernibility analysis

Figure 3-5 describes the results of the different scenario comparisons. Detailed discernibility analysis results are available in appendix A, Table A-3 to Table A-12. The results showed that scenario S2 reduces 6.5 kg CO₂ eq. of GWP compared to S1, whereas S3 saves 7.6

kg CO₂ eq. Despite the same increase amount for recyclable PET in both S2 and S4 (10% of F_1), the GWP saving differs because the decisions made in S2 and S4 affect the supply chain differently. In Figure 2, a decision made in scenario S2 will subsequently increase the weight of shipment in T_5 and T_6 , amount to be handled in MRF, weight of shipment in T_7 and T_8 , yield loss from reclamation process, and amount to be recycled. On the other hand, in scenario S4, it will affect the supply chain by increasing the amount to be recycled only. For this reason, scenario S4 shows preferable environmental benefits than scenario S2. When it comes to comparing scenarios S3 and S5, because the maximum amount to be able to increase the recyclable PET from S3 (29.6% of F_1) is higher than S5 (12.2% of F_1), S3 shows better environmental benefit than S5 for all impact indicator results.

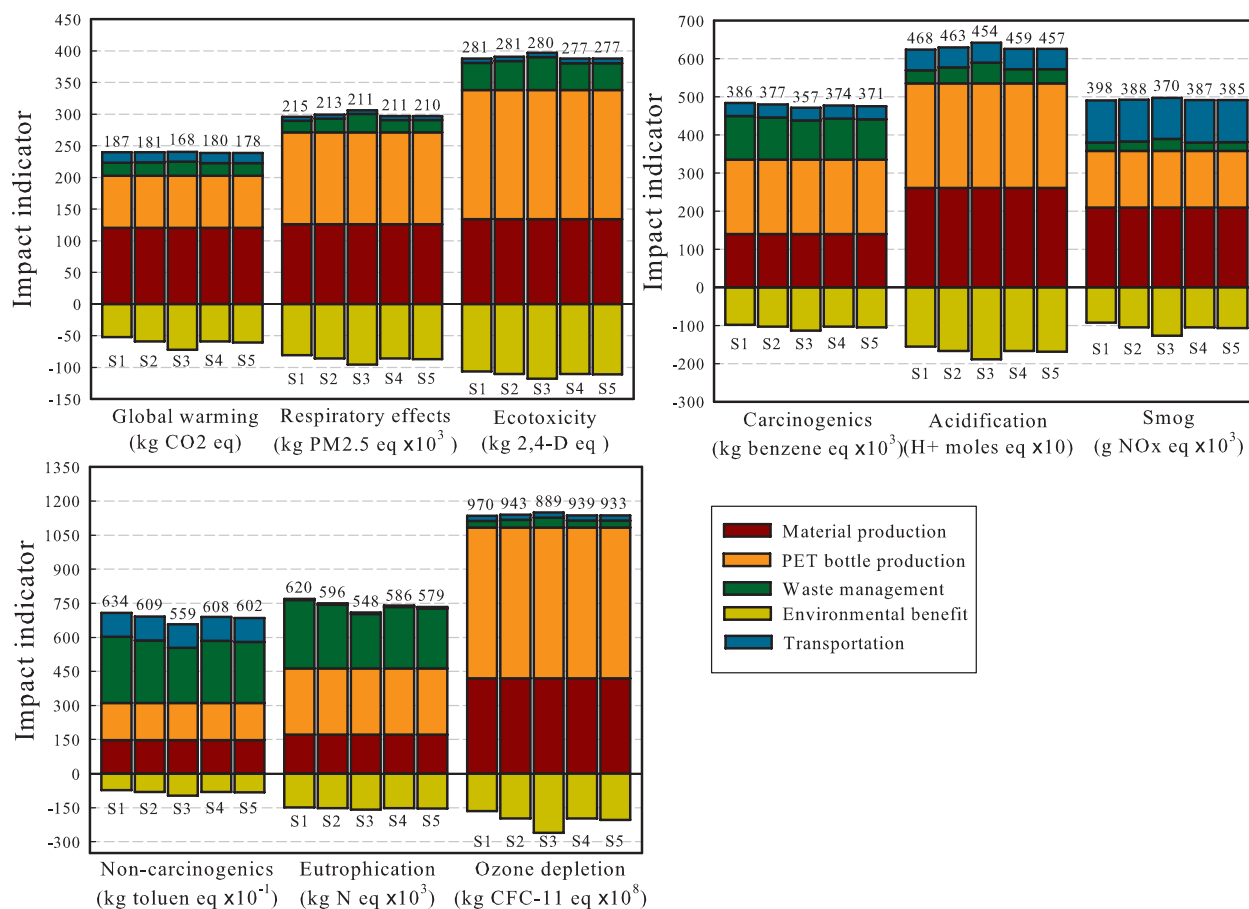


Figure 3-5. Results of scenario comparison; number on top of bar indicates the total of the impact indicator

In order to objectively compare scenario 'c' and scenario 'r', an additional analysis was conducted by hypothetically reducing 1 kg of PET from yield loss and PCB collection waste as shown in Figure 3-6. Additionally a scenario for 1 kg reduction of PET from F₁ (source reduction) was also compared. The results show that 1 kg PET reduction in yield loss produces the most environmental benefit in GWP, non-carcinogenic, eutrophication and ozone depletion. The main contributing section to differentiate the total GWP impact indicator is the environmental benefit section, which favors more environmental benefit of yield loss reduction than source reduction. In the case of non-carcinogenics, eutrophication and ozone depletion, not only in the environmental benefit section, but also the waste management section plays a major

role to generate higher environmental benefit for yield loss reduction than source reduction. For the rest of the impact indicators, source reduction produced the highest environmental benefit.

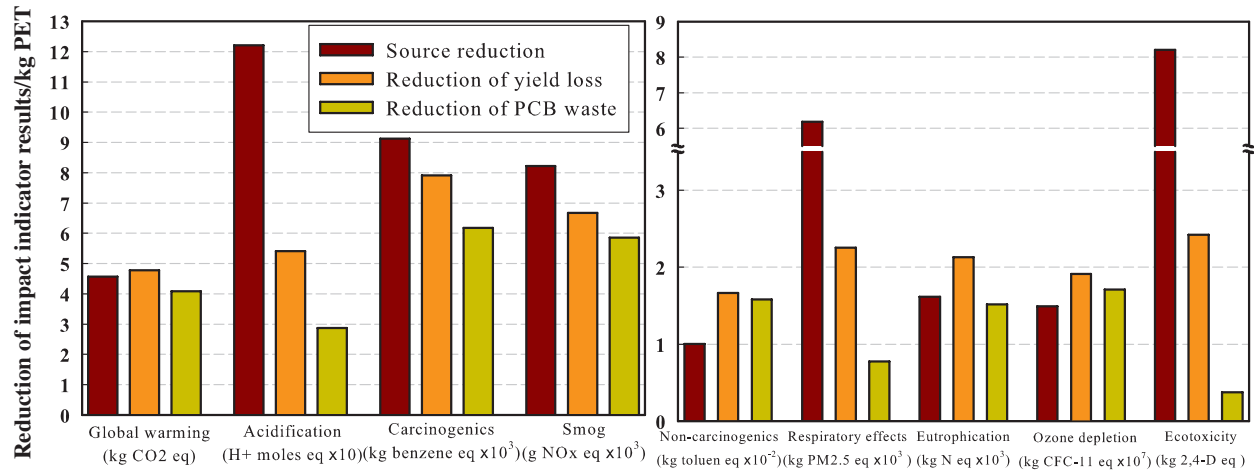


Figure 3-6. Comparison of environmental benefit for 1 kg PET reduction of F₁ (source reduction), PCB collection waste and yield loss

3.5 Conclusions

The environmental footprint of the life cycle of non-alcoholic single-serve size PET beverage bottles in the state of California was modeled. Five scenarios were established to evaluate the effect of increasing recyclable PET from reducing different PET waste sources: PCB collection waste and yield loss from recycling of PET. Scenario ‘c’ represents the hypothetical scenario to increase the recyclable PET contents in the system to reduce PCB collection waste, whereas scenario ‘r’ describes the effect of recyclable PET increase by reducing the yield loss of the reclamation process. Scenario ‘c’ suggests a possible environmental benefit by improving PCB collection system, whereas scenario ‘r’ may be interpreted as the potential environmental credit generated by improving yield efficiency in the reclamation process. The LCA model was divided into five sections to help to find the ‘hot spot’,

in the system: 1. Material production, 2. PET bottle production, 3. Waste management, 4. Environmental benefit, and 5. Transportation

A contribution analysis revealed that the main environmental burden is contributed by the PET bottle production section in acidification (27.4 H⁺ moles eq.), carcinogens (0.195 kg benzene eq.), non-carcinogens (1631.7 kg toluene eq.), respiratory effects (0.145 kg PM_{2.5} eq.), ozone depletion (6.65 x 10⁻⁶ kg CFC-11 eq.) and ecotoxicity (204.4 kg 2,4-D eq.). The material production section was the main source of GWP (120.4 kg CO₂ eq.), eutrophication (0.171 kg N eq.), and smog (0.209 g NO_x eq.).

A discernibility analysis showed that scenario 'r' has a larger environmental benefit than scenario 'c' in every impact indicator result. Comparing PET reduction in yield loss of reclamation (kg), PCB collection waste and functional unit (source reduction), yield loss reduction has higher environmental benefits than source reduction and PCB collection waste reduction in GWP, non-carcinogenic, eutrophication and ozone depletion. Source reduction is considered as the best option in terms of acidification, carcinogenic, respiratory effects, ecotoxicity and smog.

The state of California is considered to be the number one consumption and recycling state for PET beverage bottles in the US, representing a 70% recycling rate (CalRecycle 2013). In the other words, PCB collection system in the California is well established, and it indicates that the possibility to achieve PCB collection waste reduction may be relatively lower than the yield loss reduction of the reclamation process. This conclusion is only based on the results of this study without the consideration of the difficulty level of each technology development. This conclusion, however, can help to determine which option needs to be prioritized to manage the

environmental burden of non-alcoholic single-serve PET beverage bottles in the state of California.

Chapter 4. META-ANALYSIS OF LIFE CYCLE ASSESSMENT STUDIES OF THE PET BEVERAGE BOTTLE SYSTEMS ⁴

4.1 Abstract

A systematic review, specifically a meta-analysis, was performed to review the life cycle assessment (LCA) literature on the polyethylene terephthalate (PET) beverage bottle system. The goals of this study were to evaluate the variation of the environmental impact in each life cycle stage of the PET beverage bottle system and to identify the sources of variation by using the global warming potential (GWP) and energy consumption (EC) impact indicators. A total of 212 LCA studies of the PET beverage bottle system were screened, which yielded 23 studies including 4 life cycle inventory (LCI) databases, 6 LCA full reports and 13 LCA journal articles. The estimates for the 12 disaggregated life cycle stages of the PET beverage bottle system were collected from all the 23 studies and harmonized. The variation was mostly attributed to the PET bottle weight per liter, the efficiency of injection stretch blow molding (ISBM), the product loss during filling and delivery, the post consumer bottle (PCB) collection and sorting efficiency of the material recovery facility (MRF), the material efficiency of recycling, the calorific value of PET and the efficiency of electrical energy generation from the incineration facility. A statistical assessment of the central tendency and variation of the harmonized datasets was performed. The largest contribution to GWP and EC was found from bottle grade PET resin production. The largest variation of GWP and EC indicators was for incineration of plastic waste due to a large variation in electricity efficiency for energy recovery from the incineration facility. This

⁴ Chapter 4 was submitted as DongHo Kang, Rafael Auras, Susan Selke. 2014. *Meta-Analysis of Life Cycle Assessment Studies of PET Beverage Bottle System*. Under Review

indicates that improvement of the environmental performance of the PET beverage bottle system can be achieved by optimizing the electricity recovery efficiency.

4.2 Introduction

Life cycle assessment (LCA) is known as a holistic and regular approach for evaluating the environmental impact of products and/or systems through a comprehensive “cradle to grave” examination. LCAs track the environmental impacts generated from all activities that transpire over the life of a product system, including upstream and downstream processes from the operational phase (Burkhardt *et al.* 2012). Traditionally, LCA studies evaluate the environmental impact of systems or a product as they are presently, referred to as attributional LCA - ALCA. From this perspective, LCA can be considered as reductionism. Reductionism is the philosophical position where a complex system is nothing, but the sum of its parts, and an account of it can be reduced to accounts of individual constituents (2002). In this manner, the environmental burden of the total system is the sum of the environmental burdens of individual processes and constituents.

Over the last decade, the LCA literature has exponentially increased (Figure 4-1). Despite the extensive LCA literature, few attempts have been made to synthesize and to summarize previous research (Brandão *et al.* 2012). Such attempts often start with a review. Depending on the purpose, the scope and structure of a review can be varied to provide a survey of previous publications, critique current work, or summarize projections about future discoveries (Zumsteg *et al.* 2012). Among the various review types, a systematic review is a comprehensive literature search performed in a transparent and unbiased way (Neely *et al.* 2010).

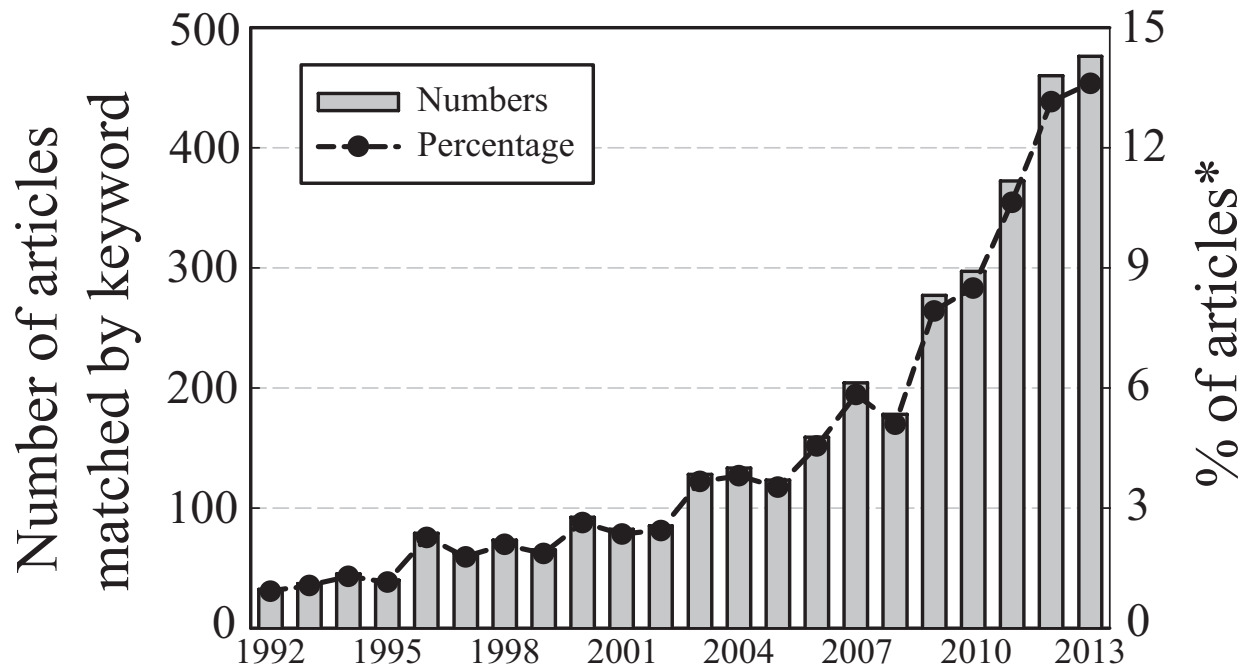


Figure 4-1. Number of articles selected by keywords (histogram) with the percentage of articles (dotted line) from 1992 to 2013 based on a search of Web of Science with the keywords “life cycle assessment” and “environmental assessment,” accessed on October 13, 2014; * percentage of selected articles with the keyword LCA of the total number of articles.

Meta-analysis is a part of the systematic review. It is performed by melding data from multiple studies with additional mathematical analyses to answer questions that cannot be addressed by existing individual studies, or by increasing the sample size (*i.e.*, the number of estimates) to improve the certainty or impact of known findings (Zumsteg *et al.* 2012). In other words, meta-analysis is a quantitative statistical technique aimed at combining the results of several studies to test the pooled data for statistical significance (Zamagni *et al.* 2012). In the course of methodological development of LCA, meta-analysis has recently emerged as a tool to structure the present LCA studies and organize unexplored areas, questions, and research priorities to further develop LCA (Zamagni *et al.* 2012).

To the best of the authors' knowledge, among the total of 20 LCA meta-analysis studies (Lenzen *et al.* 2002; Farrell *et al.* 2006; Larson 2006; Sartori *et al.* 2007; Villanueva *et al.* 2007; von Blottnitz *et al.* 2007; Werner *et al.* 2007; Sovacool 2008; Bhat *et al.* 2009; Mondelaers *et al.* 2009; Ortiz *et al.* 2009; De Vries *et al.* 2010; Kubiszewski *et al.* 2010; von Falkenstein *et al.* 2010; Whitaker *et al.* 2010; Heath *et al.* 2011; Santero *et al.* 2011; Sunde *et al.* 2011; Burkhardt *et al.* 2012; Manik *et al.* 2013), only one study focused on packaging options (von Falkenstein *et al.* 2010), where the environmental performance of beverage cartons was compared with alternative packaging systems based on the information provided in 22 reported LCA studies. The results of that study were presented by ranking the different packaging options by their environmental performance, allowing comparison of the environmental assessment of the beverage packages. However, this ranking method leads to a limitation in the study interpretation since it cannot answer questions such as which life cycle stage contributes the most to the total environmental burden, and it also cannot be used to differentiate the environmental performance between the different types and stages of the beverage packages.

LCA studies of beverage packaging are increasing, which could be attributed to the generation of the large environmental burden when this type of packaging is produced and disposed. In 2012, 193 billion beverage packaging units were sold in the US, representing 176 billion US dollars (Euromonitor International 2013f). Among the different types of plastic beverage packages, polyethylene terephthalate (PET) represented 38 % of the total beverage packages sold in 2012 in the US (Euromonitor International 2013a). Due to this large volume and subsequent considerable environmental burden, there may be an opportunity for significant reduction of the environmental burdens of the PET beverage bottle system by identifying any 'hot spots' in its life cycle.

As a result, the main goal of this study is using meta-analysis by taking into consideration different LCA studies from the reductionism standpoint to address the following objectives: 1) to evaluate the variation of the environmental impact in each life cycle stage of the PET beverage bottle system, and 2) to identify the source of variation in each life cycle stage. Overall, the goal of this study is to better understand the variability in the results of the PET beverage LCA studies, so that better-informed decisions can be made.

4.3 Materials and Methods

4.3.1 Life cycle process description

The overall life cycle of the PET beverage bottle system is described in Figure 4-2. In order to apply the harmonization process, the system was divided into 4 main phases: upstream, transportation, downstream and environmental benefit. The life cycle of the PET beverage bottle starts with raw material acquisition, such as crude oil to produce the purified terephthalic acid (PTA) and ethylene glycol (EG) to produce the amorphous PET resin (APET). After the solid-state polymerization process of APET, bottle grade PET resin is produced. In this study, an alternative scenario to produce the APET is also considered, which is producing plant-based PTA by utilizing benzene, toluene, and xylene (BTX) as the process intermediates (Akanuma *et al.* 2014). Using bottle grade PET resin, the PET beverage bottle is produced by injection stretch blow molding (ISBM). During ISBM, post-industrial plastic waste is produced. Then, the PET bottle is filled with beverage and packed using secondary packaging. The transportation phase includes the delivery of PET beverage bottles and collection of post-consumer PET bottles (PCB). The uncollected PCB is considered as municipal solid waste (MSW), mostly managed by incineration and landfill. In the downstream phase, after the PCBs are collected, they are

delivered to the material recovery facility (MRF) to separate the bottle components, such as caps and labels, and to produce baled PET. The baled PET is introduced to the recycling facility to produce the recycled PET resin. Depending on the material efficiency of the recycling process, varying amounts of waste are produced. In this system, 3 main routes are considered to generate environmental benefit; replacing the virgin APET resin in the system (closed loop recycling), replacing the virgin APET resin outside of the system (open loop recycling) and energy recovery from incineration.

To facilitate the analysis of the results, the life cycle stages were coded as series X, U, T and D. Code series X was only included in the narrative review and excluded in the statistical analysis since this data was already included in the U code series as cradle to gate data. The code series U involves the upstream phase, including bottle grade PET resin production (U1), PET bottle production (U2), filling process (U3) and secondary packaging production (U4). The code series T is for transportation, specifically delivery of filled beverage bottles to customers (T1) and collection of PCB (T2). The code series D belongs to the downstream phase: material recovery process (D1), recycling (D2) and landfill (D3). The code series E represents the environmental benefit phase, specifically the environmental benefit of closed loop (E2) and open loop (E3) recycling and energy recovery by incineration (E1). The environmental impact of incineration (E1) is considered as the summation of the environmental burdens of combusting the waste and the environmental benefit of energy recovery from the combustion process.

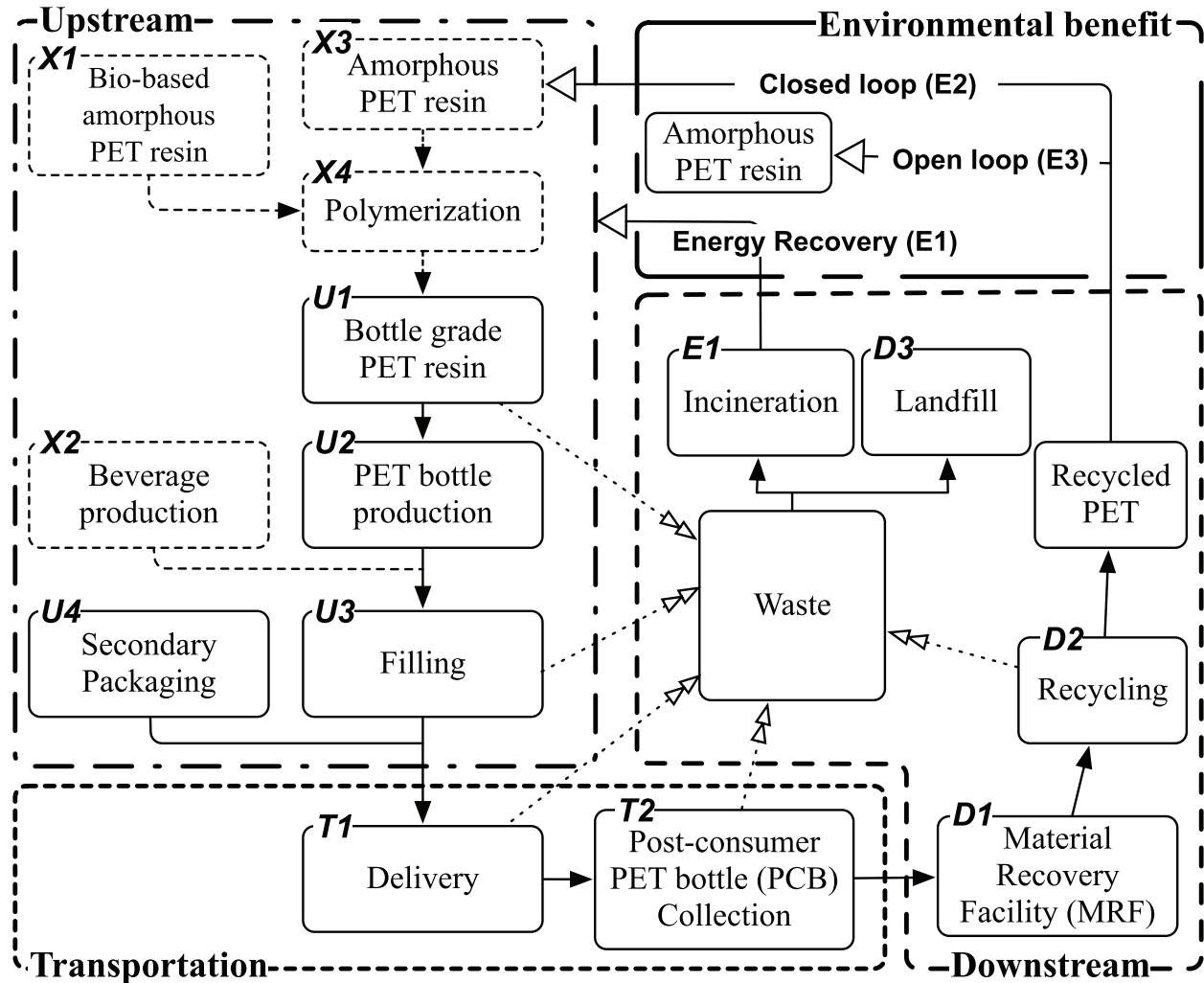


Figure 4-2. Life cycle of PET beverage bottle system describing the upstream, transportation, downstream and environmental benefit stages used in the harmonization process; the box letter indicates the life cycle stage; X series (dashed line boxes) were excluded from the cluster analysis; Incineration stage (E1) is the summation of the environmental burden (combustion) and environmental benefit (energy recovery)

4.3.2 Literature gathering and screening approach

An extensive search of the English-language literature yielded 212 journal articles, full reports, life cycle inventory (LCI) databases with keywords ‘life cycle assessment and PET’ or ‘life cycle assessment and polyethylene terephthalate’ or ‘life cycle assessment and beverage packaging’. Each study was independently subjected to the screening process, consistent with the screening methodology of the LCA harmonization project (Heath *et al.* 2012). Even though some of the literature reported Global Warming Potential (GWP) (kg CO₂ eq) or energy consumption (EC) (MJ/kg) estimates for only some of the disaggregated life cycle stages of the PET beverage bottle system, they were included in the literature gathering to increase the number of estimates. For example, Chilton *et al.*, (Chilton *et al.* 2010) studied the end of life scenario for PET beverage bottles, especially closed loop recycling and thermal recovery from incineration. Even though this study did not fully analyze the life cycle of the PET beverage bottle system, it was selected in the pool of references to collect data for recycling and incineration.

The screening process eliminated some of the initially collected references based on several gross discriminators (Figure 4-3). Literature published in 1999 or after, and that reported the impact assessment at the characterization level, and provided a contribution analysis for the PET beverage bottle system was selected. The literature that did not meet these previous conditions was excluded. Several LCI databases from SimaPro 7.3.3 and LCA reports were also investigated and included if they met the screening criteria. Of the 212 references collected, 13 LCA journal articles (Arena *et al.* 2003; Chilton *et al.* 2010; Nakatani *et al.* 2010; Shen *et al.* 2010; Intini *et al.* 2011; Pasqualino *et al.* 2011; Shen *et al.* 2011; Amienyo *et al.* 2013; Cleary 2013; Kuczenski *et al.* 2013; Akanuma *et al.* 2014; Manfredi *et al.* 2014; Papong *et al.* 2014), 4 LCI databases (Sylvatica 2009; Franklin Associates 2010) and 6 LCA full reports (Dettore 2000;

Raadal *et al.* 2003; Detzel *et al.* 2004; Jelse *et al.* 2009; Kuczenski *et al.* 2011; Doublet 2012) met the screening criteria. Detailed screening results for each article are included and described in appendix B and C.

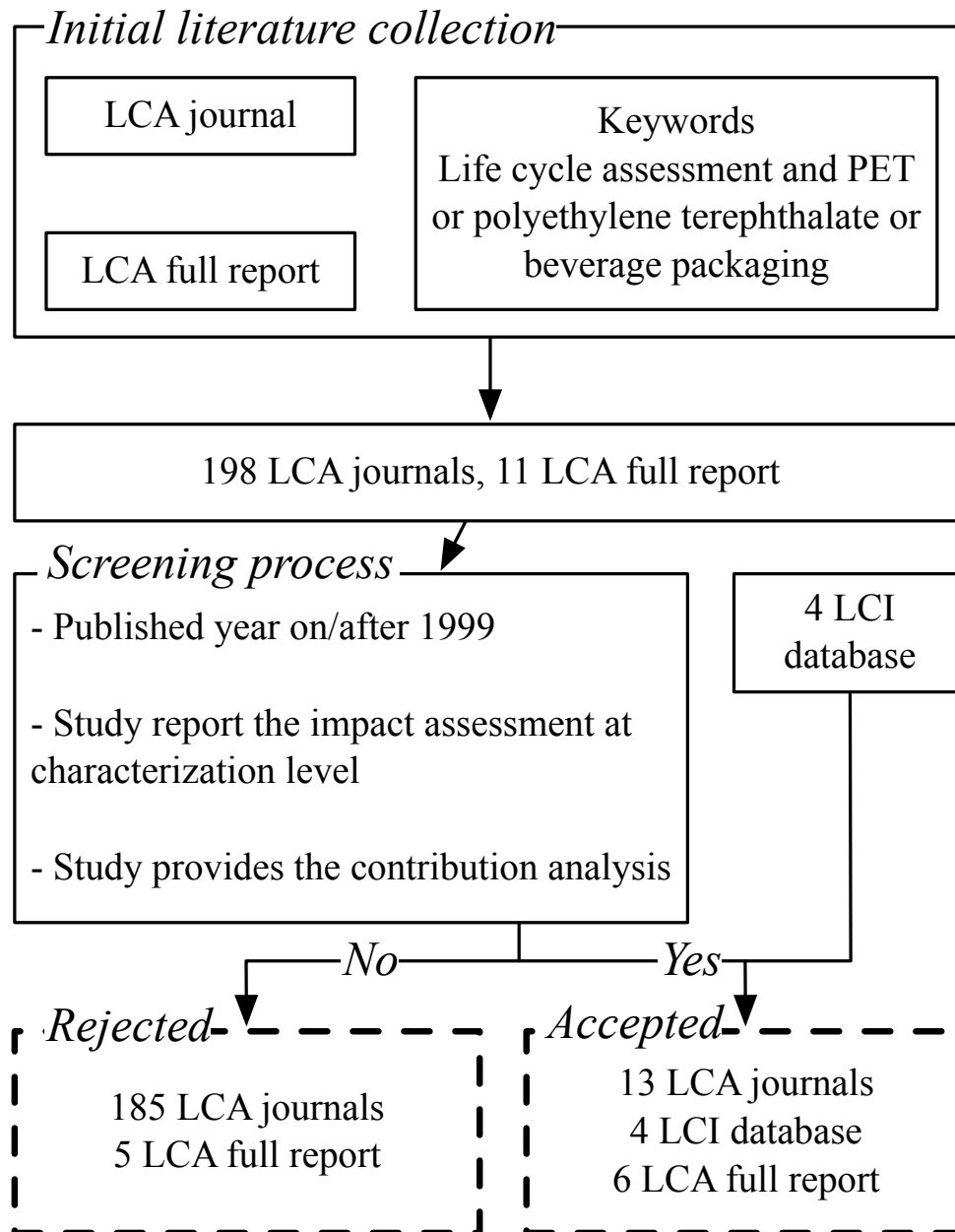


Figure 4-3. Flow diagram of literature collection and screening process

4.3.3 Harmonization approach

Two levels of harmonization have commonly been used. The more resource-intensive level is well described in the study conducted by Farrell et al. (Farrell *et al.* 2006) where they depicted the harmonization process of the results of LCAs of ethanol by carefully disaggregating a subset of the available literature estimates of life cycle greenhouse gas (GHG) emissions. By this process, a meta-model was generated based on adjusted parameter estimates, realigned system boundaries within each life cycle phase, and a review of all data sources. A less resource-intensive harmonization process can be applied to a larger set of literature estimates of environmental emissions at a more unrefined level (Hsu *et al.* 2012; Warner *et al.* 2012). Because the literature passing the final screening generally did not provide enough detail to apply the more intensive approach, the less-intensive harmonization approach was chosen for meta-analysis of the PET beverage bottle system. Under the less-intensive harmonization approach, GWP and EC indicator estimates were extracted at face value and converted to consistent units before being harmonized.

The harmonization process was performed using equations (4-1) and (4-2)

$$GWP \left(\frac{kg \ CO_2eq.}{kg \ of \ FU} \right) = \sum_{i=1}^{12} \frac{GWP_i}{(kg \ of \ material_i | kg \ of \ FU)} \quad (i = U1, U2 \dots E2, E3) \quad (4-1)$$

$$EC \left(\frac{GJ}{kg \ of \ FU} \right) = \sum_{i=1}^{12} \frac{EC_i}{(kg \ of \ material_i | kg \ of \ FU)} \quad (i = U1, U2 \dots E2, E3) \quad (4-2)$$

where GWP and EC are the impact indicator values per kg of functional unit (FU) of each study. This calculation is used in most LCA studies of the PET beverage bottle system. The numerators, GWP_i and EC_i , are the impact indicator values at the i th life cycle stage (total 12 life cycle stages) described in Figure 4-2. The denominator calculates the kg of output in i th life cycle stage with respect to kg of FU in each study.

4.3.4 Statistical analysis of the data

Statistical analysis of the central tendency and the variability of the harmonized datasets were conducted to characterize estimates of GWP and EC indicator values in each life cycle stage using R package (version 3.0.2) (R Core Team 2013). The central tendency is described as both medians and arithmetic means of the datasets. Variability of the datasets also is reported using multiple parameters, including the standard deviation (SD), the range (i.e., the maximum value minus the minimum value), and the interquartile range (IQR) (i.e., the 75th percentile value minus the 25th percentile value). To compare the size of variability among estimates, the value of IQR divided by the median (i.e., RELIQ = Interquartile range divided by the median) was used. It was considered that there is small, medium and large variability in estimates if the RELIQ value is less than or equal to 0.4, higher than 0.4 and less than or equal to 1.5, and higher than 1.5, respectively. The discussion in this study focuses on the median, IQR and RELIQ because these are more robust indicators of dataset central tendency and spread than the mean, SD, or range. The median and IQR are not heavily influenced by the dataset outliers and by the distribution of the datasets. In addition to central tendency and variability, K-means cluster analysis was conducted to analyze the statistical differences among the estimates as a function of the life cycle stage. K-means clustering is designed to group estimates, rather than variables, into a collection of K clusters (Johnson *et al.* 2007). The appropriate number of clusters is determined by comparing the within-cluster sum of squares for a number of cluster solutions.

Additionally, one-way analysis of variance (ANOVA) was performed to identify the factors (*i.e.*, the predictor variable) affecting the weight of PET bottles per liter (*i.e.*, the response variable). From the 13 studies passing the final screening criteria and personal measurements, 42 data points were obtained. Four predictor variables were selected: beverage types, regions, year

and volume with different levels. One of the assumptions to conduct the ANOVA is that the predictor variables are not correlated to each other. If factors are correlated to each other (multicollinearity), many problems can arise, such as 1) Adding or deleting a predictor variable changes the regression coefficients; 2) The extra sum of squares associated with a predictor variable varies; 3) The estimated standard deviations of the regression coefficients become large when the predictor variables in the regression model are highly correlated with each other; and 4) The estimated regression coefficients individually may not be statistically significant even though a definite statistical relation exists between the response variable and the set of predictor variables (Kutner *et al.* 2005). To check the multicollinearity issue, the variance inflation factor (VIF) is often considered. The rule of thumb indicates if the VIF value is in excess of 10, then there is a multicollinearity issue (Kutner *et al.* 2005). After confirming the significant factors, a multiple comparison of factor level means was conducted using the Tukey's test from the R package 'agricolae' (Mendiburu 2014).

The overall purpose of this statistical analysis was to summarize the current state of LCA literature for the PET beverage bottle system. Despite the reasonably large number of collected high quality studies, we acknowledge that they may not represent every possible case for the PET beverage bottle system. Consequently, the probability distribution of the harmonized datasets also may not represent the probability distribution for the actual GWP and EC of the PET beverage bottle system.

4.4 Results and Discussion

4.4.1 Source of variability for the weight of PET bottles per liter

Prior to the harmonization process, the sources of variability were evaluated. Table 4-1 indicates the results of the ANOVA for factors affecting the PET bottle weight per liter. The types of beverage, regions of market for the beverage, year, and volume of the beverage bottle were chosen as predictor variables for the PET bottle weight per liter. There were five types of beverages (carbonated soft drinks (CSD), water, juice, milk and alcohol), three different regions (North America, Europe and Asia), two different time scales (before 2010 and in or after 2010) and three different volumes (i.e., equal or lower than 0.5 L, higher than 0.5 and equal or lower than 1.0 L, higher than 1.0 L)

According to the ANOVA results, the types of beverage, regions and volume were statistically significant for the PET weight of the FU at the 95% confidence level (95% CL). The VIF was used to check for multicollinearity among the factors (Kutner *et al.* 2008). None of the variables has multicollinearity issues since all the VIF were much lower than 10 (Table 4-1).

Table 4-1. ANOVA analysis for the different factors affecting the PET bottle weight per liter considered in the meta-analysis

Variables	DF	Sum of Squares	Mean of Squares	F value	Pr(>F)	VIF
Beverage types	4	4540.8	1135.2	9.773	2.782E-05	1.074
Regions	2	1378.0	689.0	5.932	0.006	1.171
Year	1	101.7	101.7	0.8752	0.357	1.065
Volume	2	1310.3	655.15	5.640	0.008	1.245
Residuals	32	3716.9	116.15			
Total	41	11047.7				

Figure 4-4 describes the results of Tukey's test for evaluating the statistical differences among types of beverage and regions. For the types of beverage, it was clearly shown that alcohol was statistically significantly different from CSD, water, juice and milk. Except for the alcohol PET bottle, the other PET beverage bottles have fairly consistent PET bottle weight per liter. For the regions, North America and Europe had no statistically significant differences. Due to lack of data representation for Asia, it may not be appropriate to conclude that Asia had statistically higher PET bottle weight per liter than North America and Europe. The beverage bottle over than 1.0 L has statistically significantly different weight than the others with volume lower than 0.5 L and/or between 0.5 and 1L. The statistical differences of PET bottle weight per L as function of different factors imply the importance of the harmonization process. That is, the harmonization process normalized the effect of this significant difference rooted from different factors.

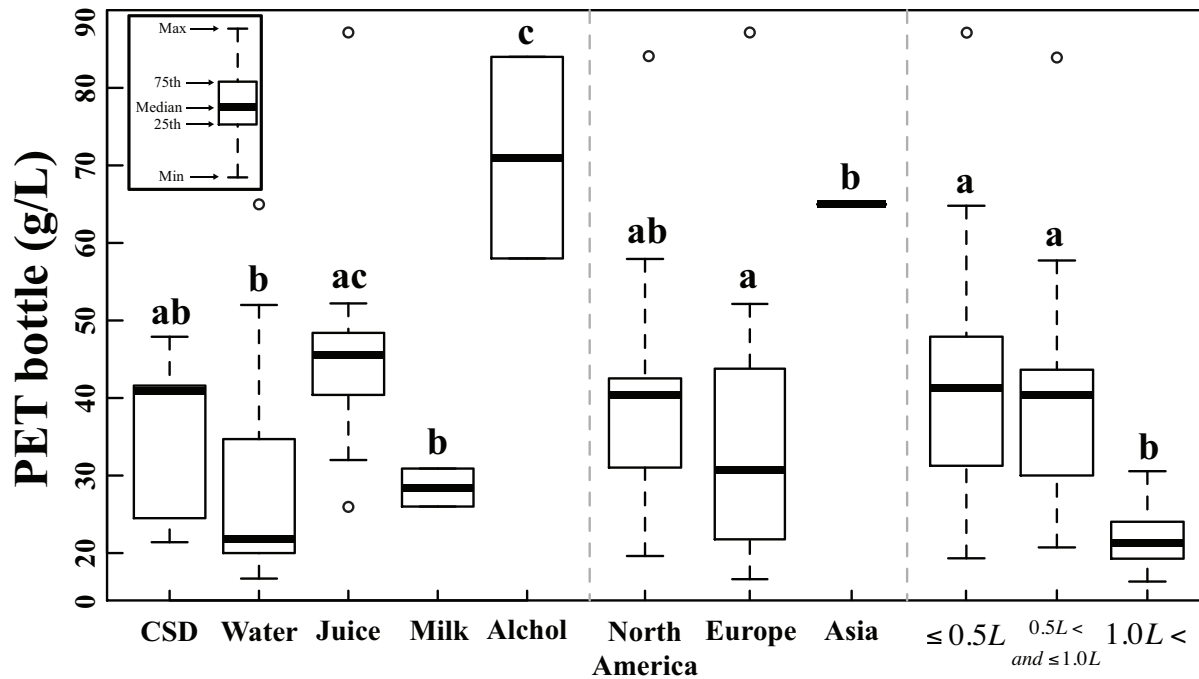


Figure 4-4. Box plots comparing the FU as a function of types of beverage and regions; different letters on top of the whisker indicate statistically significant differences at the 95% confidence level

4.4.2 Sources of variability for the supply chain of the PET beverage bottle

Other sources affecting the variability of the datasets were selected for the life cycle of the PET beverage bottle system, such as the efficiency of ISBM, product loss during filling and distribution, secondary packaging, PCB and MRF efficiency, material efficiency of the recycling process, calorific value of PET, and efficiency of electrical energy recovery from the incineration facility (Table 4-2). During ISBM, post-industrial waste is produced. The median ISBM efficiency was 96.67% with IQR of 3.88%. This indicates this source has relatively small variability ($RELIQ = 0.04$). During filling and distribution, the median loss was 1.525% with IQR 1.39%, indicating medium variability ($RELIQ = 0.91$) due to different filling processes, such as hot filling or aseptic filling. Consistency was found in the type of secondary packaging

for the PET beverage bottle system (*i.e.*, shrink film made of low-density polyethylene (LDPE), corrugated boxes and wood pallets). The efficiency of PCB collection and the MRF had a median of 81.5% with IQR 11.8%, showing that there is relatively small variability (RELIQ = 0.14) of efficiency among different collection methods, such as drop-off and curbside collection in different regions. Material efficiency of recycling had a median of 80% with IQR 5.95%, implying that the PET recycling technique is relatively consistent (RELIQ = 0.07). Electricity efficiency of energy recovery from combustion of waste had relatively medium variability with median 28.85% and IQR 14.08% (RELIQ = 0.49).

Table 4-2. Sources of variability for the ISBM, filling, efficiency of PCB collection and MRF, material efficiency of recycling, calorific value of PET and electricity efficiency of energy recovery from incineration facility

Sources	Central tendency		Variability		RELIQ
	Mean	Median	SD	IQR	
Efficiency of ISBM (%)	95.16	96.67	4.06	3.88	0.04
Product loss during filling and delivery (%)	1.783	1.525	1.21	1.39	0.91
PCB and MRF efficiency (%)	79.89	81.5	13.9	11.8	0.14
Material efficiency of recycling (%)	80.79	80.00	8.14	5.95	0.07
Calorific value of PET (MJ/kg)	23.01	23.03	0.05	0.05	0.00
Electricity efficiency of energy recovery from incineration facility (%)	34.45	28.85	14.57	14.08	0.49

4.4.3 Harmonized Results

Harmonized results are described in Table 4-3 and Figure 4-5. The X series consists of amorphous PET resin production from a petroleum-based or plant-based, solid-state polymerization and beverage production. The X series values are not considered in the cluster analysis for several reasons. In the case of X3 and X4, the environmental burden is already included in the PET bottle grade resin production (U1). Thus, in order to avoid duplicate counting, X3 and X4 were excluded from the cluster analysis. X1 represents the GWP (kg CO₂ eq / kg of FU) and EC (GJ / kg of FU) of bio-based amorphous PET resin, with median 4.28 and IQR 2.68 (RELIQ = 0.63) and median 0.069 and IQR 0.011 (RELIQ = 0.16), respectively. The relatively large variability of GWP and EC in X1 is because most data were based on lab-scale production, not from pilot or commercial production. Potential production of PET from renewable resources is, however, receiving a lot of attention in the beverage packaging industry. According to the Coca-Cola Company, they decided to make an additional investment in the full-scale commercial production of 100% plant-based PET plastic packaging, using Virent's bio-based paraxylene, BioFormPXTM (Mohan 2014). Eventually, production improvements for bio-based PET resin production are expected to reduce the GWP and EC, but at this stage, it was not included in the cluster analysis since it does not represent a common commercial technology. X2 indicates the beverage production stage, showing median of 0.82 with IQR 2.57 for GWP (kg CO₂ eq / kg of FU) (RELIQ = 3.13) and median of 0.025 with IQR 0.093 for EC (GJ / kg of FU) (RELIQ = 3.72). X2 has large variability not because of technological efficiency, but due to different beverage types, namely, CSD, water, juice and beer. Specifically, beer (2.16 kg CO₂ eq/L and 0.0523 GJ/L) (Pasqualino *et al.* 2011) has much higher GWP and EC than juice (0.029 kg CO₂ eq/L and 0.0002 GJ/L) (Pasqualino *et al.* 2011), water (0.004 kg CO₂ eq/L and 0.00002

GJ/L) (Pasqualino *et al.* 2011) and CSD (0.080 kg CO₂ eq/L and 0.00428 GJ/L) (Amienyo *et al.* 2013), mainly due to the consumption of barley and hops for beer production. As previously stated, X2 was not included in the cluster analysis.

The U series includes the PET bottle grade resin production (U1), PET bottle production (U2), filling (U3) and secondary packaging production (U4). GWP (kg CO₂ eq / kg of FU) and EC (GJ / kg of FU) of U1 have small variability with 2.96 median and 0.74 IQR (RELIQ=0.28) for GWP, and 0.078 median and 0.015 IQR (RELIQ=0.256). U2 has 1.22 median with 0.62 IQR (RELIQ=0.54) for GWP, and 0.026 median with 0.007 IQR (RELIQ=0.310) for EC, respectively. GWP and EC of U3 have relatively high variability due to different filling processes; especially hot filling and aseptic filling. One of the factors contributing to the large variability in filling is the percent of product loss rate, as described in Table 2. Another factor is that hot filling consumes more steam, whereas the aseptic process requires more electricity consumption to maintain a controlled atmosphere during filling (Manfredi *et al.* 2014). U4 represents the secondary packaging production, with 0.416 median and 0.365 IQR for GWP (kg CO₂ eq / kg of FU), and 0.013 median and 0.008 IQR for EC (GJ / kg of FU). GWP and EC of T1 and T2 tend to rely on the transportation scenario of each study instead of vehicle efficiency. T2, however, is also affected by different collection rates in the collection system (Table 2), such as drop-off centers and curbside programs. GWP (kg CO₂ eq / kg of FU) and EC (GJ / kg of FU) of D1 are 0.15 median and 0.31 IQR (RELIQ= 2.06) and 0.002 median and 0.004 IQR (RELIQ= 1.97), respectively. The main reason of this large variability is from the different levels of detail in the inventory databases. According to Intini and Kühtz (Intini *et al.* 2011), a plant consumes 43 kWh of electricity and 3.4 L of diesel for 1 ton of input plastic, whereas in the Franklin report (Franklin Associates 2010), 16.4 kWh of electricity, 2.25 L of natural gas, 1.84 L of diesel and

2.5 L of propane with 40 kg of plastic waste was consumed for 1 ton of input plastic. The large variability in D2 (RELIQ for GWP and EC was 1.35 and 1.71, respectively) was rooted in different recycling processes, such as chemical, semi-chemical and mechanical recycling. The lowest GWP and EC was found from mechanical recycling (0.96 kg CO₂ eq/kg of PET and 0.013 GJ/kg of PET) (Shen *et al.* 2010), as also well described in the WRAP report (Michaud *et al.* 2010). D3 represents the landfill, reporting 0.175 median with 0.33 IQR (RELIQ= 1.91) for GWP (kg CO₂ eq / kg of FU) and 0.0002 median with 0.001 IQR (RELIQ=5.82) for EC (GJ / kg of FU). Due to different waste management scenarios for each study, large variability was found in this life cycle stage. For example, in work conducted by Nakatani et al. (Nakatani *et al.* 2010), the end of life scenario was only focused on PET waste, whereas Amineyo et al. (Amienyo *et al.* 2013) considered PET waste, secondary packaging waste and waste water. GWP (kg CO₂ eq / kg of FU) and EC (GJ / kg of FU) of E1 is a summation of environmental burdens from combustion and environmental benefits from energy recovery. Large variation (RELIQ for GWP and EC was 2.29 and 8.70, respectively) was reported due to medium variation in efficiency of electrical energy recovery from the incineration facility, as shown in Table 4-2. Another reason for this large variation in the estimate of E1 is because of different waste management scenarios applied. E2 and E3 indicate the environmental benefits of closed loop and open loop recycling, respectively. As shown in Table 4-3, GWP and EC of E2 are consistent (RELIQ for GWP and EC was 0.4 and 0.3, respectively), whereas E3 has medium variability (RELIQ for GWP and EC was 1.0 and 0.4, respectively). The mean and SD of GWP and EC for each life cycle stage are presented in appendix D Table D-1.

Table 4-3. Harmonized results with median and IQR for GWP and EC for the life cycle stages of PET beverage bottle.

Life cycle stage	GWP (kg CO ₂ eq / kg of FU)			EC (GJ / kg of FU)		
	Median	IQR	RELIQ	Median	IQR	RELIQ
X1	4.28	2.68	0.625	0.0686	0.0106	0.155
X2	0.823	2.57	3.13	0.0252	0.0925	3.67
X3	2.44	0.440	0.180	0.0759	0.00175	0.0230
X4	0.165	0.0845	0.512	0.00290	0.000987	0.341
U1	2.76	0.765	0.277	0.0761	0.0195	0.256
U2	1.20	0.641	0.536	0.0279	0.00866	0.310
U3	0.794	1.06	1.34	0.00580	0.00585	1.01
U4	0.416	0.365	0.877	0.0134	0.00811	0.605
T1	0.454	1.06	2.33	0.0133	0.0183	1.38
T2	0.0400	0.0440	1.10	0.000410	0.000500	1.22
D1	0.150	0.309	2.06	0.00190	0.00374	1.97
D2	0.830	1.12	1.35	0.00740	0.0126	1.71
D3	0.175	0.334	1.91	0.000200	0.00116	5.82
E1	1.32	3.02	2.29	-0.00816	0.0708	8.70
E2	-2.15	0.788	0.366	-0.0575	0.0146	0.254
E3	-1.68	1.65	0.977	-0.0436	0.0187	0.429

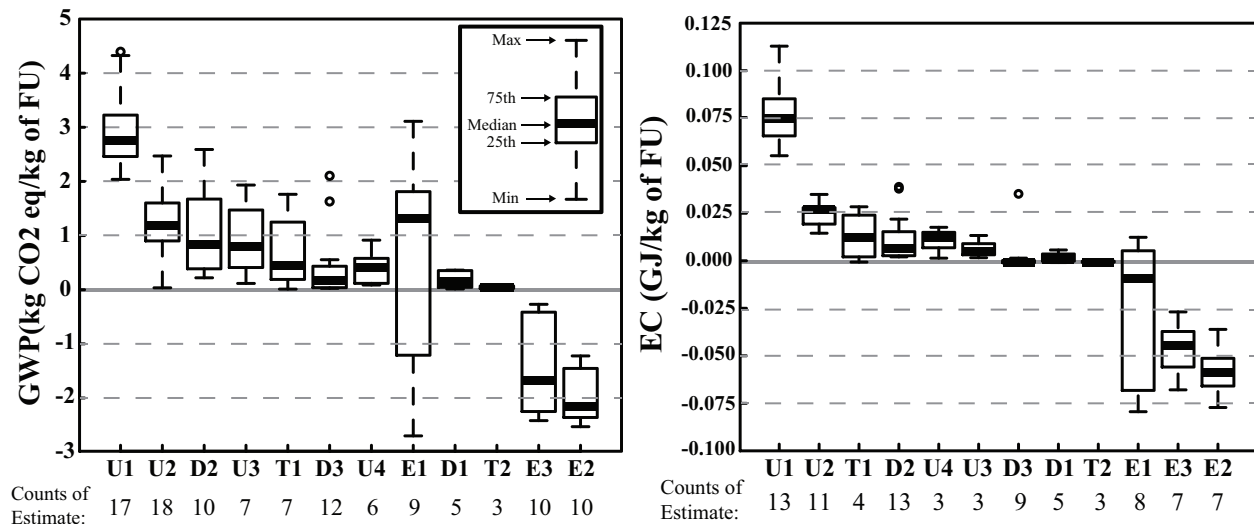


Figure 4-5. Box plots of harmonized results; “Counts of Estimate” indicate the number of estimates from independent studies that were harmonized.

4.4.4 Cluster analysis

Cluster analysis is a technique in which no assumptions are made concerning the number of groups or the group structure (Johnson *et al.* 2007). In this study, *K-means* clustering was applied. MacQueen (MacQueen 1967) suggests the term *K-means* for describing an algorithm that assigns each item to the cluster having the nearest centroid. In *K-means* clustering, *K* numbers of initial clusters need to be defined. One of the methods to define the initial number of clusters is using a scree plot (Johnson *et al.* 2007). In Figure 4-6 (left), the within groups sum of square errors (SSE) is described as a function of the cluster solution. An appropriate cluster solution is defined as that at which the reduction in SSE slows dramatically producing an “elbow” in the plot of SSE against cluster solutions when more than 90% of the total variation is explained. In Figure 4-6 (left), there is an “elbow” at the 4 cluster solution suggesting that solutions higher than 4 clusters do not have a substantial impact in the total SSE. Figure 4-6 (right) describes the results of cluster analysis with 4 clusters. The center of the circles indicates

the mean, and the radius of the circles shows the SSE. The red circle contains most of U1 estimates, whereas the blue circle covers most of U2. Due to the large variability in E1, estimates of E1 are distributed in the black, green and red circles. The green circle includes most of the rest of the estimates, except E2 and E3, which belong to the black circle. The total variation covered by the 4 clusters was 94.0%.

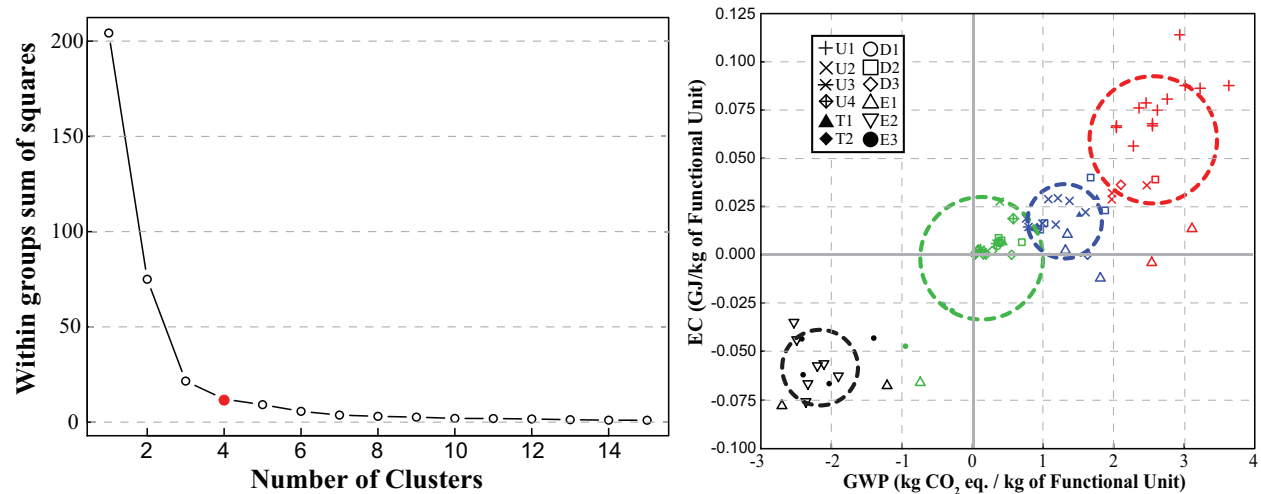


Figure 4-6. Scree plot for SSE as function of cluster solution (left), results of cluster analysis (right)

4.5 Limitations

The aim of this study was to evaluate the variability of GWP and EC estimates in each life cycle stage of the PET beverage bottle system. However, to provide a more comprehensive perspective of the environmental impacts of the PET beverage bottle system, other parameters, such as human health impacts and water contamination, should be assessed.

In this study, two impact indicators were chosen to harmonize the results: GWP and EC. GWP is known as the most often quantified environmental impact with international agreement (Bare *et al.* 2012). There are, however, several impact indicators representing EC, such as non-

renewable energy consumption (NREC), cumulative energy demand (CED) and primary energy demand (PED). Despite the slight differences among these EC indicators, they were considered as equal in this study to harmonize the EC estimates.

During data collection, it was found that most of the journal articles reported the total GWP and EC estimate values, and described the estimates for each disaggregated life cycle stage in a stacked bar chart. To determine the values from the stacked bar chart, Adobe® Illustrator® was used to measure the length of each stack and then determine the contribution for each phase. This methodology allowed us to increase the sample size, but it also may increase the inaccuracy in the harmonization. A graphical explanation of extracting the values from the stacked bar charts is provided in Figure C-1 of appendix C.

Another potential limitation of this study is that some of the selected studies may not represent statistically independent samples. There are three potential issues: multiple estimates reported in the same reference, multiple estimates from the same or similar author groups publishing serially, and multiple references citing the same sources of input data. This effect was not considered in this study.

4.6 Conclusions

Meta-analysis was applied to the existing published literature of LCA for PET beverage bottle systems. Initial criteria selection for the meta-analysis yielded 212 references. Through the screening process, 13 LCA journal articles, 4 LCI database entries and 6 LCA full reports were selected for the statistical analysis. The PET beverage bottle system life cycle was divided into 4 main phases: upstream, transportation, downstream and environmental benefit. Each phase was further disaggregated. A harmonization process was performed to obtain the GWP and EC estimates for each disaggregated life cycle stage.

Statistical assessments of the central tendency and variability were performed. The life cycle stage for GWP and EC with the largest contribution was bottle grade PET resin production (2.76 median with 0.77 IQR for GWP (kg CO₂ eq / kg of FU) and 0.076 median with 0.020 IQR for EC (GJ / kg of FU)). The largest IQR of GWP and EC was found in the incineration of waste (1.317 median with 3.02 IQR for GWP (kg CO₂ eq / kg of FU) and -0.008 median with 0.071 IQR for EC (GJ / kg of FU)) due to large variation in efficiency of electrical energy recovery from the incineration facilities. The environmental performance of incineration relies heavily on the efficiency of the incineration technology, so it can be improved by employing the most efficient technology for energy recovery. Cluster analysis revealed that 4 main clusters could categorize all the estimates. The first group contained most of the U1 estimates, implying that bottle grade PET resin production can be statistically separated from other life cycle stages. The second group includes most of the U2 and E1 estimates, while the third group covers the rest of the life cycle stage estimates, except E2 and E3.

Among the many sources of variability, the variability of incineration with energy recovery (E1) was partially influenced by technology efficiency. It was also found that the largest variation of GWP and EC was found in E1. This may imply that the best possible option to improve the environmental performance of the PET beverage bottle system can be achieved by employing the highest efficiency electrical energy recovery for incineration of plastic waste. Moreover, the largest GWP and EC contributing life cycle stage was the bottle grade PET resin production, which endorses development of lightweight PET bottles as an effective strategy to reduce the total environmental burden of the PET beverage bottle system. This study could be used to inform future advancement in reducing the environmental burdens of the PET beverage bottle system.

Chapter 5. A PRELIMINARY SYSTEM DYNAMICS AND LIFE CYCLE ASSESSMENT APPROACH TO DETERMINE THE GLOBAL WARMING POTENTIAL OF PET BEVERAGE BOTTLE IN THE STATE OF CALIFORNIA

5.1 Abstract

A system dynamics and life cycle assessment (LCA) approach was preliminarily applied to construct a dynamic assessment of the global warming potential (GWP) of PET beverage bottles in the state of California. The goals of this study were to conduct a contribution analysis of the historical GWP of PET beverage bottle system and to evaluate the impact of recycled PET (RPET) content and crude oil price over time on PET beverage bottles in terms of CO₂ tax (\$/ton) and GWP. In order to construct the GWP model, the GWP estimates obtained from the LCA and its probability distribution of each life cycle stage from Chapter 4 were used.

Approximately 67% of total GWP was contributed by the upstream phase of the PET beverage bottle system including the production of the PET resin, the manufacture of the PET bottle, bottle filling and the production of secondary packaging. The GWP value of PET beverage bottle systems in 2010 (180.05 ± 55.4 kg CO₂ eq) was also compared with the results of Chapter 3 (187.4 ± 28.4 kg CO₂ eq.), which indicates that the GWP model in this chapter was properly established to calculate the total GWP.

The effect of RPET content and crude oil price on CO₂ tax was evaluated through 12 hypothetical scenarios. Under the scenario where the crude oil price will be constantly low, the CO₂ tax (\$/ton) was expected to increase due to the high favor to use virgin PET (VPET) resin. It has, however, relatively minor impact compared to the effect of RPET content in PET bottles. By

increasing from 20% to 60% and 60% to 100%, the expected CO₂ tax and GWP saving averaged 32.4 and 19.8 million dollars and 0.81 and 0.5 billion kg CO₂ eq., respectively.

5.2 Introduction

During 2012, the US consumed a total of 193 billion beverage packaging units, equal to 176 billion US dollars (Euromonitor International 2013e). Among the many types of beverage packaging, polyethylene terephthalate (PET) is the largest plastic used for beverage packaging, accounting for 38 percent of the total beverage packaging units in the US (Euromonitor International 2013a). The US market for PET beverage packaging has gradually increased from 67 billion units in 2008 to 85 billion units in 2013 due to the increasing demand for bottled water, functional drinks, ready-to-drink tea, and flavored milk drinks delivered in PET containers (Euromonitor International 2010). The state of California consumed the largest number of bottles and cans among all the US states in 2012, about 11 percent of the total US beverage packaging units sold (Calrecycle 2013b). With 2400 certified recycling centers, 601 curbside recycling programs (CalRecycle 2014) and the California Beverage Container Recycling Litter Reduction Act, the state of California is also the number one PET recycling state, reporting a recycling rate of 70 percent for PET beverage bottles in 2012 (Calrecycle 2013b).

There are many socio-economic factors affecting beverage consumption, such as prices and demographics. Some of the available studies (Grimm *et al.* 2004; Storey *et al.* 2006; Bere *et al.* 2008) were designed to find factors influencing the preference and consumption of different beverage type whereas other available studies were focused on forecasting the demand for beverages using a Translog demand system (Yen *et al.* 2004), GM(1,1) model of Grey theory (Lin *et al.* 2002), and the three-stage demand model (Rickertsen 1998). Among the many socio-

economic factors, prices do provide a partial answer to estimate the demand of beverage (Yen *et al.* 2004). Even though beverage consumption varies depending on demographic characteristics (Forshee *et al.* 2003), an increase in per capita regular carbonated soft drink consumption was reported (Nielsen *et al.* 2002; French *et al.* 2003; Nielsen *et al.* 2004). With a positive population growth expected by the US Census Bureau (US Bureau of the Census 2012), it is safe to assume that population growth is a significant factor contributing to the demand for beverages.

Life cycle assessment (LCA) is known as a holistic method to evaluate the environmental impact of products or systems. One of the limitations known in LCA is that life cycle inventory analysis assumes that input parameters are constants or fixed functions in time. This limitation stems from the inherent nature of LCA, but it also limits the opportunities to account for temporal and spatial effects. Consequently, most LCA models predominantly reflect steady-state conditions (Kloepffer 2008). This is because fixed input parameters preclude consideration of the dynamics of the product system. The term, dynamics, refers that the system changes over time considering internally and externally generated forces.

PET beverage bottles have a relatively short life span and a dynamic market, which can respond in complex ways to management interventions. The emergent behavior is often very different from the expected behavior, and this difference can result in misapplied effort on the part of managers and policy makers (Stasinopoulos *et al.* 2012). Therefore, it is important to understand the possible responses of the whole system to potential interventions, such as product demand, resource supply, and government policy (Stasinopoulos *et al.* 2012).

In this study, system dynamics was applied in the LCA model presented in Chapter 3 and averaged estimates of global warming potential at each life cycle stage in the PET beverage bottle system from Chapter 4 to test ‘what if’ scenarios. Scenarios of relevance were set up to

achieve the following objectives: 1) The contribution analysis of historical GWP of the PET beverage bottle system, and 2) The impact of recycled PET content and crude oil price over time on PET beverage bottles in terms of CO₂ tax (\$/ton) and global warming potential (kg CO₂ eq.)

5.3 Materials and Methods

5.3.1 General description of the model

A system dynamics and LCA models were coupled to model the GWP of the PET beverage bottle model developed in Chapter 3 to account for the changing factors of the wider system. Figure 5-1 explains the variables included and excluded in this study. There are two types of variables included, endogenous and exogenous. Endogenous variables are the variables affected by other variables from inside of the system, while exogenous variables are derived from outside of the system. As endogenous variables, global warming potential (GWP) from the life cycle of the PET beverage bottle, crude oil price, PET bottle demand, recycled PET (RPET) price, mass flow of PET beverage bottles, and amount of RPET in the market were included. As for exogenous variables, the recycling rate of California, population of California, RPET content in PET bottles, and CO₂ tax were included. Due to the lack of data and limitation of the system boundary, the effect of crude oil price on RPET and GWP credit from exported RPET were excluded in this study.

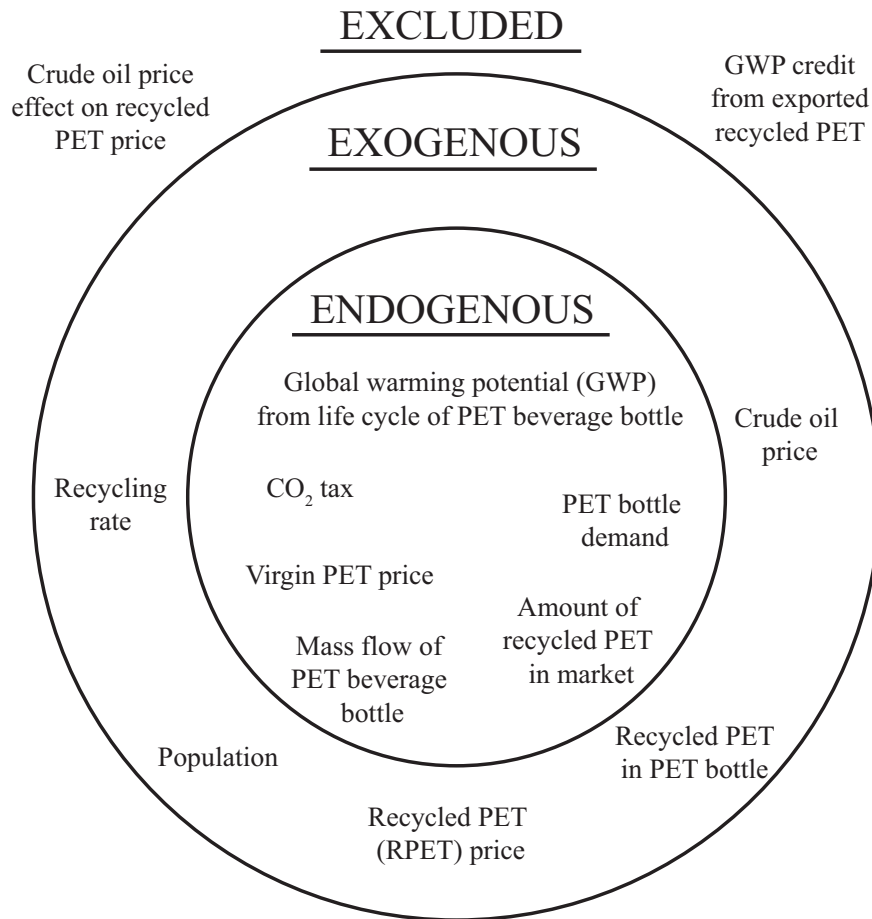


Figure 5-1. Bull's eye diagram of the current study; *endogenous* variables are any variables affected by a parameter in the system, whereas *exogenous* variable is any parameter originated from outside the system.

The geographical boundary of this study was defined as the state of California, and the time scale was from 1988 to 2035. The product of this study is PET beverage bottles consumed and demanded in the state of California. The model incorporates two main components: life cycle assessment of PET beverage bottle system and PET resin consumed and demanded for PET bottle in California. The hypothesis concerning the main interactions embodied in these two main components is represented in the causal loop diagram (Figure 5-2). The amount of PET

resin demanded for PET bottles in California is driven by the population of California and the crude oil price. It is supplied by virgin PET (VPET) and RPET available in California. RPET available in California, however, also replaces the amount of VPET used for PET bottles in California. The price of VPET is driven by crude oil prices and CO₂ tax, and it affects the amount of VPET and RPET available for PET bottles in California. If VPET price increases, then the preference for VPET decreases, and simultaneously the preference for RPET increases. Another main component is the life cycle assessment (LCA) of the PET beverage bottle system. In this study, GWP is only considered as the result of LCA of the PET beverage bottle system. More GWP causes a larger CO₂ tax, which will affect the VPET price.

The concept explained in Figure 5-2 assumes that there is a reinforcing loop and a balancing loop acting simultaneously. The reinforcing loop describes more PET bottle demand will cause more PET resin required, which will also increase the GWP. The balancing loop explains that more RPET resin introduced for PET beverage bottles will reduce the amount of VPET resin required, which will reduce the GWP.

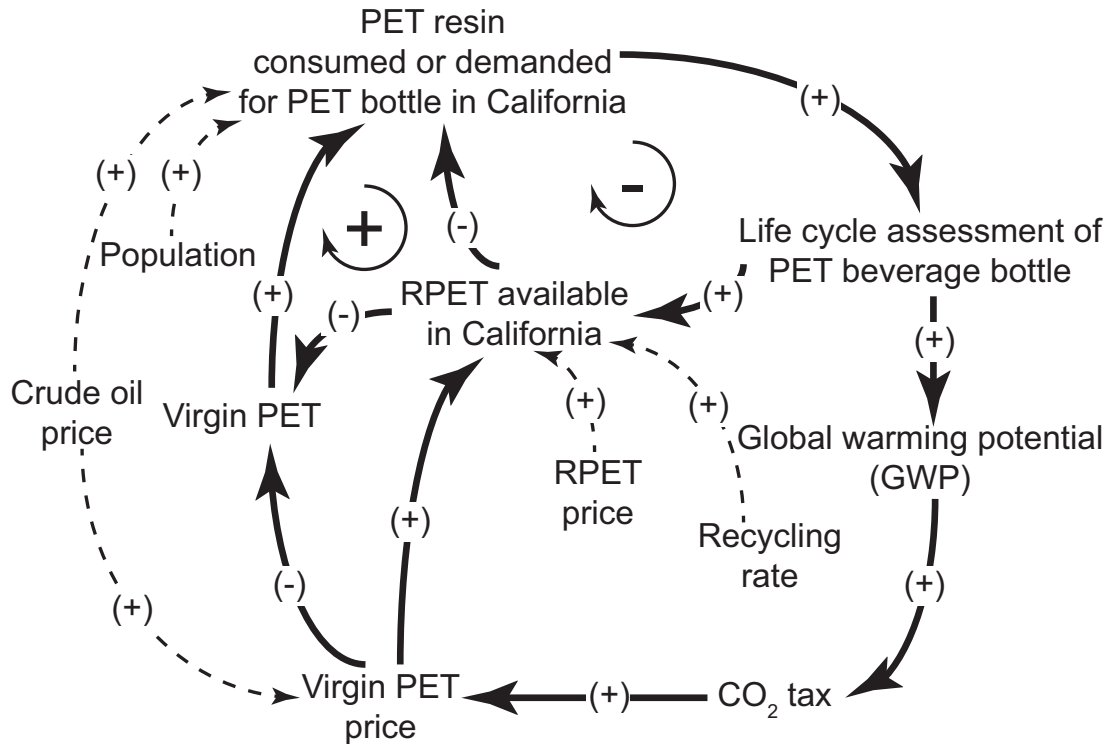


Figure 5-2. A causal loop diagram of this study. The *text elements* represent system state variables, and the *arrows* represent influence links. A *plus (+) and minus (-) signs on the arrows* indicate link polarity. A *plus and minus sign* indicates that an increase/decrease in the value of the variable at the *tail of the arrow* will cause the increase/decrease for the value of the variable at the *head of the arrow*. *Solid arrows* indicate endogenous relationships, whereas *dashed arrows* represent exogenous relationship. *270-degree circles* indicate the *reinforcing (+) or balancing (-)* loop

In order to perform the required computations, a stock-and-flow model was constructed using the system dynamics software STELLA[®] (version 10.0.4) (isee systems 2013). The structural arrangement of this model is summarized in Figure 5-3. It is composed of modules (rounded squares), stocks (squares), variables (circles), flows (double-lined arrows), influence links (single-lined arrows) and flow rates (tap symbol). Modules contain the separate stock-and-

flow model inside. For example, the module 'PET' contains the flow 'population' and 'future crude oil price' to fill up the stock 'PET demand'. The stock is where the materials are accumulated, and the stock changes over time through the actions of a flow. For example, the stock 'Recycled PET' is changed by inflow 'RPET in' and outflow 'RPET out' and 'RPET back'. The variable influences the rate of flow based on the hypothesis and the assumption explained in sub section 5.3.2. For example, the flow 'RPET in' is changed depending on the variable 'Recycling rate' by an influence link. Dashed lined boxes with code F1 and F2 indicate the parameters selected for setting up the scenarios.

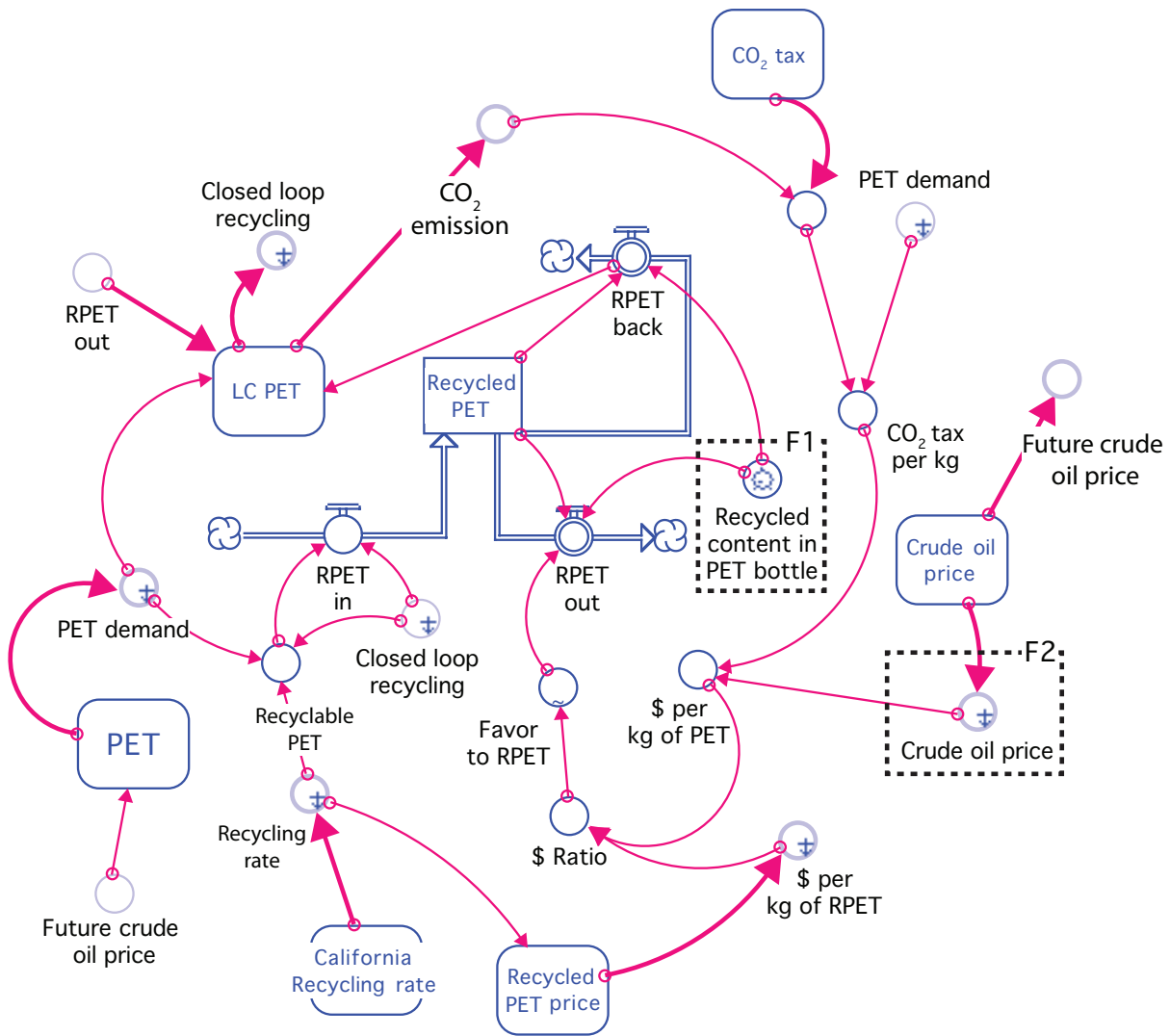


Figure 5-3. A stock-and-flow model. *Square boxes* represents stocks (e.g. 'Recycled PET'), *Rounded square boxes* represent the module, containing another stock-and-flow model inside (e.g. 'PET'), *Circles* indicate the variables (e.g. 'Recycling rate'), the *double-lined arrows* represent flows (e.g. 'RPET in'), the *single-lined arrows* represent influence links (e.g. the variable of 'Recycling rate' influences the variable of 'Recyclable PET'). *Dashed square boxes* indicate the factors selected for this study; Recycled content in PET bottle, Crude oil price

5.3.2 Module description and assumptions

As explained above, each module contains a separate stock-and-flow model. The description and assumption of each module is explained as follow;

5.3.2.1 Module ‘PET’

The module ‘PET’ includes the stock-and-flow model to predict the PET beverage bottle demand using two variables: population and crude oil price. It was assumed that population and crude oil price are significant factors for the PET beverage bottle market. In order to satisfy the time scale of this study, historical population data and a projection of population in California were determined for 1988 to 2035 (CA DOF 2013; US Bureau of the Census 2014). Also, historical and projections of crude oil prices were collected (US EIA 2010; 2014). According to the US Energy Information Administration (2010), the dataset for projection of crude oil prices was constructed based on 4 hypothetical situations, compared to a reference case; high and low economic growth, and high and low oil price. Depending on the different views of economic growth determined by labor force growth and productivity, the reference case assumed average 2.4 percent of GDP growth per year, whereas average 3.0 percent and 1.8 percent of GDP growth per year was assigned to high and low economic growth scenarios, respectively. The high oil price situation depicts a future world oil market in which conventional production is restricted by political decisions and economic access to resources, such as use of quotas, fiscal regimes, various degrees of access restrictions by the major producing countries decreasing their oil production, and consuming countries turning to high-cost unconventional fuel production to satisfy demand (US EIA 2010). The low oil price case depicts a future world oil market in which non-OPEC producing countries develop stable fiscal policies and investment regimes directed at

encouraging development of their resources (US EIA 2010). These four different scenarios were selected as one of the parameters in this study.

In order to develop the model to predict the PET bottle demand, historical population and crude oil price from 1988 to 2013 were used. When it comes to deal with data in economics and business, many regression applications involve time series data. For such data like the historical population and crude oil price, the error terms in the regression model are frequently correlated positively over time (Kutner *et al.* 2005). This effect is called autocorrelation or serial correlation. One of the methods to test if there is an autocorrelation issue is Durbin-Watson test (Durbin *et al.* 1950). The Durbin-Watson test calculates the statistic (D), and if the D is close to 2, then there is no autocorrelation issue. Table 5-1 describes the results of ordinary least squares (OLS) and Durbin-Watson statistic, which confirms there is an autocorrelation issue (D=0.5380) between population growth and oil price. The model of OLS is illustrated in equation (5-1)

Table 5-1. Results of ordinary least square (OLS) with Durbin-Watson statistic (D)

Variables	Coefficient	Standard Error	t value	$P > t $	95% Confidence interval	
Constant	-2.24×10^{10}	3.16×10^9	-7.08	0.000	-2.89×10^{10}	-1.58×10^{10}
Population	725.12	104.0864	6.97	0.000	509.801	940.440
Price	4.65×10^7	1.02×10^7	4.55	0.000	2.54×10^7	6.77×10^7
<i>Adjusted R</i> ² = 0.95 Durbin-Watson statistic = 0.5380						

$$\text{PET demand} = 725.12(\text{population}) + 4.65 \times 10^7(\text{price}) - 2.24 \times 10^{10} + e_i \quad (5-1)$$

Due to serial correlation in the error terms of OLS, a first order autoregressive error model described in equation (5-2) was used. Specifically, the Cochrane-Orcutt estimation (Cochrane *et al.* 1949) was employed. In this estimation a procedure is used to adjust the OLS for serial correlation in the error term. The estimation is composed of three steps; estimation of the autocorrelation parameter (ρ), fitting of the transformed model, and a test for need to iterate (Kutner *et al.* 2005).

$$Y_t = \beta_0 + \beta_1 X_t + \varepsilon_t, \quad \varepsilon_t = \rho \varepsilon_{t-1} + \mu_t \quad (5-2)$$

where ρ is a autocorrelation coefficient that $|\rho| < 1$, μ_t are independent $N(0, \sigma^2)$

Table 5-2 describes the results of Cochrane-Orcutt estimation with adjusted R^2 , results of Durbin-Watson statistic (D), and autocorrelation coefficient (ρ). The Durbin-Watson statistic confirms that the autocorrelation issue is better addressed but not completely resolved (D=1.2287). Although not perfect, based on the results presented in Table 5-2, equation (5-3) is proposed to predict the demand for PET bottles in California. Historical PET bottle consumption and PET bottle demand predicted by the Cochrane-Orcutt estimation and linear regression are described in Figure 5-4. Despite the better goodness of fit in linear regression, the Cochrane-Orcutt estimation model was used to avoid the autocorrelation issue. It was also found that a good matching occurs between 2000 and 2013 in the Cochrane-Orcutt estimation model.

Table 5-2. Results of Cochrane-Orcutt estimation with adjusted R^2 , results of Durbin-Watson statistic (D), and autocorrelation coefficient (ρ)

Variables	Coefficient	Standard Error	t value	$P > t $	95% Confidence interval	
Constant	-4.12×10^{10}	4.90×10^9	-8.40	0.000	-5.13×10^{10}	-3.10×10^{10}
Population	1300.218	144.7761	8.98	0.000	999.9703	1600.465
Price	1.29×10^7	7018022	1.84	0.080	-1662275	2.74×10^7
<i>Adjusted $R^2 = 0.87$ Durbin-Watson statistic = 1.228741 $\rho(\rho) = 0.7584352$</i>						

$$\text{PET demand}_t = 1300.22(\text{population})_t + 1.29 \times 10^7 (\text{price})_t - 4.12 \times 10^{10} + u_t \quad (5-3)$$

where $u_t = 0.7584u_{t-1} + e_t$, e_t = Residual from ordinary least square (OLS)

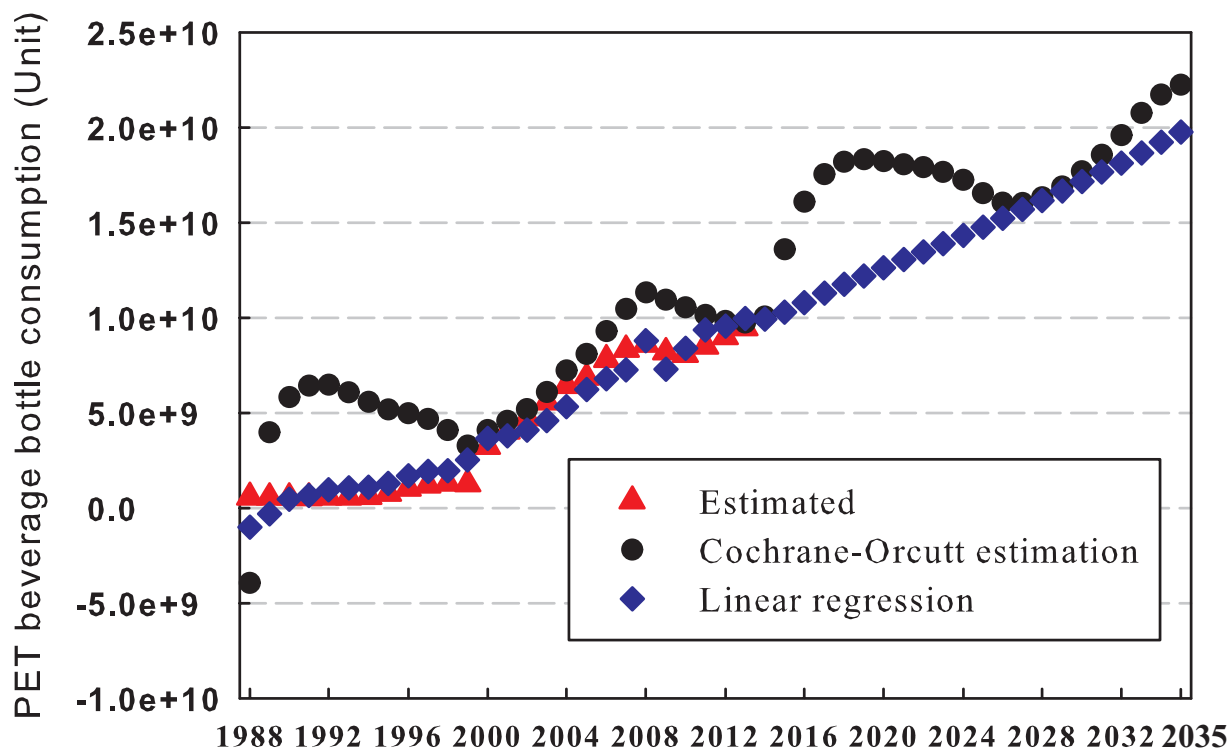


Figure 5-4. PET bottle consumption in California (red triangles) and PET bottle demand predicted by Cochrane-Orcutt estimation (black circles) and OLS (blue diamonds)

5.3.2.2 Module ‘LC PET’

Figure 5-5 describes the two stock-and-flow models designed in the Module ‘LC PET’. The mass flow model starts with the bottle grade PET resin production (U1). The amount of bottle grade PET resin is calculated based on the PET bottle consumed and demanded in California. One PET beverage bottle was assumed to equal 0.0202 kg. All the waste was managed in three routes: landfill, incineration with energy recovery and recycling. The destination of recycled PET was designed in three ways: export, open loop recycling and closed loop recycling. The amount of PET for closed loop recycling is considered as available RPET for PET beverage bottles. A detailed description of the life cycle of PET beverage bottles was provided in Chapter 4. Based on mass flow of life cycle of PET beverage bottle, GWP is

calculated using the GWP model. The GWP estimates of each life cycle stage from Chapter 4 are implemented in the GWP model. In order to define the best probability distribution of GWP estimates for each life cycle stage, the corrected Akaike information criteria (AICc) (Akaike 1974) was used. The best probability distribution, mean and standard deviation (SD) of GWP estimates for each life cycle stage are described in Table 5-3. Detailed information of the AICc and log likelihood results to find the best probability distribution is explained in appendix E.

Table 5-3. The value of variables used in module 'LC PET' with probability distribution

Variable	Description	Value (Mean $\pm$ SD)	Probability distribution
U1 CO ₂ C	GWP estimates for PET bottle grade resin production (U1)	2.88 $\pm$ 1.26	Lognormal
U2 CO ₂ C	GWP estimates for PET bottle production (U2)	1.22 $\pm$ 0.60	Normal
U3 CO ₂ C	GWP estimates for filling process (U3)	1.06 $\pm$ 0.40	Exponential
U4 CO ₂ C	GWP estimates for secondary packaging (U4)	2.37 $\pm$ 0.97	Exponential
T1 CO ₂ C	GWP estimates for distribution of bottle (T1)	1.37 $\pm$ 0.52	Exponential
T2 CO ₂ C	GWP estimates for post-consumer PET bottle (PCB) collection (T2)	20.76 $\pm$ 12.0	Exponential
D1 CO ₂ C	GWP estimates for material recovery process (MRF) (D1)	5.42 $\pm$ 2.42	Exponential
D2 CO ₂ C	GWP estimates for recycling (D2)	0.77 $\pm$ 2.17	Lognormal
D3 CO ₂ C	GWP estimates for landfill (D3)	0.17 $\pm$ 4.20	Lognormal
E1 CO ₂ C	GWP estimates for incineration with energy recovery (E1)	0.38 $\pm$ 1.98	Normal
E2 CO ₂ C	GWP estimates for environmental benefit of closed loop recycling (E2)	-2.00 $\pm$ 0.45	Normal
E3 CO ₂ C	GWP estimates for environmental benefit of open loop recycling (E3)	-1.44 $\pm$ 0.85	Normal
U2 S1 (%)	Yield loss from injection stretch blow molding	95.16 $\pm$ 4.06	Normal
U3T1 S2 (%)	Product loss during filling and delivery	1.78 $\pm$ 1.21	Normal
D1 S3 (%)	PCB collection and MRF efficiency	79.89 $\pm$ 13.89	Normal
D2 S4 (%)	Recycling efficiency	80.79 $\pm$ 8.14	Normal
Landfill ratio	Ratio to control landfill amount	0~1	Range
Closed ratio	Ratio to control closed loop recycling amount	0~1	Range
Export ratio	Ratio to control the export of RPET amount	0~1	Range

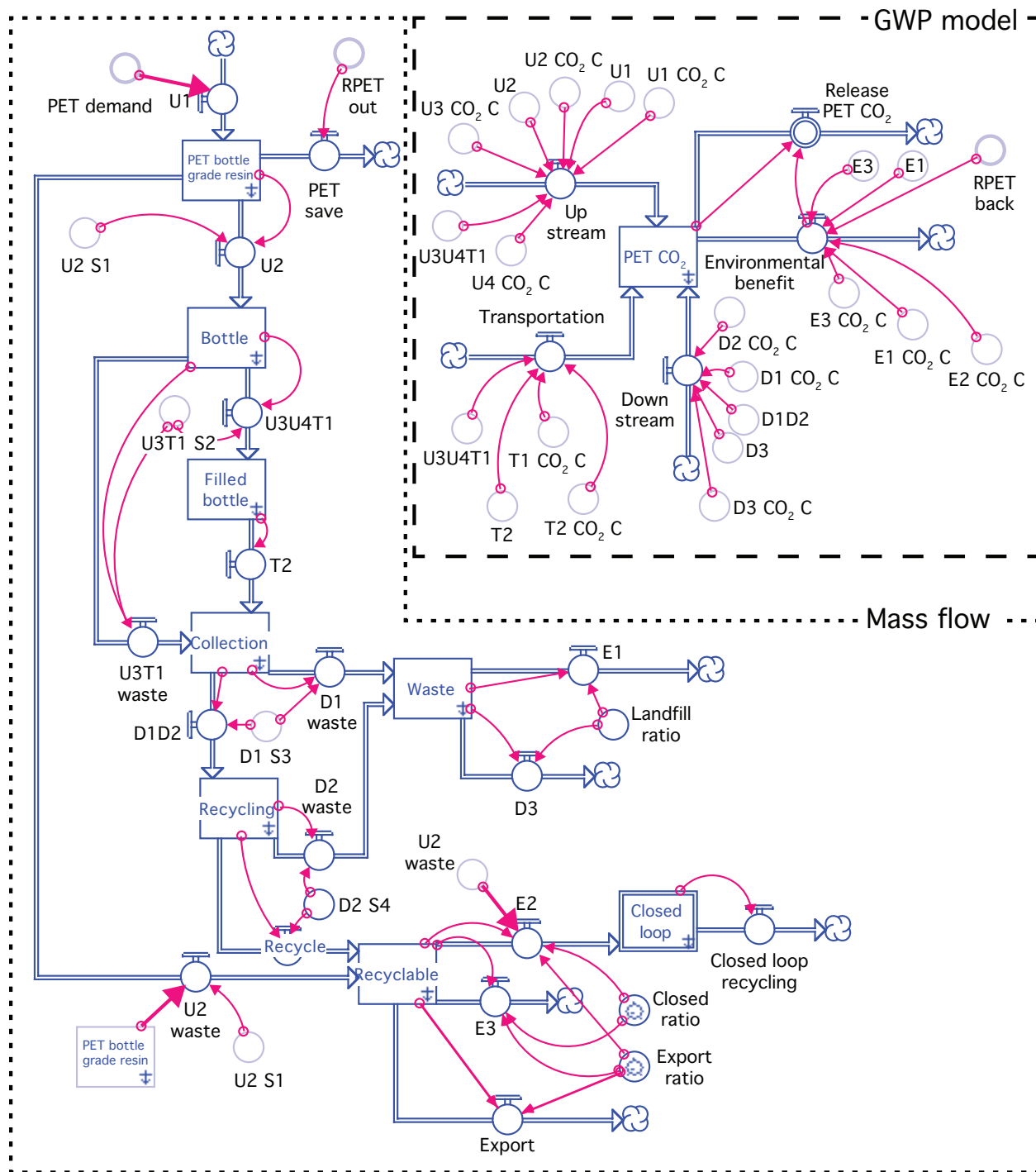


Figure 5-5. Stock-and-flow model of module 'LC PET'. It contains two stock-and-flow models, mass flow of PET beverage bottles and GWP model of PET beverage bottles. The codes used in module 'LC PET' were defined in Chapter 4 (ex. U1, U2 etc.)

5.3.2.3 Module ‘California recycling rate’

The recycling rate model was constructed based on the change of California Refund Value (CRV). CRV is defined as “the amount paid by consumers at the checkout stand and paid back to consumers when they recycle eligible aluminum, plastic, glass and bi-metal beverage containers at one of California’s approximate 2500 certified recycling centers.” It was established in Division 12.1 of Chapter 1290 (AB2020) as the California Beverage Container Recycling and Litter Reduction Act, effective September 29, 1986 (CalRecycle 2013c). CRV is paid on several types of beverages such as carbonated and noncarbonated water, soft drinks, energy drinks, coffee, tea, beer and 100% fruit juice in containers less than 46 fluid ounces (CalRecycle 2013a). Table 5-4 explains CRV changes over time. In this study, CRV change was assumed to be the biggest factor affecting the CRV PET recycle rate in future years.

Table 5-4. CRV of different volume and year (Calrecycle 2013b)

Year	Volume		Enactment
	Smaller than 24 ounce	24 ounce and larger	
1987~1988	1 cent		AB 2020, Chapter 1290
1989~1991	2 cents for a single beverage container 5 cents for every two beverage containers		SB 1221, Chapter 1339
1992~2003	2.5 cents	5 cents	
2004~2006	4 cents	8 cents	AB 28, Chapter 753
2007~present	5 cents	10 cents	AB 3056, Chapter 907

Figure 5-6 (top) shows the CRV recycling rate from 1988 to 2013. The vertical dashed line indicates when the CRV value was increased by a new enactment. In this study, we assumed that the future CRV recycling rate will follow the trend between 2007 and 2013, where recent

enactment is established. Figure 5-6 (bottom) shows the linear regression of the CRV recycling rate from 2007 to 2013. To simplify the relationship between recycling rate and time, we decided to use extrapolated linear regression obtained from 2007 to 2013 to predict the future CRV recycling rate. The maximum CVR recycling rate was bounded to 1.00.

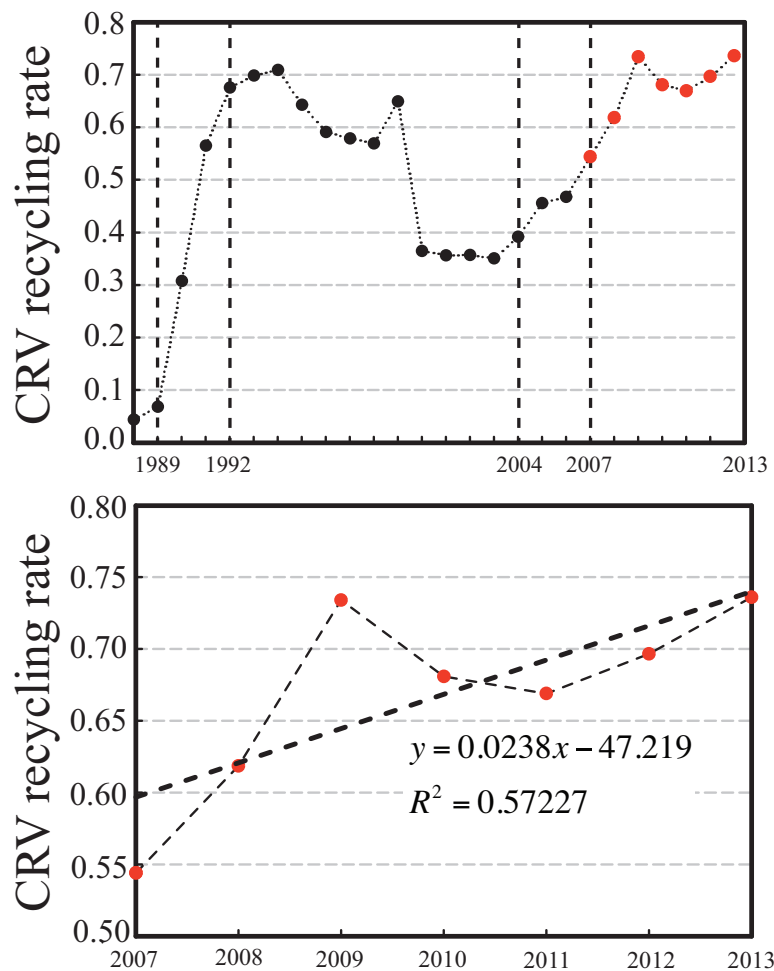


Figure 5-6. CRV recycling rate from 1988 to 2013; vertical dashed line indicates when the CRV increased (top). Linear regression of CRV recycling rate from 2007 to 2013 used in this study to predict the future CRV recycling rate (bottom)

5.3.2.4 Module ‘CO₂ tax’

CO₂ tax, often called a carbon tax, is a tax on greenhouse gases. It is a market-based policy instrument that can be used to achieve a cost-effective reduction in emissions (Parry *et al.* 2012). A carbon tax uses the power of market price signals to encourage the reduction of greenhouse gas emissions from a variety of sources (C2ES 2013). The major greenhouse gas is carbon dioxide (CO₂), which is largely generated from burning fossil fuels. A number of countries have initiated carbon taxes, such as Finland, Netherlands, Norway, Sweden, Denmark, Costa Rica, United Kingdom, Switzerland and so on. Although the US has not yet taken up the issue of a national price on carbon, there are six carbon-pricing proposals that have been introduced or released in draft form. Five would initiate a carbon tax, also called a “carbon pollution fee”, and one would establish a cap-and-dividend program, which is a cap-and-trade program that would rebate program revenues to consumers (C2ES 2013). Among the six proposals, the Sanders-Boxer proposal was used in this study. This proposal recommends that \$20 per ton carbon tax will be set up and it will rise 5.6 percent per year over a 10-year period. It was assumed that the carbon tax proposed by Sanders-Boxer would be applied from 2014 onward.

5.3.2.5 Module ‘Crude oil price’

This module consists of historical and projected crude oil prices from 1988 to 2035 (US EIA 2010; 2014). As described in Section 5.3.2.1, projections of crude oil prices were constructed based on 4 hypothetical situations: high and low economic growth, and high and low oil price. In this study, these 4 hypothetical situations were selected as one of the parameters to evaluate the effect on GWP value and CO₂ emissions and CO₂ tax saving.

5.3.2.6 Module ‘Recycled PET price’

The module ‘Recycled PET price’ contains the dataset of historical prices for post-consumer PET clean flake from 1988 to 2013 (Crain Communications Inc. 2014), and the linear regression for predicting the post-consumer PET clean flake price. It was assumed that the price of recycled PET is largely influenced by the recycling rate. As described in Section 5.3.2.3, the recycling rate from 2007, when a new enactment was made for CRV, was assumed to drive the future trend of recycled PET. Thus, it was used to establish the linear regression (Figure 5-7 bottom) model for predicting future RPET price. Additionally, data transformation was made to increase the coefficient of determination (R^2), in which the predictor variable was converted from the recycling rate to the recycling rate divided by post-consumer PET clean flake price. Although this model does not account for the increase in the price of crude oil, it will be used as a preliminary model for this work.

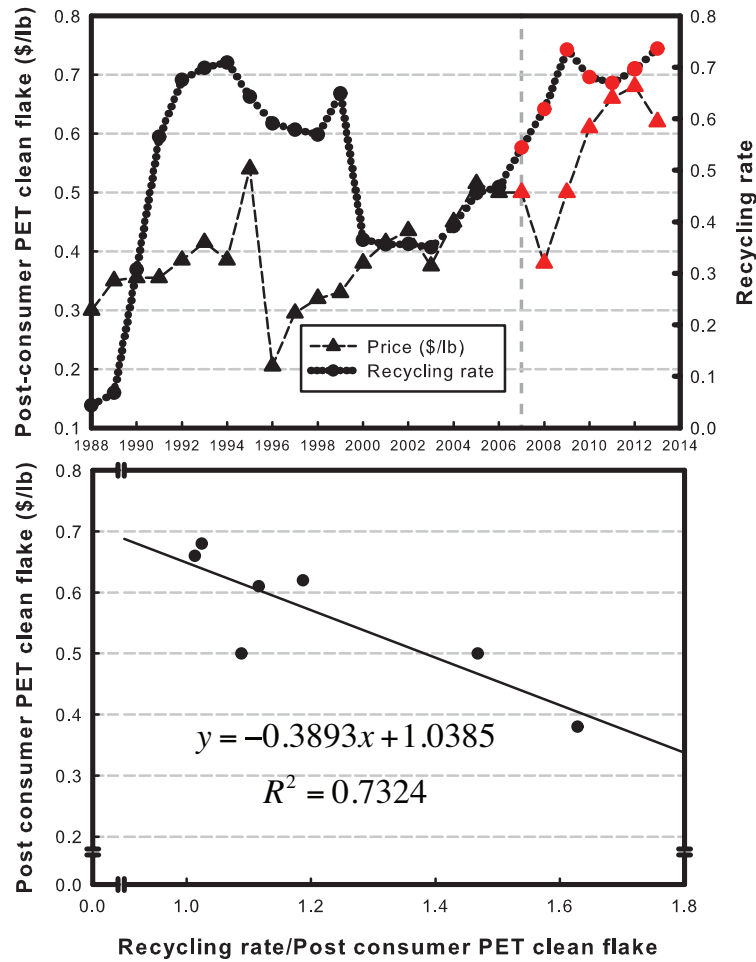


Figure 5-7. Historical price of post-consumer PET clean flake and recycling rate from 1988 to 2013 (top). The linear regression used to project the future price of post-consumer PET clean flake (bottom)

5.3.3 Other variables

As described in Figure 5-3, the modules are connected to other variables. The variable ‘CO₂ emissions’ comes from the module ‘LC PET’, which is the cumulative GWP value (kg CO₂ eq.) from the life cycle of the PET beverage bottle. Then, this variable is used to calculate the CO₂ tax per kg of PET beverage bottles (\$/kg). The variable ‘Crude oil price’ is converted to the price of VPET resin (\$/kg). The conversion factor from crude oil price to VPET resin price was

taken from the Lulea University of Technology report (Gervet 2007). The variable 'CO₂ tax per kg' was added to the variable '\$ per kg of PET'. The variable '\$ Ratio' is the ratio between VPET and RPET price (RPET price divided by VPET price). Next, this variable was introduced to the variable 'Favor to RPET', which describe the logical relationship between price and demand. That variable has a range of 1 to 5, and it has negative exponential relationship with the variable '\$ Ratio'. On the other side of Figure 5-3, the variable 'Recyclable PET' is calculated by multiplying the variables 'PET demand' and 'Recycling rate'. The variable 'Recyclable PET' and 'Closed loop recycling' is introduced to flow 'RPET in' as available RPET resin for PET beverage bottles. Depending on the variables 'Favor to RPET' and 'Recycled content in PET bottle', the amount of RPET for PET beverage bottle was determined. The rest of the RPET (variable 'RPET back') is also considered as an environmental benefit due to closed loop recycling.

5.4 Results and discussion

In order to answer the objectives of this study, the analysis was conducted in two parts. First, the contribution analysis of GWP indicator for the life cycle of PET beverage bottle from 1988 to 2013 (section 5.4.1) was conducted. Second, the effect of RPET content in PET bottle and crude oil price and CO₂ taxes was evaluated. The hypothetical scenarios were established to test the stated hypothesis, that RPET content in PET bottles and crude oil price have significant effects to reduce the CO₂ taxes and the GWP emissions.

5.4.1 Historical GWP of life cycle of PET beverage bottle

Figure 5-8 describes the historical GWP and recycling rate of PET beverage bottles in California from 1988 to 2013. Several assumptions were made regarding the end of life scenario. One of the assumption was that 80% of total recycled PET was exported. The amount of RPET exported was handled by the cut-off method, which considered that RPET and VPET are separate systems. Thus, there is no environmental benefit acquired from exported RPET. Of the remaining 20% of RPET, 10% was managed by closed loop recycling, while the other 10% was recycled through open loop recycling. The 10% RPET managed by closed loop recycling was added to the available RPET that can be used for PET bottles. The available RPET was the summation of RPET managed by closed loop recycling and RPET calculated by recycling of PET beverage bottle in California. It was assumed that the available RPET, except RPET from closed loop recycling, was introduced from outside of the system boundary. That is, the GWP generated by the production of available RPET derived from outside of the system boundary was ignored. Based on the RPPC law (CalRecycle 2013d) in California, it was assumed that 20% of the total available RPET was used for PET beverage bottles. The end life scenario for waste was assumed to be 80% landfill and 20% incineration with energy recovery.

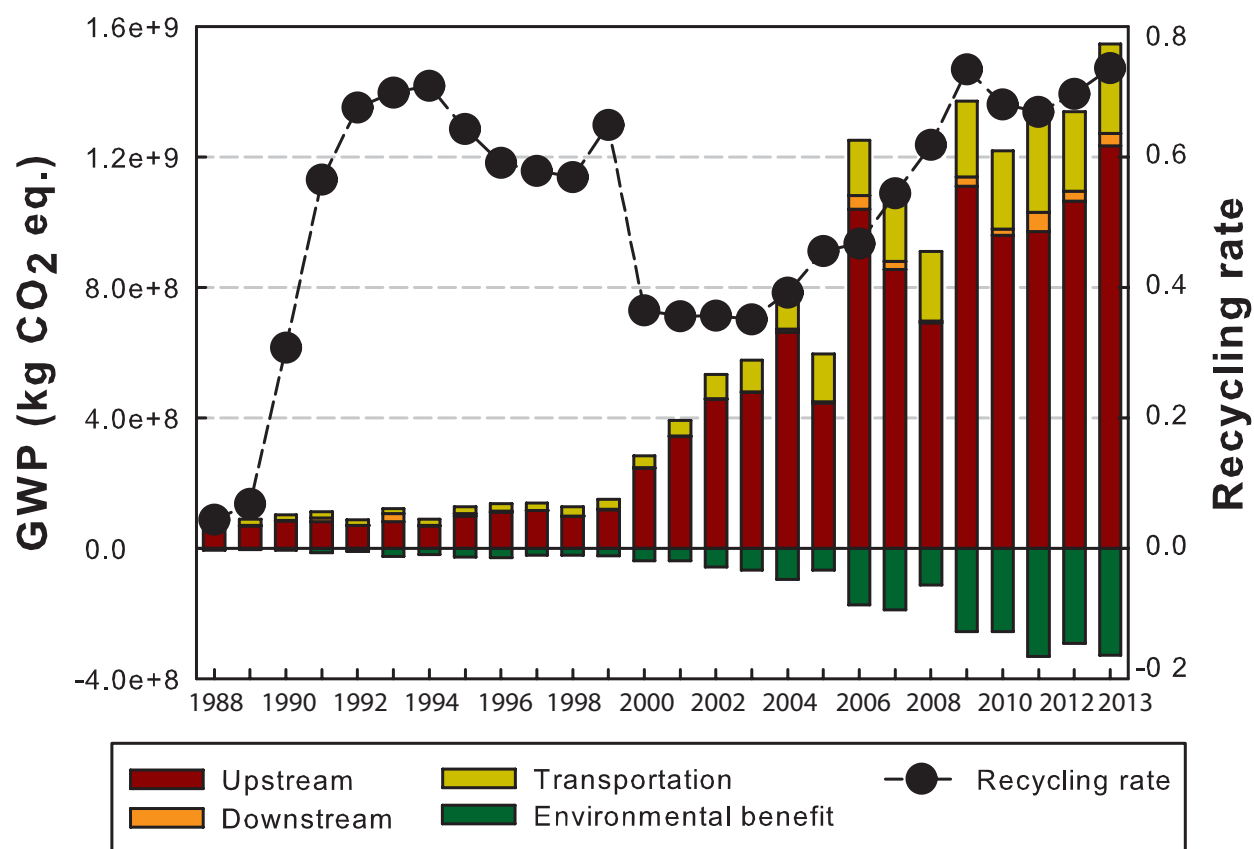


Figure 5-8. Historical GWP (stacked bar) and recycling rate (dot line with black circle) of PET beverage bottle in California from 1988 to 2013; upstream includes PET resin production, PET bottle production, filling and secondary packaging production, downstream contains MRF and recycling, transportation is composed of delivery of PET bottle and collection of PCB, environmental benefit includes the energy recovery from incineration and the benefit from open loop and closed loop recycling

Due to randomness in the GWP estimate of each PET life cycle stage, the average GWP value was calculated by averaging 10 replications. Total GWP has exponentially increased from 1999 to 2008. One of the reasons may be due to the decrease in recycling rate between 1999 and 2004. Another reason is due to the increase of PET beverage bottles in the market. The total

GWP has stabilized from 2009 to 2013 due to market saturation of PET beverage bottles and the increased recycling rate.

The upstream phase dominates the GWP over the entire period, $67.4 \pm 4.7\%$ of total GWP. As described in Chapter 4, the upstream phase contains the VPET resin production (U1), PET bottle production (U2), filling (U3), and secondary packaging (U4). It implies that the trend of the total GWP is highly correlated with the upstream phase. The next GWP contributing phase was transportation, generating $16.8 \pm 2.9\%$ of the total GWP. It is composed of delivery (T1) and PCB collection (T2). The smallest GWP contribution was found in the downstream phase ($2.56 \pm 3.5\%$ of total GWP). The environmental benefit phase saved $13.3 \pm 4.4\%$ of the total GWP.

To validate the processes for this model, the total GWP was compared with the results from Chapter 3. Based on the functional unit (34.212 kg of PET resin to deliver 1000 L of beverage), Chapter 3 estimated a 187.4 ± 28.4 kg CO₂ eq. in 2010, whereas this model reported 180.05 ± 55.4 kg CO₂ eq. in 2010 for the same functional unit. So, this comparison indicates that the GWP model in this study may be properly established to calculate the total GWP of PET beverage bottle.

5.4.2 Sensitivity analysis to evaluate the effect of RPET content in PET bottles and crude oil price on CO₂ tax

In order to evaluate the effect of RPET content in PET bottles and crude oil price on the CO₂ tax, several scenarios were established. Table 5-5 describes the hypothetical scenarios with codes and two adjustable parameters. One of the parameters depicts the projection of crude oil price under 4 different market situations: high and low economic growth and high and low oil

price. Another parameter is the amount of RPET content in PET bottles: 20%, 60% and 100%.

Except for these two parameters, the other parameters were fixed based on the same assumptions made in the contribution analysis for the historical GWP of PET beverage bottles.

Table 5-5. Scenarios established in this study with scenario code and two parameters implemented

Scenario code	Crude oil price	RPET content in PET bottle
he20	High economic growth	20%
le20	Low economic growth	20%
ho20	High oil price	20%
lo20	Low oil price	20%
he60	High economic growth	60%
le60	Low economic growth	60%
ho60	High oil price	60%
lo60	Low oil price	60%
he100	High economic growth	100%
le100	Low economic growth	100%
ho100	High oil price	100%
lo100	Low oil price	100%

Figure 5-9 describes the CO₂ tax results in the different scenarios. Figure 5-9 (a), (b) and (c) indicate the CO₂ tax of different RPET content in PET bottles. Figure 5-9 also contains the CO₂ tax results of 4 different cases of crude oil prices. For these, only the low oil price case had an effect. Low oil price causes high favor in using VPET and low favor in using RPET.

Consequently, more GWP is produced and larger amount of CO₂ tax should be paid. On the

other hand, the amount of RPET in PET bottles shows clear differences among scenarios. As more RPET was included in the PET bottle, less CO₂ tax was incurred. When the RPET content became 100%, the CO₂ tax even decreased from 2014 to 2029, and it will bounce back. This implies that the amount of RPET content in PET bottles has more significant effect than the crude oil price changes.

Additionally, to compare the Cochrane-Orcutt and OLS estimation methods to extrapolate the PET bottle consumption in the state of California from 2014 to 2035, an additional low oil price scenario was used. Figure 5-9 showed that the overall trend of CO₂ tax was not fully changed. Instead, the intensity of the CO₂ tax was reduced from the Cochrane-Orcutt estimation results to the OLS results, which implies that future trends of CO₂ tax will not be radically changed by the different model of predicting the PET bottle demand. It is, however, very important to emphasize that accurate PET bottle demand will determine the accurate CO₂ tax saving as well as GWP reduction. Therefore, future work will be oriented to determine further extrapolation models of PET bottle demand.

CO₂ tax (\$) for PET beverage bottle

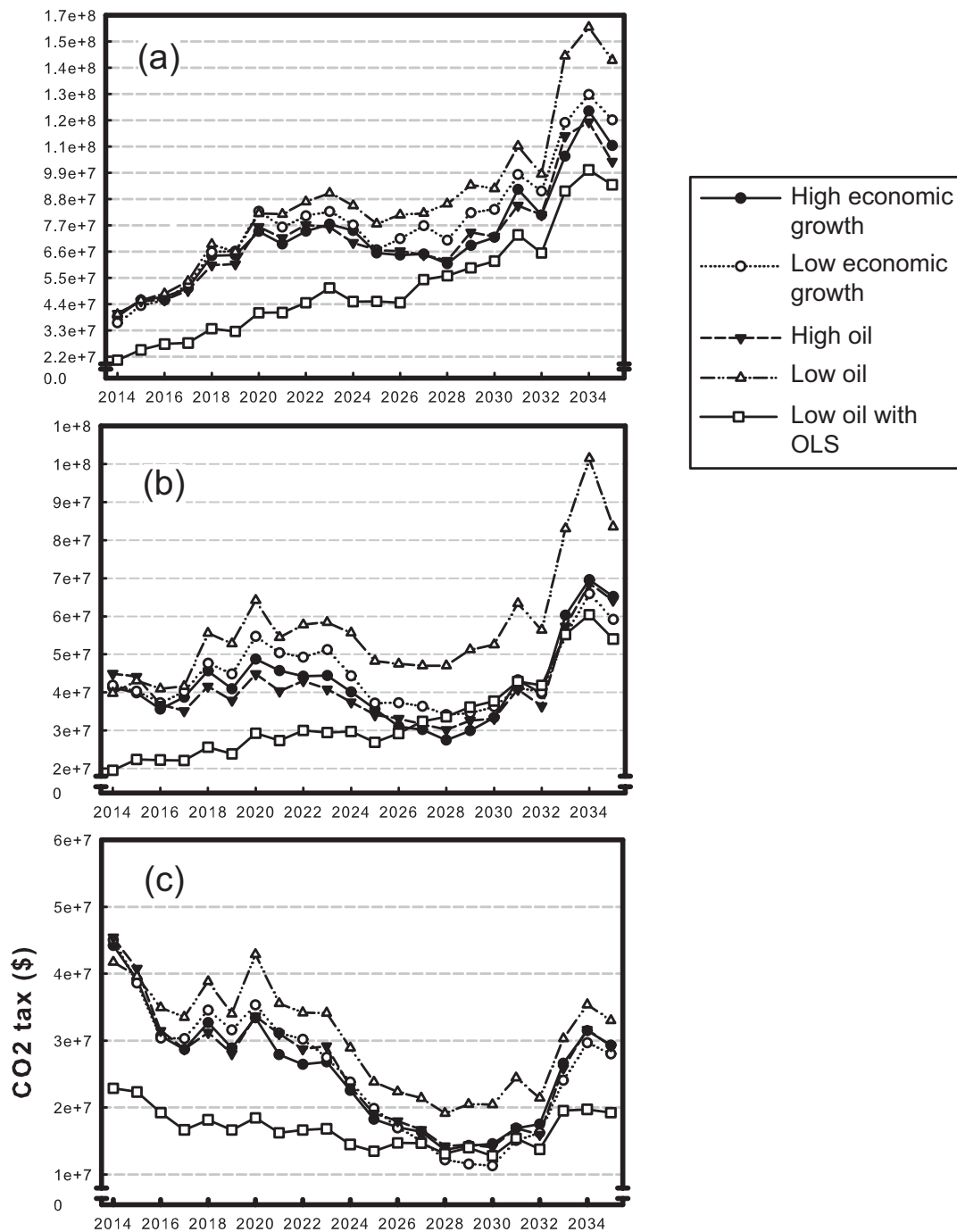


Figure 5-9. CO₂ tax in different scenarios; (a) 20% RPET content in PET bottle, (b) 60% RPET content in PET bottle, (c) 100% RPET content in PET bottle. To compare the quality fitting of the Cochrane-Orcutt estimation, the OLS fitting for the low oil price scenario is also obtained.

Table 5-6 describes the CO₂ tax and GWP in the different scenarios in 2014, 2024 and 2034 with averaged increasing rate of CO₂ tax from 2014 to 2035. In 2014, the CO₂ tax in all the scenarios is between 36.2 and 45.2 million dollars, and the GWP ranges from 1.81 to 2.27 billion kg CO₂ eq. With 20% of RPET in PET bottles, the CO₂ tax will increase in all crude oil scenarios with an average of 5~7% increasing rate. When the RPET content in the PET bottle increased to 60%, the average increasing rate decreased to around 2 to 5% from 2014 to 2035. Finally, with 100% RPET content in the PET bottles, an average of -1~1% increasing rate of CO₂ tax was expected from 2014 to 2035. In 2024, by increasing the RPET content from 20% to 60%, an average of 32.4 million dollars of CO₂ tax and 0.81 billion kg CO₂ eq. will be saved. At 100% RPET content in PET bottle, an average of 52.2 million dollars of CO₂ tax and 1.3 billion kg CO₂ eq. will be avoided in a comparison of 20% RPET in the PET bottle scenario.

Table 5-6. CO₂ tax (million dollar) and GWP (billion kg CO₂ eq.) in different scenario for every 10-year and averaged increasing rate from 2014 to 2035

Scenario code	CO ₂ tax (million dollar) (GWP (billion kg CO ₂ eq.))			Averaged increasing rate of CO ₂ tax 2014 to 2035
	Year 2014	Year 2024	Year 2034	
he20	38.8 ± 8.2 (1.94 ± 0.41)	74.8 ± 6.8 (1.87 ± 0.17)	125 ± 13.0 (2.08 ± 0.22)	6%
le20	36.2 ± 7.5 (1.81 ± 0.38)	77.2 ± 8.1 (1.93 ± 0.20)	132 ± 5.5 (2.20 ± 0.09)	7%
ho20	40.1 ± 7.0 (2.00 ± 0.35)	69.8 ± 12 (1.74 ± 0.30)	120 ± 13 (2.00 ± 0.22)	5%
lo20	39.7 ± 7.9 (1.99 ± 0.40)	85.3 ± 9.2 (2.13 ± 0.23)	160 ± 15 (2.67 ± 0.25)	7%
he60	41.3 ± 10 (2.06 ± 0.51)	40.1 ± 3.4 (1.00 ± 0.085)	69.5 ± 6.1 (1.16 ± 0.10)	3%
le60	41.8 ± 14 (2.09 ± 0.69)	44.4 ± 2.0 (1.11 ± 0.050)	65.9 ± 6.7 (1.10 ± 0.11)	2%
ho60	44.9 ± 11 (2.24 ± 0.53)	37.4 ± 3.0 (0.9435 ± 0.074)	68.6 ± 4.6 (1.14 ± 0.076)	3%
lo60	39.8 ± 7.6 (1.99 ± 0.38)	55.6 ± 7.6 (1.39 ± 0.19)	101.5 ± 14 (1.69 ± 0.23)	5%
he100	44.2 ± 8.0 (2.21 ± 0.40)	22.6 ± 1.6 (0.564 ± 0.040)	31.5 ± 3.3 (0.525 ± 0.056)	-1%
le100	45.0 ± 4.4 (2.25 ± 0.22)	23.8 ± 2.2 (0.595 ± 0.054)	29.7 ± 5.2 (0.495 ± 0.087)	1%
ho100	45.4 ± 4.1 (2.27 ± 0.21)	23.1 ± 2.1 (0.577 ± 0.051)	31.7 ± 5.7 (0.528 ± 0.094)	-1%
lo100	41.7 ± 5.2 (2.09 ± 0.26)	28.9 ± 2.8 (0.723 ± 0.069)	35.4 ± 3.5 (0.590 ± 0.059)	-1%

5.5 Limitations and recommendations

A system dynamics approach was preliminarily applied to calculate and predict the GWP of PET beverage bottle in California. It must be noted that such modeling is just a tool to organize vast amounts of information, and portray recognized uncertainties. That is, we construct the model based on what we already know with recognized uncertainties by computable probabilities to answer the conceivable outcomes (Carpenter *et al.* 2012). In order to perform this, it is very important to recognize the limitations and assumptions of this model, which are described as follows:

- No alternative product was considered. That is, an increased demand of PET beverage bottle does only drive more PET beverage bottle, and no alternative polymer can replace the increasing demand.
- The validation of the model to predict the PET demand was not completely successful. Even though the model used resolved the autocorrelation issue, it still may not be the best model to predict the PET demand. Future analysis is necessary to include more relevant predictor variables, such as demographic characteristic and other types of beverage packaging consumption. Another limitation of this model was derived from the Durbin-Watson test, which can only evaluate the first order autocorrelation. A generalized Durbin-Watson test is recommended to test if the error terms are correlated with high order autocorrelation.
- Non-CRV PET beverage bottles are not considered in this study, such as milk, medical food, infant formula, wine, 100% fruit juice in containers 46 ounces or more and 100% vegetable juice over 16 oz.

- The mass flow of PET beverage bottles used in module 'LC PET' is not exclusively designed for the state of California, rather it is constructed for the general mass flow of PET beverage in US, except for the 'PET demand' and RPET content for PET bottle ('RPET out') components.
- The time delay is not properly considered. For example, the PET recycling rate in 2007 will affect the RPET prices in 2007 instead of 2008.
- In this study, economic growth and technology development are not considered except during the projection of crude oil price.

5.6 Conclusion

A system dynamics model was preliminarily employed to construct a dynamic GWP model of PET beverage bottles in California, and especially to calculate the total GWP over time. Despite the fact of the preliminary approach of the model with many assumptions and limitations, some interesting results were found.

The contribution analysis of historical GWP for PET beverage bottles in California was conducted from 1988 to 2013. It was found that the upstream phase was the most GWP contributing phase with an average of 67% of total GWP. The second GWP contributing phase was the transportation phase, an average of 17% of the total GWP. The downstream phase only generated an average of 2.56% of the total GWP, which makes it the least GWP contributing phase. The environmental benefit phase saved the average $13.3 \pm 4.4\%$ of the total GWP. In order to check the accuracy of the model, the GWP value for 2010 (180.05 ± 55.4 kg CO₂ eq.) was also compared with the GWP from Chapter 3 (187.4 ± 28.4 kg CO₂ eq.), and implies that the GWP model in this study was properly established to calculate the total GWP.

Hypothetical scenarios were designed to evaluate the effect of RPET content in PET bottles and crude oil price on CO₂ tax and GWP. A total of 12 scenarios were constructed. The results showed that the RPET content in the PET bottle is a more significant factor than the crude oil price for the CO₂ tax. With the given assumptions and scenarios, 10 years from 2014, an average of 32.4 million dollars and 0.81 billion kg CO₂ eq. will be saved if RPET content in PET bottles is increased from 20% to 60%. Additionally, an average of 19.8 million dollars and 0.5 billion kg CO₂ eq. will be saved by increasing RPET content in PET bottles from 60% to 100%.

It is suggested that additional research be undertaken to further explore the dynamics of the PET beverage bottle system, to explore the response of the PET beverage bottle system to other management interventions. Moreover, this model can be improved by developing a more accurate model of the PET beverage bottle demand. Another improvement may also be made if more economic factors are introduced, such as market competition of PET beverage packaging with other types of beverage packaging and direct effect of crude oil price on RPET demand.

Chapter 6. OVERALL CONCLUSIONS and RECOMMENDATIONS

The environmental footprint of non-alcoholic single serve PET beverage bottles in the state of California was analyzed using system dynamics and life cycle assessment (LCA) approaches, specifically the global warming potential (GWP). To achieve this, the research was divided into three major parts. The first part involved an LCA of PET beverage bottles in CA, as presented in chapter 3. The second part presented a systematic review of LCA studies for PET beverage bottles using meta-analysis, as described in chapter 4. The third and last part was a preliminary attempt to couple system dynamics and LCA approaches for constructing a dynamic GWP model of PET beverage bottles in the state of CA.

As shown in the contribution analysis of chapter 3, the main environmental burden was contributed by the PET bottle production in acidification, carcinogens, non-carcinogens, respiratory effects, ozone depletion and ecotoxicity. The material production section was the main source of GWP, eutrophication and smog. Additionally, hypothetical scenarios were established to compare two different waste sources to increase the amount of recyclable PET. The scenario comparison suggested that increasing the yield efficiency of recycling shows better environmental benefit than reducing the waste during PCB collection. Moreover, this study provided an LCA model of PET beverage bottles in CA, which was then used in chapter 5.

In chapter 4, meta-analysis was applied to LCA studies of the PET beverage bottle system. Statistical assessment was performed to evaluate the central tendency and variation of the GWP and energy consumption (EC) estimates of each life cycle stage for the PET beverage bottle system. The largest contribution of GWP and EC was the bottle grade PET resin production, whereas the largest variation was found in the incineration of waste, which results from large variation in efficiency of electrical energy recovery from the incineration facilities.

The overall results implied that the best possible option to improve the environmental performance of the PET beverage bottle system is to employ the highest efficiency electrical energy recovery for incineration of plastic waste. The results also suggested that lightweight PET bottles are an effective strategy to reduce the total environmental burden of the PET beverage bottle system. The GWP indicator estimate of each life cycle stage for the PET beverage bottle system was further used in chapter 5.

In chapter 5, system dynamics and life cycle assessment approaches were applied to construct a dynamic GWP model of the PET beverage bottle system. The contribution analysis of historical GWP for PET beverage bottle showed that the upstream phase was the most GWP contributing phase with an average of 67% of total GWP, which was also consistent with the results from chapter 3. The effect of recycled PET (RPET) content in the PET bottle and crude oil price on CO₂ tax and GWP was evaluated by several hypothetical scenarios. The results indicated that the RPET content in the PET bottle is a more significant factor than crude oil price for CO₂ tax and GWP. The model estimated that an average of 32.4 million dollars and 0.81 billion kg CO₂ eq. would be saved if RPET content in PET bottle was increased from 20% to 60% in 2024. If RPET was augmented from 60% to 100% content, an average of 19.8 million dollars and 0.5 billion kg CO₂ eq. would be saved in 2024.

Because this study provided a first intent to develop a preliminary methodology for creating a dynamic environmental assessment model coupled with LCA, there are some areas that should be further investigated and improved. Specially, in chapter 5, further study is needed to construct a more accurate PET bottle demand model. This PET demand model can be improved by including more economic factors, such as market competition of PET beverage packaging with other type of beverage packaging and direct effect of crude oil price on RPET

demand. Other variables in chapter 5, such as the California recycling rate and RPET price will also require further modification to increase the future prediction power of the current model. One possible modification is to apply an auto-regressive model to solve the autocorrelation problem of the dataset.

APPENDICES

APPENDIX A: Data sources for LCI and mass flow and results of discernibility analysis

Table A-1. Data sources of PET mass flow in this study

Data description	Sources	Year
PET resin imported into US	Interactive Tariff and Trade DataWeb in United States International Trade Commission (USITC) http://dataweb.usitc.gov/	2010
PET resin produced in US	American Chemistry Council	2011
Different applications of PET resin in US	SRI Consulting report	2011
Mass flow of PET from US into California	USA Trade Online in United States Census Bureau, https://usatrade.census.gov/	2012
Transportation distances of PET mass flow between US and California	Assumed based on SRI Consulting report and Google Map	2011
Mass flow of PET resin imported and exported into California from foreign country	USA Trade Online in United States Census Bureau https://usatrade.census.gov/	2012
Transportation distances of filled PET beverage bottle	Commodity Survey Flow in United States Census Bureau http://www.census.gov/econ/cfs/	2007
PCB collection	The California Department of Resources Recycling and Recovery (CalRecycle)	2011
Transportation distances of PCB collection	Assumption based on Franklin Association Report	2010
Waste during PCB collection	Assumption based on CalRecycle report	2011
Waste during recycling of PCB	Assumption based on Franklin Association Report	2010
Bale, dirty flake and clean flake in California	Market report prepared by NewPoint Group	2009
Total PCB recycled in US	National Association for PET Container Resources (NAPCOR)	2010
Different application of recycled PET resin in US	National Association for PET Container Resources (NAPCOR)	2010

Table A-2. Inventory data sources for this LCA

Life cycle	Material process	&	Process name	Description	Database	Year	Geography
Material production	PET (Bottle grade)		Polyethylene terephthalate, granulate, bottle grade, at plant/RER WITH US ELECTRICITY	Average data for the production of bottle grade PET out of ethylene glycol, PTA and amorphous PET.	US-EI 2.2	2010	Europe
	PP cap & label		Polypropylene, granulate, at plant/RER WITH US ELECTRICITY	Aggregated data for all processes from raw material extraction until delivery at plant	US-EI 2.2	2010	Europe
PET bottle production	PET bottle		Stretch blow molding/RER WITH US ELECTRICITY	This process contains the auxiliaries and energy demand for the mentioned conversion process of plastics. The converted amount of plastics is NOT included into the dataset.	US-EI 2.2	2010	Europe & Swiss
	PP cap		Injection molding/RER WITH US ELECTRICITY				
	PP label		Extrusion, plastic film/RER WITH US ELECTRICITY				
Transportation	Distribution (Filled bottle) Curbside Deposit Delivery to MRF		Transport, single unit truck, diesel powered NREL/US	Combustion of diesel in a single-unit truck	US-EI 2.2	2008	Europe & US

Table A-2 (Cont'd)

Life cycle	Material & process	Process name	Description	Database	Year	Geography
Transportation	Drop-off collection	Transport, single unit truck, gasoline powered NREL/US	Combustion of gasoline in a single-unit truck	US-EI 2.2	2008	Europe & US
	CRV Commercial collection	Transport, combination unit truck, diesel powered NREL/US	Combustion of diesel in a combination truck	US-EI 2.2	2008	Europe & US
	Delivery to MRF					
	MRF to reclaim*	Transport, freight, rail, diesel/US WITH US ELECTRICITY	Based on European railway freight transport; instead of mix of electric and diesel trains, it includes operation of diesel train only	US-EI 2.2	2010	US
Material recovery process	Post-consumer PET recovery process	Material recovery process	Overall facility energy use reported on the MRF surveys was compared to MRF energy requirements. Electricity use reported by the facilities correlated with calculated electricity requirements	Franklin associates report	2010	US
Reclamation	PET recycling	Reclamation	The material, energy requirement and environmental emissions were collected from several reclaiming facilities	Franklin associates report	2010	US
Solidification	Solidification	Solidification	N/A	Thesis	2008	N/A

*At this stage, post-consumer PET is delivered by combination truck and train to reclamation facility

Table A-2 (Cont'd)

Life cycle	Material process	&	Process name	Description	Database	Year	Geography
Disposal	Avoided Electricity use		Electricity, medium voltage, production UCTE, at grid/UCTE WITH US ELECTRICITY	The electricity production in UCTE, the transmission network and direct SF6-emissions to air.	US-EI 2.2	2010	US & Europe
	Avoided PET use		Polyethylene terephthalate, granulate, amorphous, at plant/RER WITH US ELECTRICITY	Average data for the production of amorphous PET out of ethylene glycol and PTA. The data include material and energy input, waste as well as air and water emissions.	US-EI 2.2	2010	Europe
	Incineration of PI-PET		Disposal, polyethylene terephthalate, 0.2% water, to municipal incineration/CH WITH US ELECTRICITY	Waste-specific air and water emissions from incineration, auxiliary material consumption for flue gas cleaning. Short-term emissions to river water and long-term emisisions to ground water from slag compartment and residual material landfill.	US-EI 2.2	2010	US & Europe & Japan
	Incineration of PI-PP		Disposal, polyethylene terephthalate, 15.9% water, to municipal incineration/CH WITH US ELECTRICITY	Waste-specific short-term emissions to air via landfill gas incineration and landfill leachate. Burdens from treatment of short-term leachate (0-100a) in wastewater treatment plant (including WWTP sludge disposal in municipal incinerator).	US-EI 2.2	2010	US & Europe & Japan
	Landfill PET	of	Disposal, polyethylene terephthalate, 0.2% water, to sanitary landfill/CH WITH US ELECTRICITY	Waste-specific short-term emissions to air via landfill gas incineration and landfill leachate. Burdens from treatment of short-term leachate (0-100a) in wastewater treatment plant (including WWTP sludge disposal in municipal incinerator).	US-EI 2.2	2010	US & Europe
	Landfill PP	of	Disposal, polyethylene terephthalate, 15.9% water, to sanitary landfill/CH WITH US ELECTRICITY	Waste-specific short-term emissions to air via landfill gas incineration and landfill leachate. Burdens from treatment of short-term leachate (0-100a) in wastewater treatment plant (including WWTP sludge disposal in municipal incinerator).	US-EI 2.2	2010	US & Europe

Table A-3. Discernibility analysis¹ for GWP

			A side				
$n(A > B = \%)^3$			Waste from PCB collection			Yield loss from reclamation process	
			S1	S2	S3	S4	S5
B side		S1	- ²	0.1%	0%	0%	0%
	Waste from PCB collection	S2	99.9%	-	0%	0%	0%
		S3	100%	100%	-	99.9%	99.7%
	Yield loss from reclamation process	S4	100%	100%	0.10%	-	0%
		S5	100%	100%	0.30%	100%	-

¹ Discernibility analysis conducted with 1000 number of Monte Carlo simulation ² ‘-’ indicates no data was obtained for that comparison ³ The probability (%) of Scenario in A side has higher impact indicator than Scenario in B side out of 1000 number of Monte Carlo simulation

Table A-4. Discernibility analysis for acidification

			A side				
$n(A > B = \%)$			Waste from PCB collection			Yield loss from reclamation process	
			S1	S2	S3	S4	S5
B side		S1	-	9.4%	9.2%	0.1%	0.1%
	Waste from PCB collection	S2	90.6%	-	11.4%	0%	0%
		S3	90.8%	88.6%	-	75.8%	69.2%
	Yield loss from reclamation process	S4	99.9%	100%	24.2	-	0.2%
		S5	99.9%	100%	30.8	99.8	-

Table A-5. Discernibility analysis for carcinogenic

			A side				
$n(A > B = \%)$			Waste from PCB collection			Yield loss from reclamation process	
			S1	S2	S3	S4	S5
B side		S1	-	5.3%	5.3%	0.6%	1.1%
	Waste from PCB collection	S2	94.7%	-	6.1%	0.1%	0%
		S3	94.7%	93.9%	-	90.6%	87.6%
	Yield loss from reclamation process	S4	99.4%	99.9%	9.40%	-	0.6%
		S5	98.9%	100%	12.4%	99.4%	-

Table A-6. Discernibility analysis for non-carcinogenic

			A side				
$n(A > B = \%)$			Waste from PCB collection			Yield loss from reclamation process	
			S1	S2	S3	S4	S5
B side		S1	-	2.2%	1.2%	0.2%	0.9%
	Waste from PCB collection	S2	97.8%	-	2.4%	8.8%	0.2%
		S3	98.8%	97.6%	-	97.3%	95.4%
	Yield loss from reclamation process	S4	99.8%	91.2%	2.7%	-	0.2%
		S5	99.1%	99.8%	4.6%	99.8%	-

Table A-7. Discernibility analysis for respiratory effect

			A side				
$n(A > B = \%)$			Waste from PCB collection			Yield loss from reclamation process	
			S1	S2	S3	S4	S5
B side	Waste from PCB collection	S1	-	21.8%	21.3%	2.0%	1.3%
		S2	78.2%	-	21.8%	0%	0%
		S3	78.7%	78.2%	-	56.6%	49.5%
		S4	98.0%	100%	43.4%	-	0.7%
		S5	98.7%	100%	50.5%	99.3%	-

Table A-8. Discernibility analysis for eutrophication

			A side				
$n(A > B = \%)$			Waste from PCB collection			Yield loss from reclamation process	
			S1	S2	S3	S4	S5
B side	Waste from PCB collection	S1	-	4.9%	5.3%	0.7%	0.6%
		S2	95.1%	-	5.6%	0%	0%
		S3	94.7%	94.4%	-	90.8%	87.7%
		S4	99.3%	100%	9.2%	-	0.3%
		S5	99.4%	100%	12.3%	99.7%	-

Table A-9. Discernibility analysis for ozone depletion

$n(A > B = \%)$			A side				
			Waste from PCB collection			Yield loss from reclamation process	
			S1	S2	S3	S4	S5
B side		S1	-	0%	0%	0%	0%
	Waste from PCB collection	S2	100%	-	0%	0%	0%
		S3	100%	100%	-	100%	100%
	Yield loss from reclamation process	S4	100%	100%	0%	-	0%
		S5	100%	100%	0%	100%	-

Table A-10. Discernibility analysis for ecotoxicity

$n(A > B = \%)$			A side				
			Waste from PCB collection			Yield loss from reclamation process	
			S1	S2	S3	S4	S5
B side		S1	-	30.3%	29.5%	4.8%	4.9%
	Waste from PCB collection	S2	69.7%	-	30.4%	0%	0%
		S3	70.5%	69.6%	-	56.7%	52.8%
	Yield loss from reclamation process	S4	95.2%	100%	43.3%	-	4.2%
		S5	95.1%	100%	47.2%	95.8%	-

Table A-11. Discernibility analysis for smog

			A side				
$n(A > B = \%)$			Waste from PCB collection			Yield loss from reclamation process	
			S1	S2	S3	S4	S5
B side		S1	-	0.1%	0.1%	0%	0%
	Waste from PCB collection	S2	99.9%	-	0.2%	0.8%	0%
		S3	99.9%	99.8%	-	99.4%	99.3%
	Yield loss from reclamation process	S4	100%	99.2%	0.6%	-	0%
		S5	100%	100%	0.7%	100%	-

Table A-12. The results of discernibility analysis with mean and standard deviation for each impact indicator

Impact category	Unit	S1	S2	S3	S4	S5
GWP	kg CO ₂ eq	187.4 ± 29 ^a	180.9 ± 30 ^b	168.1 ± 32 ^c	179.8 ± 28 ^d	178.1 ± 29 ^e
Acidification	H ⁺ moles eq	46.8 ± 10.5 ^a	46.3 ± 11.1 ^b	45.4 ± 11.4 ^c	45.9 ± 10.3 ^{c,d}	45.7 ± 10.6 ^e
Carcinogenic	kg benzene eq	0.386 ± 0.421 ^a	0.377 ± 0.226 ^b	0.357 ± 0.493 ^c	0.374 ± 0.290 ^d	0.371 ± 0.339 ^e
Non-carcinogenic	kg toluene eq ×10 ³	6.342 ± 13.1 ^a	6.089 ± 5.27 ^b	5.592 ± 11.5 ^c	6.075 ± 7.81 ^d	6.017 ± 5.49 ^e
Respiratory effect	kg PM _{2.5} eq	0.2147 ± 0.0711 ^a	0.2134 ± 0.0774 ^a	0.2110 ± 0.0836 ^a	0.2110 ± 0.0667 ^{a,b}	0.2102 ± 0.0709 ^{a,c}
Eutrophication	kg N eq	0.6205 ± 0.421 ^a	0.5961 ± 0.403 ^b	0.5484 ± 0.637 ^c	0.5863 ± 0.526 ^d	0.5788 ± 0.746 ^e
Ozone depletion	kg CFC-11 eq ×10 ⁻⁶	9.70 ± 1.64 ^a	9.43 ± 1.58 ^b	8.89 ± 1.59 ^c	9.39 ± 1.57 ^d	9.33 ± 1.61 ^e
Ecotoxicity	kg 2,4-D eq	281.37 ± 202 ^a	280.77 ± 248 ^a	279.58 ± 198 ^a	277.49 ± 254 ^{a,b}	276.64 ± 218 ^{a,c}
Smog	g NO _x eq	0.3978 ± 0.0561 ^a	0.3885 ± 0.0645 ^b	0.3701 ± 0.0625 ^c	0.3871 ± 0.0555 ^d	0.3848 ± 0.0589 ^e

* Different subscript in the same row indicate statistically significantly different at the 85 percent of probability in Monte Carlo simulation

APPENDIX B: Screening results for meta-analysis

Appendix B provides the literature screening forms with the references that passed the final screening criteria. The screening forms contain the type of reference with titles, identification number of accepted references, title of reference, author, year, information of references, such as volume, issue, report number, DOI. The forms also mention the goal, functional unit, boundary of the study, information of LCA software, and brief summary of the LCI databases. Lastly, the form presents the GWP and EC results of each study per life cycle stage with the description of where this value was taken from.

Table B-1. Screening results

Journal	The International Journal of Life Cycle Assessment			No	1
Keyword search	PET or polyethylene terephthalate or beverage packaging				
Title	PET bottle reverse logistics-environmental performance of California’s CRV program				
Author	Brandon Kuczenski, Roland Geyer				
Year	Volume	Issue	doi		
2013	18	2	10.1007/s11367-012-0495-7		
Goal and scope					
Goal	To compare the three main end-of-life pathways followed by CRV PET bottles (landfilling, curbside collection, and consumer drop-off) To evaluate the potential environmental improvement that could be obtained through PET recycling by comparing the impacts of secondary production against those of equivalent primary production				
Functional unit (FU)	The delivery of 1 L of beverage to a California consumer in single use PET bottles during the years 2007-2009 35.8 g of PET / L, 5 g of PP/L				
Boundary	U1-2, D1-D3				
Inventory analysis					
Software		SimaPro 7.3.3			
Data source		Ecoinvent v2.01, US LCI, various literature			

	Impact Assessment				
Method	CML 2001 and TRACI 2.0				
Screening output	U1	U2	D1	D2	D3
EC (GJ/kg of FU)	0.0668	0.0287	0.00466	0.0164	0.002
GWP (kg CO ₂ eq./kg of FU)	2.55	1.973	0.353	1.02	0.28
Values were taken from Figure 3 and 4					

Table B-1 (Cont'd)

Journal	The International Journal of Life Cycle Assessment		No	2
Keyword search	PET or polyethylene terephthalate or beverage packaging			
Title	Life cycle environmental impacts of carbonated soft drinks			
Author	David Amienyo, Haruna Gujba, Heinz Stichnothe, Adisa Azapagic			
Year	Volume	Issue	doi	
2013	18	1	10.1007/s11367-012-0459-y	

Goal and scope	
Goal	1. To estimate the environmental impacts and identify the 'hot spot' in the life cycle of carbonated drinks produced and consumed in the UK 2. To analyze how the environmental impacts may be affected by the type and size of different packaging typically used in the UK 3. To estimate the life cycle impacts from the whole carbonated drinks sector, based on the findings from the first two goals of the study and a UK market analysis
Functional unit (FU)	1 L of a carbonated drinks of 0.5L PET bottle (47.9 g/L PET body, 6.1 HDPE top, 0.7 PP) and 2L PET bottle (21.4 g/L PET body, 1.5 HDPE, 0.6 PP)
Boundary	X2, U1-3, E2

Inventory analysis	
Software	GaBi
Data source	Drink manufacturer, CCaLC, Ecoinvent and GaBi

	Impact Assessment for 0.5 L PET bottle					
Method	PED (Primary energy demand) (GJ/kg), Global warming (kg CO ₂ eq.)					
Results	U1	U2	X2	U3	D3	E2
EC (GJ/kg)	0.0660	0.0220	0.0448	0.0144	0.0363	-0.035
GWP (kg CO ₂ eq.)	2.038	1.602	0.837	0.794	2.103	-2.53
Values were taken from Figure 5, 7, 12 and 13						

Table B-1 (Cont'd)

Journal	The International Journal of Life Cycle Assessment		No	3
Keyword search	PET or polyethylene terephthalate or beverage packaging			
Title	Life cycle energy and GHG emissions of PET recycling: change-oriented effects			
Author	Li Shen, Evert Nieuwlaar, Ernst Worrell, Martin K. Patel			
Year	Volume	Issue	doi	
2011	16	6	10.1007/s11367-011-0296-4	

Goal and scope	
Goal	To analyze the effect of increased recycling in different forms
Functional unit (FU)	350 kg of PET bottles and 650 kg of PET fibre
Boundary	X1, X4, U1, E2-3

Inventory analysis	
Software	N/A
Data source	Latest eco-profile published by plasticsEurope, Various literature, Ecoinvent database V2

	Impact Assessment				
Method	NREU (GJ/kg), Global warming (kg CO2 eq.)				
Results	U1	X4	X1	E2	E3
EC (GJ/kg)	0.0668	0.00525	0.07	-0.044	-0.0436
GWP (kg CO2 eq.)	2.04	0.288	0.78	-2.49	-2.418
Values were taken from Table 2, Figure 3 and 6, F3 calculated by SimaPro with Impact 2002+					

Table B-1 (Cont'd)

Journal	The International Journal of Life Cycle Assessment		No	4
Keyword search	PET or polyethylene terephthalate or beverage packaging			
Title	Life-cycle assessment of domestic and transboundary recycling of post-consumer PET bottles			
Author	Jun Nakatani, Minoru Fujii, Yuichi Moriguchi, Masahiko Hirao			
Year	Volume	Issue	doi	
2010	15	6	10.1007/s11367-010-0189-y	

Goal and scope	
Goal	Compare the recycling and disposal scenarios of Japanese post-consumer PET bottles
Functional unit (FU)	Disposal of 1 kg of Japanese waste PET bottles
Boundary	D3, E1-E3

Inventory analysis	
Software	N/A
Data source	Various published reports and database, field surveys in China

	Impact Assessment			
Method	Fossil resource consumption (GJ/kg), Global warming (kg CO ₂ eq.)			
Results	D3	E1	E2	E3
EC (GJ/kg)	0.0005	-0.00414	-0.0628	-0.0622
GWP (kg CO ₂ eq.)	0.04	2.54	-1.90	-2.4
Values were taken from Figure 2 and 4				

Table B-1 (Cont'd)

Journal	The International Journal of Life Cycle Assessment		No	5
Keyword search	PET or polyethylene terephthalate or beverage packaging			
Title	Recycling in buildings: an LCA case study of a thermal insulation panel made of polyester fiber, recycled from post-consumer PET bottles			
Author	Francesca Intini, Silvana Kuhtz			
Year	Volume	Issue	doi	
2011	16	4	10.1007/s11367-011-0267-9	

Goal and scope	
Goal	To define the energy and environmental profile of the finished products
Functional unit (FU)	1.065 kg of insulation panel
Boundary	X3, D1-2, E3

Inventory analysis	
Software	Simapro v 7.2
Data source	Various published reports and database

	Impact Assessment			
Method	Energy consumption (EC) (GJ/kg), Global warming (kg CO2 eq.)			
Results	X3	D1	D2	E3
EC (GJ/kg)	-	0.000916	0.0074	-
GWP (kg CO2 eq.)	3.27	0.044	0.41	-2.25
Values were taken from Table 4, 7 and 8, S2 and S3 calculated by SimaPro with Impact 2002+				

Table B-1 (Cont'd)

Journal	The International Journal of Life Cycle Assessment		No	6
Keyword search	PET or polyethylene terephthalate or beverage packaging			
Title	A preliminary LCA case study: comparison of different pathways to produce purified terephthalic acid suitable for synthesis of 100% bio-based PET			
Author	Yasuhiko Akanuma, Susan E. M. Selke, Rafael Auras			
Year	Volume	Issue	doi	
2014	19	6	10.1007/s11367-014-0725-2	

Goal and scope	
Goal	To compare the environmental burdens of bio-based PET resin with three different PTA production method scenarios
Functional unit (FU)	1 kg of PET resin
Boundary	X1, U1
Scenarios	Muconic acid
	Isobutanol
	Benzene, toluene and xylene (BTX)

Inventory analysis	
Software	SimaPro 7.3.3
Data source	Ecoinvent v2.0, US-EI and US LCI, various literature

	Impact Assessment						
Method	NREU (Primary energy demand) (GJ/kg), Global warming (kg CO ₂ eq.)						
Results	U1	X1			Benefit of X1		
		1	2	3	1	2	3
EC (GJ/kg)	0.0887	0.0819	0.0672	0.0478	-	-	-
GWP (kg CO ₂ eq.)	3.013	7.1	6.81	4.31	-1.966	-0.463	-0.887

Table B-1 (Cont'd)

Journal	The International Journal of Life Cycle Assessment		No	7
Keyword search	PET or polyethylene terephthalate or beverage packaging			
Title	Life Cycle Assessment of a Plastic Packaging Recycling System			
Author	Umberto Arena, Maria Laura Mastellone, Floriana Perugini			
Year	Volume	Issue	doi	
2003	8	2	10.1007/BF02978432	

Goal and scope	
Goal	To acquire information which allows one to quantify the real environmental advantage of recycling of PET and PE containers
Functional unit (FU)	1 kg of flakes of recycled or virgin PET
Boundary	T2, D1-3, E1, E3

Inventory analysis	
Software	N/A
Data source	Data provided by CoRePla (the Italian Consortium for plastic recycling)

	Impact Assessment								
Method	Energy consumption (EC) (GJ/kg), Global warming (kg CO ₂ eq.)								
Results	T2	D1	D2				D3	E1	E3
			1	2	3	4			
EC (GJ/kg)	0.0004	0.00016	0.0035	0.00314	0.0038	0.0035	0	0.0134	-
GWP (kg CO ₂ eq.)	-	-	-	-	-	-	1.63	3.11	-1.97
Values were taken from Figure 4 and 7, paragraph of page 94,									

Table B-1 (Cont'd)

Journal	Resources, Conservation and Recycling			No	8
Keyword search	PET or polyethylene terephthalate or beverage packaging				
Title	A life cycle assessment of the closed-loop recycling and thermal recovery of post-consumer PET				
Author	Tom Chilton, Stephen Burnley, Suresh Nesaratnam				
Year	Volume	Issue	doi		
2010	54	12	10.1016/j.resconrec.2010.04.002		

Goal and scope	
Goal	To compile a life cycle assessment (LCA) inventory to quantify and compare the environmental emissions from recovering value from post-consumer PET by the recycling and thermal recovery routes
Functional unit (FU)	The management of 1 tonne of post-consumer PET soft drink bottles
Boundary	U2, T2, D1-2, E1-2

Inventory analysis	
Software	SimaPro 7.1
Data source	Various literature and SimaPro database (ETH-ESU 96)

	Impact Assessment					
Method	Energy consumption (EC) (GJ/kg), Global warming (kg CO ₂ eq.)					
Results	U2	T2	D1	D2	E1	E2
EC (GJ/kg)	-	-	-	-	-	-
GWP (kg CO ₂ eq.)	0.035	0.0083	0.0136	0.220	-2.073	-1.223
Value was calculated by SimaPro with Impact 2002+ using Table 8 and 10						

Table B-1 (Cont'd)

Journal	Resources, Conservation and Recycling			No	9
Keyword search	PET or polyethylene terephthalate or beverage packaging				
Title	Open-loop recycling: A LCA case study of PET bottle-to-fibre recycling				
Author	Li Shen, Ernst Worrell, Martin K. Patel				
Year	Volume	Issue	doi		
2010	55	1	10.1016/j.resconrec.2010.06.014		

Goal and scope	
Goal	To understand the environmental impacts of recycled PET fibre compared to virgin PET To apply different allocation methods for this open-loop-recycling case
Functional unit (FU)	1 tonne of fibre
Boundary	D2, E1, E3

Inventory analysis	
Software	N/A
Data source	Data from three recycled PET fibre producers, Ecoinvent v2.0
Scenario	1. Mechanical recycling 2. Semi-mechanical recycling 3. Chemical recycling

Method	Impact Assessment						
Results	D2			E1	E3		
	1	2	3		1	2	3
EC (GJ/kg)	0.013	0.023	0.039	0.01053	-0.0432	-0.0474	-0.0290
GWP (kg CO ₂ eq./kg)	0.96	1.88	2.59	1.345	-1.399	-0.950	-0.289
Value were taken from Table 5 and Figure 14							

Table B-1 (Cont'd)

Journal	Journal of Cleaner Production			No	10
Keyword search	PET or polyethylene terephthalate or beverage packaging				
Title	Comparative assessment of the environmental profile of PLA and PET drinking water bottles from a life cycle perspective				
Author	Seksan Papong, Pomthong Malakul, Ruethai Trungkavashirakun, Pechda Wenunun, Tassaneewan Chom-in, Manit Nithitanakul, Ed Sarobol				
Year	Volume	Issue	doi		
2014	65		10.1016/j.jclepro.2013.09.030		

Goal and scope	
Goal	To assess the life cycle environmental performance of drinking water bottles made of polylactic acid produced from cassava in comparison with similar PET bottles produced in Thailand
Functional unit (FU)	1000 units of 250 ml drinking water bottles (16.26 kg of PET resin)
Boundary	U1-2, T2, D3, E1, E3

Inventory analysis	
Software	N/A
Data source	Field data at the actual sites in Thailand, various literature, the Ecoinvent database, national life cycle inventory databases of Thailand, research reports

	Impact Assessment					
Method	CML2 baseline 2000					
Results	U1	U2	T2	D3	E1	E3
EC (GJ/kg)	0.114	0.0156	0.00130	0.00023	-0.01218	-0.0258
GWP (kg CO ₂ eq./kg)	2.937	1.18	0.0962	0.0249	1.8114	-0.415
Values were taken from Figure 3, 4 and 9						

Table B-1 (Cont'd)

Journal	Journal of Cleaner Production			No	11
Keyword search	PET or polyethylene terephthalate or beverage packaging				
Title	Life cycle assessments of wine and spirit packaging at the product and the municipal scale: a Toronto, Canada case study				
Author	Julian Cleary				
Year	Volume	Issue	doi		
2013	44		10.1016/j.jclepro.2013.01.009		

Goal and scope	
Goal	To compare the net life cycle impacts of five types of 1 L wine packages and four types of 750 mL spirit packages To compare the net life cycle impacts from existing wine and spirit packaging consumption
Functional unit (FU)	The packaging required for 1 L of wine and 750 mL of spirits (58 g and 63 g of PET, respectively)
Boundary	U1-3, T1, D3, E2

Inventory analysis	
Software	SimaPro 7.2
Data source	Field data and Laboratory data, US EcoInvent (US-EI) database

Method	Impact Assessment ReCiPe v1.02								
Results	U1		U2		U3	T1	D3	E2	
	1	2	1	2				1	2
EC	-	-	-	-	-	-	-	-	-
GWP	4.359	4.325	1.453	1.442	0.4797	0.3564	0.3128	-1.454	-1.436
Values were taken from Figure 1, F7 data taken from refilling process									

Table B-1 (Cont'd)

Journal	Journal of Food Engineering			No	12
Keyword search	PET or polyethylene terephthalate or beverage packaging				
Title	The carbon footprint and energy consumption of beverage packaging selection and disposal				
Author	Jorgelina Pasqualino, Montse Meneses, Francesc Castells				
Year	Volume	Issue		doi	
2011	103			10.1016/j.jfoodeng.2010.11.005	

Goal and scope	
Goal	To evaluate the environmental impact of producing and disposing of several types of beverage packaging To determine the environmental profile of each product's life cycle
Functional unit (FU)	Packaging required to contain 1 litre of beverage
Boundary	X2, U1-2, T1, D3, E1, E2

Inventory analysis	
Software	N/A
Data source	Field data and Ecoinvent v2.1, various literature
Beverage	1. Juice, 2. Beer, 3. Water

	Impact Assessment								
	U1	U2	X2			T1	D3	E1	E2
			1	2	3				
EC	0.0863	0.0288	0.0056	0.254	0.0016	0.0295	0.00249	0.00219	-0.0668
GWP	3.225	1.075	0.806	10.49	0.311	1.762	0.0886	1.317	-2.332
Values were taken from Figure 6 and Table 4									

Table B-1 (Cont'd)

Journal	Journal of Food Engineering			No	13
Keyword search	PET or polyethylene terephthalate or beverage packaging				
Title	Comparative Life Cycle Assessment of hot filling and aseptic packaging systems used for beverages				
Author	Michele Manfredi, Giuseppe Vignali				
Year	Volume	Issue	doi		
2015	147		10.1016/j.jfoodeng.2014.09.018		
Goal and scope					
Goal	To evaluate and compare the environmental impacts of the hot filling and aseptic packaging systems by identifying the inputs and outputs for both processes and their impacts				
Functional unit (FU)	0.5 L of orange juice packaged in one-way PET bottles				
Boundary	U2-4				

Inventory analysis					
Software	SimaPro 7.3				
Data source	Ecoinvent v2.2, Data from designers and manufacturing companies				
Beverage	1. Hot filling 2. Aseptic filling				

	Impact Assessment				
Method	ReCiPe				
Results	U2		U3		U4
	1	2	1	2	
	-	-	-	-	-
GWP (kg CO ₂ eq./kg)	0.345	0.901	1.933	1.904	0.3795
Values were taken from Table 4 and 5					

Table B-1 (Cont'd)

Journal	Government report	No	14
Department	California Department of Resources Recycling and Recovery		
Title	Life Cycle Assessment of Polyethylene Terephthalate (PET) Beverage Bottles Consumed in the State of California		
Author	Brandon Kuczenski, Roland Geyer		
Year	Publication number	Web address (Accessed on Oct. 24. 2014)	
2011	DRRR-2014-1487	http://www.calrecycle.ca.gov/Publications/Documents/1487%5C20141487.pdf	

Goal and scope	
Goal	To estimate the environmental impacts of the plastic bottle product system and to evaluate the environmental benefits that result from recycling
Functional unit (FU)	The delivery of beverages packaged in single-use bottles made from 1 kg PET resin to California consumers
Boundary	U1-2, T2, D1-2

Inventory analysis	
Software	GaBi
Data source	US LCI, Ecoinvent, PlasticsEurope, PE International

	Impact Assessment				
Method	TRACI and CML				
Results	U1	U2	T2	D1	D2
EC (GJ/kg of FU)	0.0749	0.036	0.0003	0.0019	0.0065
GWP (kg CO ₂ eq./kg of FU)	2.62	2.47	0.04	0.15	0.699
Values were taken from Figure 3.1 and Figure 4.1					

Table B-1 (Cont'd)

Journal	Research center report		No	15
Center	Stiftelsen Ostfoldforskning			
Title	Environmental Assessment of Non-Refillable-Recyclable and Refillable PET Bottles Used as Packaging for Drinks in Norway			
Author	Hanne Lerche Raadal, Cecilia Askham Nyland, Ingunn Saur Modahl, Ole Jorgen Hanssen			
Year	ISBN number	Web address (Accessed on Oct. 24. 2014)		
2003	82-7520-509-3	http://ostfoldforskning.no/uploads/dokumenter/publikasjoner/95.pdf		
Goal and scope				
Goal	To carry out an environmental comparison of today's system for refillable PET and a system for non-refillable-recyclable PET used as drink packaging for mineral water, squash and water			
Functional unit (FU)	Production and transport of packaging and waste management of used packaging that is necessary in order to distribute 1000 L drinks to the consumer (in Norway)			
Boundary	U1-2, U4, T1, E2			

Inventory analysis	
Software	SimaPro 5.1
Data source	SimaPro database, PETCORE, Actual data from stakeholders

Method	Impact Assessment				
Results	U1	U2	U4	T1	E2
EC (GJ/kg of FU)	0.05636	0.01879	0.00248	0.000404	-0.05644
GWP (kg CO ₂ eq./kg of FU)	2.28	0.76	0.0863	0.0108	-2.105
Values were taken from Figure 6.3 and Figure 6.6					

Table B-1 (Cont'd)

Journal	Research center report	No	16
Center	Swedish Environmental Research Institute		
Title	LCA of Tetra Pak and alternative packaging on the Nordic market		
Author	Kristian Jeise, Elin Eriksson and Elin Einarson		
Year	Web address (Accessed on Oct. 24. 2014)		
2009	http://www.tetrapak.com/se/documents/lca%20nordics%20report%202009.pdf		

Goal and scope	
Goal	To assess the environmental performance of the individual packaging systems as well as the results of the comparisons of the environmental performance of the packages at each Nordic national market
Functional unit	Distribution of 1 litre of milk or juice or 0.5 litre of portion-packed beverage or small portion packed beverage
Boundary	U1-2, U4, T1, E3

Inventory analysis	
Software	GaBi 4
Data source	GaBi database, Plastics Europe, European Federation of Corrugated Board Manufacturers (FEFCO), Various literature

Method	Impact Assessment (CML2001)				
Results	U1	U2	U4	T1	E3
GWP (kg CO ₂ eq./kg of FU)	3.918	1.768	0.117	0.984	-0.270
Values were taken from Figure 16					

Table B-1 (Cont'd)

Journal	Research center report	No	17
Center	IFEU GmbH		
Title	LCA of one way PET bottles and recycled products		
Author	Andreas Detzel, Jurgen Giegrich, Martina Kruger, Sandra Mohler, Axel Ostermayer		
Year	Web address (Accessed on Oct. 25. 2014)		
2004	https://www.ifeu.de/oekobilanzen/pdf/LCA%20fuer%20PET%20Einwegsysteme%20erstellt%20fuer%20PETCORE%20%28Sept%202004%29.pdf		

Goal and scope	
Goal	The use of PET one-way-bottles for carbonated mineral water, non-carbonated mineral water and soft drinks was compared to the most reasonable refillable glass bottle system for the same beverage
Functional unit (FU)	Packaging system required to deliver 1000 litres of beverage to the consumer
Boundary	U1-4, T1, D2, D3

Inventory analysis	
Software	N/A
Data source	IFEU database, Various literature

Method	Impact Assessment						
Results	U1	U2	U3	U4	T1	D2	D3
EC (GJ/kg of FU)	0.0679	0.0162	0.0027	0.0187	0.0059	0.0062	0
GWP (kg CO ₂ eq./kg of FU)	2.55	0.992	0.116	0.579	0.454	0.386	0.554
Values were taken from Figure 5							

Table B-1 (Cont'd)

Journal	Master Thesis	No	18
Institute	Swiss Federal Institute of Technology Zurich (ETH)		
Title	LCA of Rivella and Michel soft drinks packaging		
Author	Genevieve Doublet		
Year	Web address (Accessed on Oct. 25. 2014)		
2012	http://www.esu-services.ch/fileadmin/download/doublet-2012-masterarbeit.pdf		

Goal and scope	
Goal	To compare the environmental impacts of the glass and PET bottles by conducting an LCA on Rivella and Michel packaging To decide whether or not glass bottles used in catering should be replaced by PET bottles
Functional unit (FU)	Delivering 9.9 L of Rivella drink in one refillable 33 cl glass bottle refilled 30 times or in 19.8 PET bottles of 50 cl Delivering 15 L of Michel juices in one refillable 100 cl glass bottle refilled 15 times or in 20 PET bottles of 75 cl
Boundary	U1-U4, T1

Method	Impact Assessment				
Results	U1	U2	U3	U4	T1
GWP (kg CO ₂ eq./kg of FU)	3.195	1.065	1.04	0.453	0.023
Values were taken from Table 3.3					

Table B-1 (Cont'd)

Journal	Master Thesis	No	19
University	University of Michigan		
Title	Comparative Life-Cycle Assessment of Bottled vs. Tap Water Systems		
Author	Christopher G. Dettore		
Year	Report No.	Web address (Accessed on Oct. 25. 2014)	
2009	CSS09-11	http://css.snre.umich.edu/css_doc/CSS09-11.pdf	

Goal and scope	
Goal	To compare various scenarios for delivering drinking water to consumers in the United States
Functional unit	1000 gallons of drinking water delivered to the consumer
Boundary	U1-4, T1, D3, E2

Method	Impact Assessment						
Results	U1	U2	U3	U4	T1	D3	E2
EC (GJ/kg of FU)	0.0877	0.0293	0.0058	0.0134	0.0207	0.0002	-0.0575
GWP (kg CO ₂ eq./kg of FU)	3.632	1.210	0.340	0.915	1.513	0.194	-2.198
Values were taken from Table 2.1 and Appendix H							

APPENDIX C: Example of the procedure to collect the GWP and EC estimates

Appendix C presents an example of the procedure to collect the GWP and EC estimates from the literature when only stacked bar charts were provided.

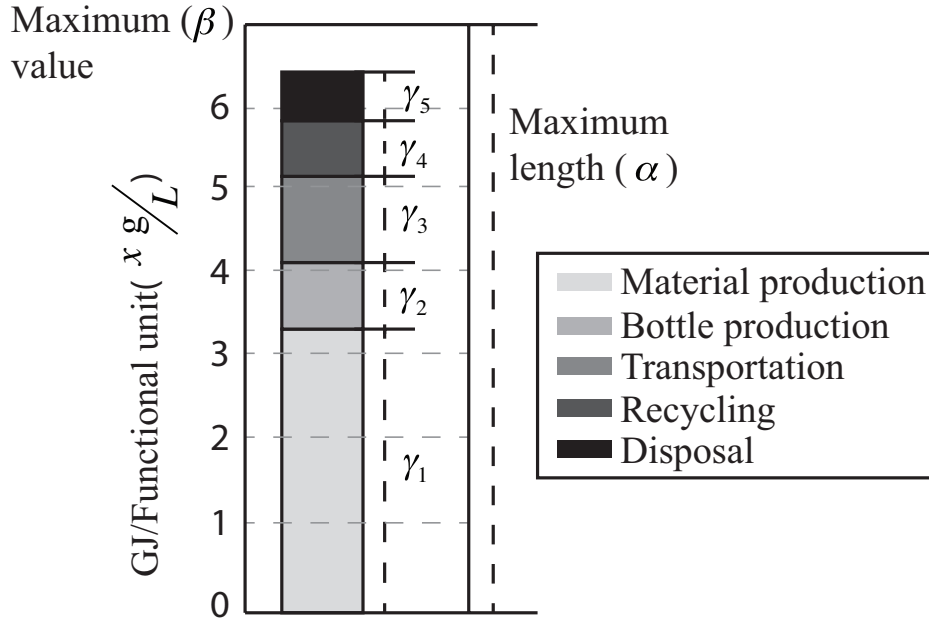


Figure C-1. Illustration of how to extract the GWP and EC from stacked bar chart

Where

x (g/L): Functional unit (FU) of study

α : Length of contribution analysis plot

β : Maximum value of contribution analysis plot

γ_i : Length of each life cycle phase

$$\frac{\beta \gamma_i}{\alpha} \times \frac{1}{x} \times 1000 = \text{Value of } i\text{th cycle phase per kg of FU} \quad (\text{III-1})$$

APPENDIX D: Harmonized results of meta-analysis

Table D-1. Harmonized results with mean and SD for GWP and EC

Life cycle stage	GWP (kg CO ₂ eq / kg of FU)		EC (GJ / kg of FU)	
	Mean	SD	Mean	SD
X1	3.9210	2.413	0.0667	0.014135
X2	3.1110	4.925	0.0765	0.119928
X3	2.6050	0.463	0.0759	0.001750
X4	0.1795	0.081	0.0032	0.001424
U1	2.9587	0.737	0.0777	0.014543
U2	1.2228	0.621	0.0257	0.006629
U3	0.9438	0.730	0.0076	0.006062
U4	0.4216	0.309	0.0115	0.008271
T1	0.7290	0.704	0.0141	0.013361
T2	0.0482	0.045	0.0007	0.000548
D1	0.1845	0.166	0.0029	0.002766
D2	1.0209	0.787	0.0134	0.012967
D3	0.4544	0.685	0.0038	0.010804
E1	0.3778	2.099	-0.0253	0.038665
E2	-2.0028	0.476	-0.0569	0.013833
E3	-1.4391	0.891	-0.0454	0.015305

APPENDIX E: Probability distribution analysis for the GWP estimates of each life cycle stage

Table E-1. Probability distribution analysis for the GWP estimates of each life cycle stage

Distribution	Upstream				Transportation		Downstream			Environmental benefit		
	U1	U2	U3	U4	T1	T2	D1	D2	D3	E1	E2	E3
Log likelihood												
Normal	-18.41	-16.45	-7.19	-0.91	-6.94	5.69	2.45	-11.27	-11.96	-18.92	-6.24	-12.51
Logistic	-18.73	-16.69	-7.51	-1.09	-7.29	5.52	2.12	-11.46	-11.03	-19.41	-6.69	-13.11
Weibull	-18.88	-17.56	-6.16	-0.23	-4.35	6.19	3.45	-9.31	-1.04	NA	NA	NA
Gamma	-17.55	-19.16	-6.21	-0.29	-4.14	6.17	3.45	-9.18	-1.43	NA	NA	NA
Lognormal	-17.27	-23.61	-6.58	-0.54	-5.22	6.05	3.09	-8.99	-0.02	NA	NA	NA
Exponential	-35.44	-21.62	-6.60	-0.82	-4.79	6.10	3.45	-10.21	-2.53	NA	NA	NA
Corrected Akaike Information Criteria (AICc)												
Normal	41.68	37.70	21.38	9.82	20.88	4.63	5.11	28.25	29.26	43.83	18.20	30.74
Logistic	42.31	38.18	22.02	10.18	21.58	4.95	5.77	28.63	27.39	44.81	19.09	31.94
Weibull	42.62	39.92	19.32	8.45	15.71	3.62	3.09	24.33	7.41	NA	NA	NA
Gamma	39.95	43.12	19.43	8.58	15.28	3.66	3.10	24.07	8.19	NA	NA	NA
Lognormal	39.40	52.03	20.17	9.09	17.44	3.89	3.83	23.70	5.37	NA	NA	NA
Exponential	73.74	46.04	18.19	7.64	14.58	1.80	1.10	24.13	8.40	NA	NA	NA

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