ENVIRONMENTAL LIFE CYCLE DRIVEN DECISION MAKING IN PRODUCT DESIGN

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ENVIRONMENTAL LIFE CYCLE DRIVEN DECISION MAKING IN PRODUCT DESIGN

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To My Parents, Jingdong Lu and Yanling He

To My Husband, Yanbing Yu and Son, David Yu

With Love

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SUMMARY

There is growing interest in the assessment of products from a life cycle perspective. Product life cycles are often dominated by extensive chemical supply chains that lead up to the materials contained in the products and the overwhelming contribution that the production of these chemicals make to the overall life cycle due to their energy intensity. Hence, chemical engineers are uniquely positioned to carry out significant components of this assessment because of their skills in chemical process design and analysis. Furthermore, the complexity and extent of life cycle concerns creates opportunities for new process systems tools to be developed to support product design and analysis.

The specific thesis objectives are threefold. The first is to develop a systematic methodology to optimize material selections for a product based on life cycle inventory (LCI) characteristics. The second is to use this methodology combined with sustainability assessment standards to assess whether these standards are congruent with life cycle assessment. The third is to develop an approach to design product sustainability assessment standards that are clear and consistent with life cycle principles. The overall contributions will be in the applied domain of life cycle assessment and its integration into standards setting, and in contributions to optimization tools and methods.

The three objectives will be illustrated in the domain of carpet systems. Previous research has generated a substantial database of gate-to-gate (GTG) life cycle inventories for various chemicals that make up carpet, extending from the inputs to the final carpet mill back to the natural resources such as oil, natural gas and mined calcium carbonate.

Carpet recycling is a promising alternative approach for reducing life cycle impacts and is being practiced at a growing scale in the U.S. This thesis uses the specific individual LCI gate-to-gate blocks for virgin materials and for important carpet recycling and general polymer recycling processes. A database for the GTG LCI will be used to construct a virtual chemical tree that automatically that represents the potential cradle-to-gate (CTG) use of resources. The alternatives for each possible route for the product will be generated, and optimization approaches will be applied to optimize the performance of the carpet system according to life cycle objectives.

Sustainability assessment standards are currently being developed for a range of building products, such as carpet, resilient flooring, commercial textile coverings and office furniture. This activity has been stimulated through the considerable success of the U.S. Green Building Council's (USGBC) LEED™ standard. The LEED™ Standard is points-based: the building design and construction earns points for having certain attributes or promoting certain activities. The points are totaled and then the building earns a rating based on the total being above a certain threshold. The second thesis objective is met through extending the LCI optimization methodology to represent point-based standards. A product can then be optimized to maximize the number of points it earns or to minimize its life cycle attributes. This approach can be used to evaluate the effectiveness of an emerging carpet sustainability standard, NSF-140, in integrating LCI into the standard.

The last objective, standard design, is approached through designing the tables that award points in the standard to be consistent with life cycle information. Certain minimum principles of consistency are articulated and then the designs shown to be consistent with these principles in the case that the life cycle impact assessment method maps the life cycle inventory to impact through a linear weighting.

CHAPTER 1

INTRODUCTION

1.1 Background

In the United States, carpet is the major floor covering material. Approximately 2.057 billion square yards of carpet were produced in the U.S. (The Carpet and Rug Industry Statistics). According to the annual report from CARE (Carpet America Recovery Effort, 2008), 5,038 million pounds of used carpet were generated as municipal solid waste (MSW), and only 243.4 million pounds of the used carpet were recycled. In addition, the used carpet does not significantly degrade, and the high performance synthetic fiber polymers from face and back of a carpet have significant economic value. Therefore, waste landfill (Doka, G., 2005) is a poor choice for the management of the used carpet from a sustainable development viewpoint. From the environmental responsibility and the cost saving perspective, recycling technique is becoming an important opportunity for the used carpet (Polk, M., 1994, and Craighill, A, 1996). As a result, an average of about 2 to 25 percent of used carpet recycled materials is currently involved in the carpet production system according to the Carpet Industry's Sustainability Report (2003). Additionally, 294.4 million pounds of post-consumer carpet were diverted from landfill in 2008, with 243.4 million pounds being recycled as a consequence of the government and companies efforts (Carpet America Recovery Effort Annual Report, 2008) From the state and the federal regulatory perspective, a Memorandum of Understanding (MOU) is signed between the industry, a number of states, and the Federal

EPA as a non-binding voluntary agreement to reach certain recycling targets by 2012. A third party non-profit organization, the Carpet America Recovery Effort (CARE) has been established by the industry to coordinate the activities to reach the MOU targets. In addition, the industry has made vigorous efforts to establish an ANSI standard for sustainable carpets. The ANSI standard is developed through a consensus process with the efforts of state and federal government, architectural specifications and carpet buyers, and environmental consultants. As part of the standard, the industry is especially engaged in life cycle inventory studies of carpet production systems and recycling processes.

1.2 Problem Statement: Establishing the Systems Science Base for Carpet Recycling and Sustainability

Life cycle assessment (LCA) is a commonly used method for evaluating environmental impact. Environmental impacts can differ significantly from process to process even in the same industry. Moreover, the chemical process itself is complicated with diverse operating equipments and various reaction conditions. Therefore, how to model and study the environmental impact of complex processes effectively using LCI information is a key issue.

In view of the fact that chemical processes are involved with numerous information, even though it is straight forward to model the system in the mathematical expression, when comes to the stage of solving the problem, it is difficult and time consuming due to the complex nature of the expression which involved with the integer and the non-linear programming. There are two ways to cope with the difficulty. One of them is to dig into the optimization algorithm and come up with a novel mechanism to solve the mixed integer nonlinear programming (MINLP) problem, and the other method is to express the problem properly at the beginning so that the existing solver instead of a new algorithm can solve the problem. In this dissertation, I will focus on the second method to manage the difficulty.

1.2.1 Cradle-to-Gate LCI System Synthesis

The development of Gatet-to-Gate blocks that are representative and transparent is one prerequisite for the scientific study of life cycles. The development of new recycling processes or the adoption of new materials leads to alternatives for products that involve different configurations of GTG blocks. Furthermore, it is important to ensure that different production pathways can be captured systematically, so that any potential alternatives will be included. This leads to the problem of constructing the network of GTG blocks that connects raw materials with products. Therefore, how to build the GTG network automatically is an interesting and important issue.

Once the GTG network is built, all the possible routes for producing the desired product are found. Which route is the best according to the environmental requirement? What is the system impact regarding environmental concern? Is current production system optimal for minimizing energy consumption? How can we analyze the system and make some improvements? How does recycling technology influence the configuration of the supply chain? These questions will be answered through the development of an optimization formulation.

1.2.2 Modeling for Sustainability Standards in Optimization

Sustainability standards are an important driving factor for product development in certain industries, such as carpet and buildings. Also, standards are helpful for procurement by large commercial organizations and government agencies. Standards are developed through a consensus process that often places emphasis on the categories of impacts which are based on stakeholders' previous experiences in the environmental fields. For instance, emphasis is often placed on the avoidance of solid waste through recycling and release of materials to other media during manufacturing. However, emphasis on energy efficiency, use of renewable materials, and social equity metrics, is increasing due to rising concerns about other human impacts on the environment and on global inequity. The emerging paradigm for sustainability standards is to establish a points-based reward system to allow the combination of multiple attributes of the product's performance. The products are then categorized into discrete levels based on crossing a certain threshold in the sum of points earned across categories. A key problem in this points system is allocating the points between performance attributes.

This problem is important and raises some important questions.

1. Given an existing standard, is there any connection between the points' distribution and life cycle inventory and assessment data?

2. If there is agreement that certain categories of points should reflect life cycle assessment, how should the results be mapped to points in different categories?

To examine these questions we will choose the specific example of the NSF 140 Sustainable Carpet Standard which is a points-based standard. The questions will be approached through the development of an LCI optimization tool to incorporate the evaluation and optimization of standards based products. This will contribute both to answering the above questions, and potentially lead to some interesting questions from a methodology perspective.

1. How should a points-based standard be represented in an optimization problem?

2. How can the above questions be represented and answered using optimization methods?

As standards begin to drive product design and marketing, it is considerate to reward appropriately aspects of life cycles. The information from life cycle contributes the most to resource usage and scientifically based measures of environmental impact. As a result, life cycle inventory contains lots of useful information that could help us to make the standards more comprehensive. Therefore, the research question is how to map life cycle information into standards and solve the optimization problem of designing a standard to encourage overall environmentally beneficial systems.

1.2.3 Design Sustainability Standards Using LCI information

Design of sustainability standards has taken place without a firm systematic understanding of the environmental decisions and life cycle information involved. In particular, the standard has evolved through several generations of stakeholder input to have a certain number of points awarded in different categories of activity, without a systematic understanding of whether the point allocations actually reflect improved environmental performance. In the carpet industry, the positive role of recycling, and in particular closed-loop recycling of materials from carpet back into new carpet, is not clear, since the energy involved could be more or less when examined from a cradle-to-cradle perspective. On the other hand, the GTG life cycle information would help to construct the multi-attribute standard. Carpet is not the only product for which multi-attribute standards are being developed and for which life cycle inventory is being suggested as the underpinning evaluation method. For example, sustainable forestry, other flooring surfaces, textiles, office furniture, and the Leadership in Energy and Environmental Design (LEED^{TM}) green building standard are all evolving standards and many of them have life cycle assessment components. This motivates a systematic and normative approach to incorporating life cycle assessments into standards.

1.3 Thesis Objectives

The objectives of this thesis are

1). To develop a set of transparent and representative GTG LCI blocks for carpet recycling that can be used in the optimization models. These blocks will represent both closed loop and open loop options for the use of carpet materials. A focus on the depolymerization of carpet materials will be explored for closed loop options along with polymer re-extrusion for the backing components. These GTG blocks will contribute to the growing body of scientific LCI data based chemical engineering principles.

2). To develop a life cycle optimization framework that can construct a GTG network and operate over a transparent and representative set of GTG life cycle blocks. This framework will generate a complete process network which can be optimized to meet different objectives, such as minimizing energy consumption, minimizing emissions, and minimizing use of virgin raw materials. This model will be used to test the hypothesis that closed loop recycling can be significantly sub-optimal when objectives relating to overall energy and mass consumption of a product are used to drive the decisions. This framework will contribute to simplifying the optimization process and use life cycle information to help design early in the product life cycle.

3). To develop a normative optimization model that can explore the relationship between standards setting and life cycle inventory calculations. This model will be tested in the context of a carpet standard under development through a consensus ANSI standards body. The model will be used to test the hypothesis that the standard point reward system and life cycle inventory measures are not completely aligned for carpet. The optimal solution will be used to suggest changes to the point allocation scheme that could bring the standard and life cycle assessment into closer agreement. This method will answer the question: given an existing point distribution, how do we assess the perverse incentive for products to increase their life cycle impact to increase the number of points they get?

4). To develop a normative methodology that can design standards setting using life cycle inventory information. How sustainability standards and life cycle assessment are related will be well established through this method. Also the following question will be answered: If one could design a standard, how could life cycle assessment data be used to design the standard to achieve consistency between the points and the assessment to avoid creating perverse incentives? This will contribute to identify regulatory needs and address public concerns for chemical industry.

1.4 Dissertation Overview

The chemical industry puts great emphasis on improving the energy efficiency with renewable materials and reducing the amount of emissions that enter the environment. The sustainable development across the extensive chemical supply chain is employed by synthesizing the life cycle inventory information. The study from the LCI of how each process cooperates in the life cycle supply chain and how to optimize the entire chemical system through individual processes is a necessary and meaningful subject. Namely, we will focus on the complexity with respect to model of both the system and processes using a back searching approach to evaluate the environmental impacts throughout the product's entire life cycle. Importantly, except for obtaining the objective value, the content and the sequence of the processes can also guide us on how to evaluate and improve the system for decision making. The approach will be illustrated in the domain of the EcoWorx^{TM} carpet system from the Shaw Industry & Inc.

This dissertation is comprised of seven chapters. Chapter 2 carries out the literature review of life cycle assessment, process-based and economic input-output life cycle assessment methodology, and LCA for environmental decision making. Chapter 3 describes using transparent and representative LCI data for GTG blocks modeling and the life cycle impact assessment (LCIA) method, which are the foundations for the carpet case study. Chapter 4 explains our approach to modeling the chemical system using a mathematical programming technique that involves process network construction and linear programming optimization. Chapter 5 illustrates how to integrate life cycle inventory with multi-attribute standard through mixed integer linear programming (MILP) optimization and the process network construction. Chapter 6 explores more applications of combining LCI and optimization tools to help the environmental policies and regulations decision making scientifically. Additionally, our studies can be extended to show how sustainability assessment standards can be redesigned to make them congruent with life cycle measures. Finally, Chapter 7 discusses the future work of using life cycle information to help environmental decision making.

CHAPTER 2

LITERATURE REVIEW

In this chapter we give a broad overview of life cycle assessment which is the foundation of our study. This chapter focuses on the literature review of life cycle assessment with four sections. Section 2.1 introduces the historical background of the life cycle assessment approach. Section 2.2 describes the life cycle assessment methodology in detail including process-based LCA approach, optimization of the process-based LCA, economic input-output LCA method, and LCA for environmental decision making. Section 2.3 describes the major advanced LCA tools used by both researchers and industry such as GaBi, SimaPro, TEAM^{TM}, and BEES. Section 2.4 discusses well-known existing LCA databases including the Ecoinvent database, the GaBi U.S. extension database, the database from NREL, and the EIO-LCA database.

2.1 Life Cycle Assessment Historical Background

The first documented life cycle studies date from the late 1960s (Miettinen, P., 1997), and the initial studies were focused on direct environmental impact such as energy requirements and solid wastes. Later on, other potential environmental effects were included in life cycle studies. From Hunt, R. (1996) and Fink, P. (1997), the emissions into air, water, or soil, and other environmental concerns such as human health and global warming began to play an increasing role in life cycle studies. Life cycle assessment was formalized by the Society of Environmental Toxicology and Chemistry (Fava, J.A., 1991); with the goal of capturing all the environmental impacts of a product. Finally, LCA was standardized by the International Standardization Organization through ISO 14040 and ISO 14044 standards in 1997. Since then, researchers have developed various life cycle impact assessment methods to evaluate the environmental impact. In addition, economic input-output analysis is also applied to life cycle studies. Nowadays, LCA method is widely used by many industries.

LCA is the assessment of the environmental impact such as energy (Kim, S., 2003) and emission of a product through its life cycle. The framework of LCA (Consoli, F., 1993) contains four phases in sequence as shown in Figure 2.1.

1. **Goal and scope definition** determines the system boundaries, assumptions of a study, and functional unit according to the goal of evaluating potential environmental impacts.

2. **Life cycle inventory analysis** is the basis of LCA, which quantifies material consumption and environmental emissions inside the defined boundary of the production system.

3. **Life cycle impact analysis** evaluates the potential impacts, such as global warming and fossil fuel depletion, based on the manipulation of LCI results.

4. **Interpretation** includes sensitivity and uncertainty analysis for the study, and what can be learned about the system, or what may be improved in the future.

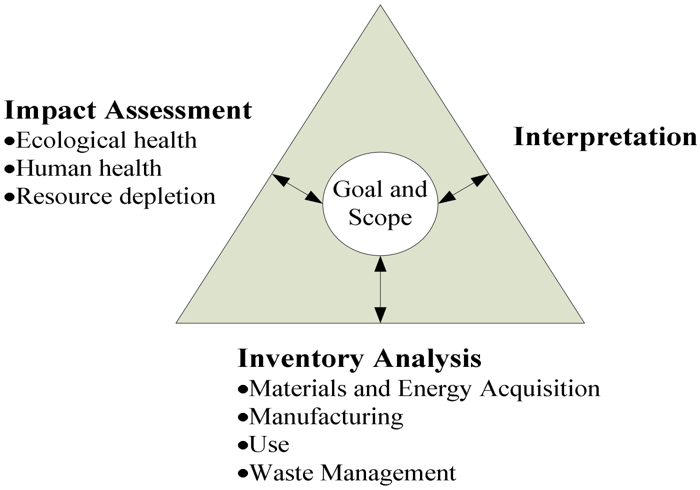


Figure 2.1: A Technical Framework for Life Cycle Assessment

Among the four phases of LCA, life cycle inventory analysis is the foundation of LCA and has the following procedures:

1. **Data Collection** is typically the most data-intensive part of LCI.

   a) Construct the particular process flow diagram;

   b) Describe each detailed process unit;

   c) Document the data and information sources.

2. **Calculation** through the application of conservation laws and thermodynamic properties.

   a) Calculate mass balance to capture all the material flow;

   b) Calculate energy balance to trace all the energy consumption throughout the system boundary.

3. **Validation of Data** reviews and revises the results from common experience and experts' comments.

The process flow diagram in Figure 2.2 is an example of flow diagram with various unit processes for PET depolymerization.

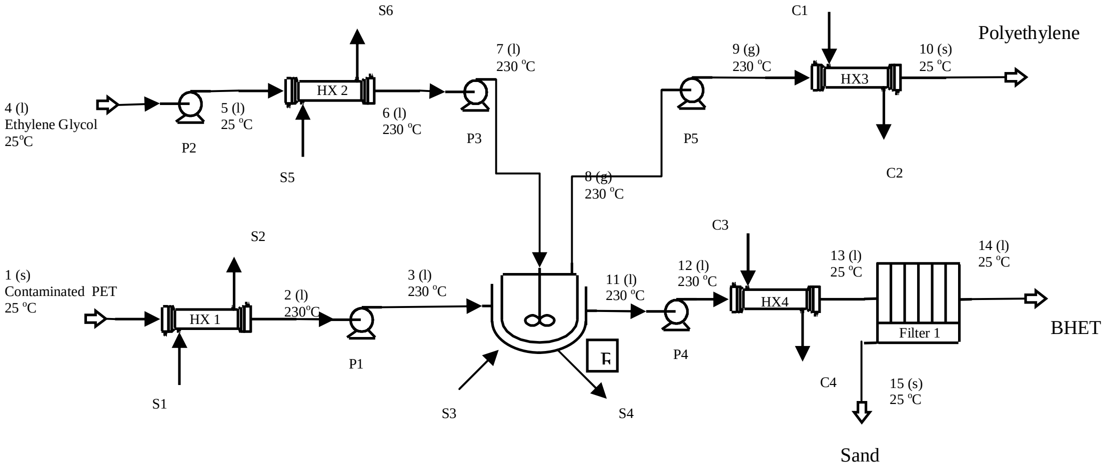


Figure 2.2: A Process Flow Diagram for PET Depolymerization

For each general LCI block, inputs are material and energy, while outputs are final product and emission as described in Figure 2.3.

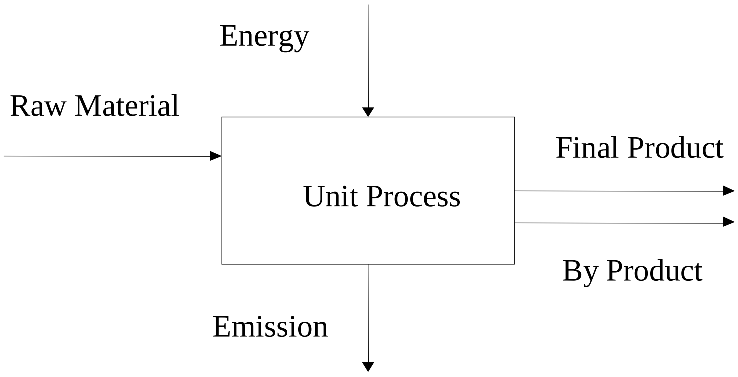


Figure 2.3: General LCI Block

In addition, the LCA glossary that is used in the following chapters will be explained below, and Figure 2.4 shows a typical LCA scope through a product life cycle.

Functional unit is a quantified reference unit for performance description of the product system. It provides a reference to relate the inputs and outputs and facilitates comparison of different systems.

Raw material is a primary or secondary (recovered and/or recycled) feedstock used in a manufacturing process.

Intermediate materials are the middle materials made from raw materials in order to make final products.

Cradle-to-grave is the LCA of the whole product life cycle from raw materials to use phase and disposal.

Cradle-to-gate is the LCA of the life cycle from raw materials to the factory product.

Gate-to-gate is the LCA of the part life cycle from one factory product to another factory product.

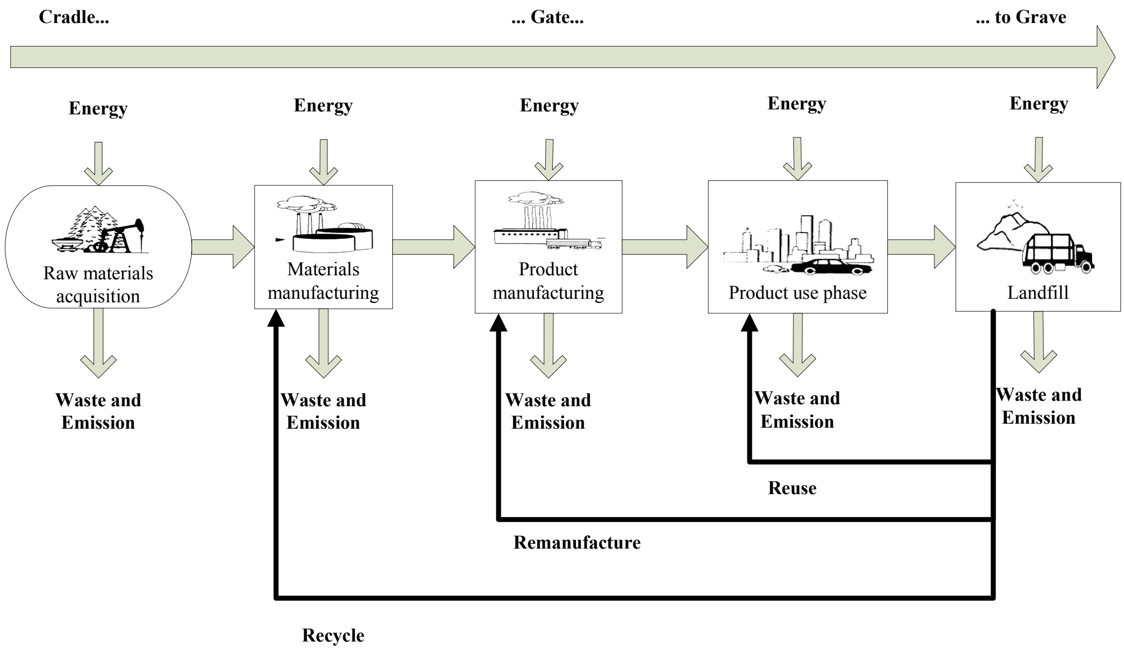


Figure 2.4: Typical LCA Scope through Product Life Cycle

The GTG LCI captures the unit operations of manufacturing from an intermediate product. The chemical product is either a commerce article or is an identifiable chemical intermediate. Consequently, numerous GTG LCI blocks can build up a process path for one product. In addition, if the original resources of the process path are raw materials such as crude oil, natural gas, or minerals, the LCI will be termed as a CTG LCI.

2.2 Life Cycle Assessment Methodology

The major LCA methods are process-based LCA and economic input-output LCA. The process-based LCA method is also named as "classical" or "traditional" LCA approach, which is developed by the effort of Society of Environmental Toxicology and Chemistry (SETAC), U.S. Environmental Protection Agency (EPA), and International Organization for Standardization (ISO). The process-based LCA approach uses physical process flow information through a product life cycle to capture resources, energy, and environmental impacts. The EIO-LCA method has been developed at Green Design Initiative from Carnegie Mellon University. The EIO-LCA method uses the structure of the flows of money in the economy to bring economic activity as quantitative input and estimate corresponding environmental impacts.

2.2.1 Process-Based LCA Method

The Process-Based LCA model shown in Figure 2.5 is based on process mass and energy balances for systems contained within the boundary. Throughout the process analysis, data and site information at various levels of detail, which reflect real systems and knowledge about specific systems, are used.

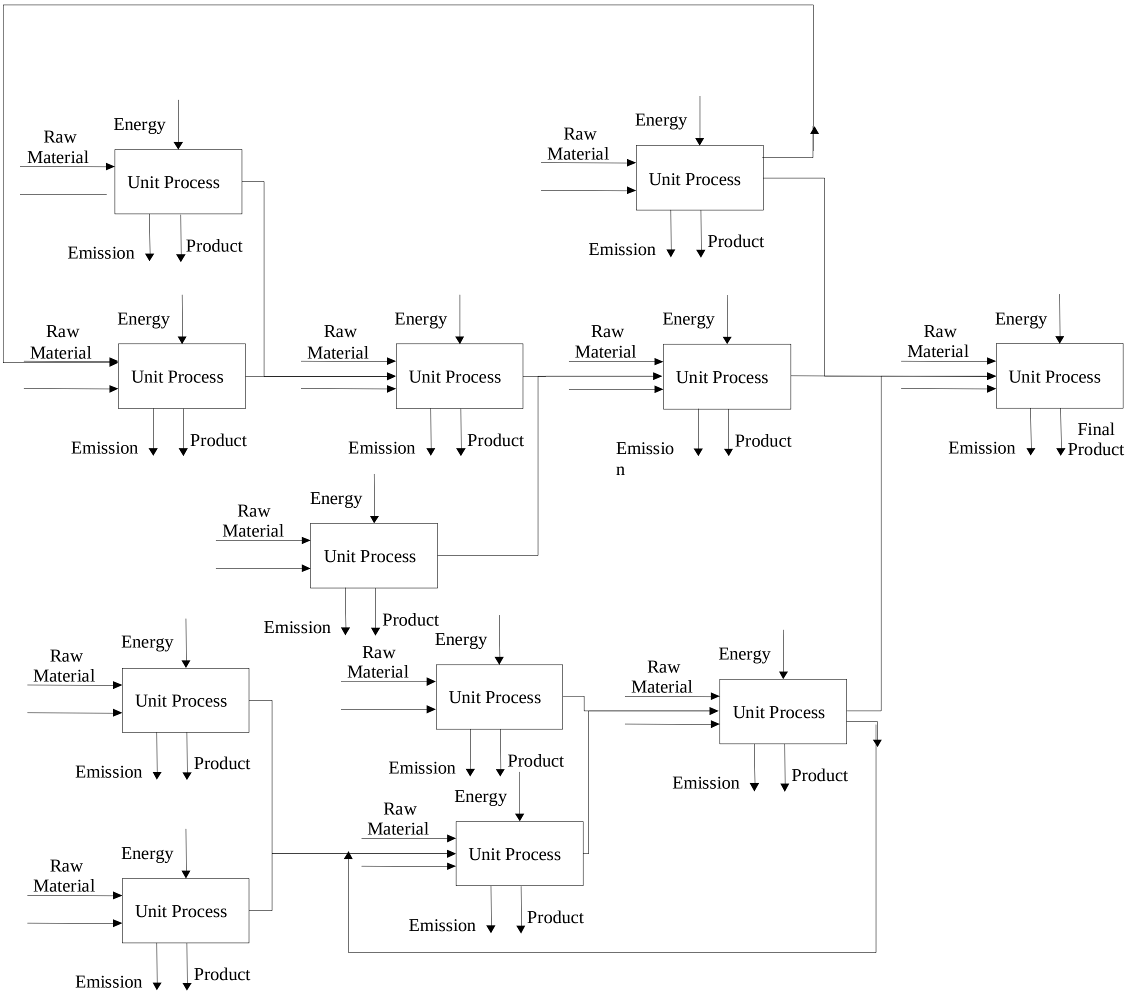


Figure 2.5: Process-Based LCA

Kim, S., and Overcash, M. (2003) utilize sources that represent accumulated engineering practice such as scientific articles, chemical encyclopedia, and patents to find relevant data for the process-based LCA.

2.2.2 Optimization of Process-Based LCA

Among life cycle assessment, life cycle inventory is based on linear relationships between the amount of activities and a set of direct measurement of environmental burdens such as energy consumption, material usage, and emissions. Therefore, linear programming can be used to model the LCA relationships for environmental studies. Figure 2.6 shows the connections between life cycle assessment and linear programming modeling. Environmental burden can be allocated in the inventory stage. The optimal solution of the linear programming presents how to improve the system from an environmental perspective. The benefit of using linear programming with LCA is that we can analyze the life cycle more accurately and evaluate how to improve the system efficiency according to different requirements. Furthermore, when additional system performances, such as economic or social performance are evaluated, multi-objective linear programming can be applied (Azapagic, A., 1999).

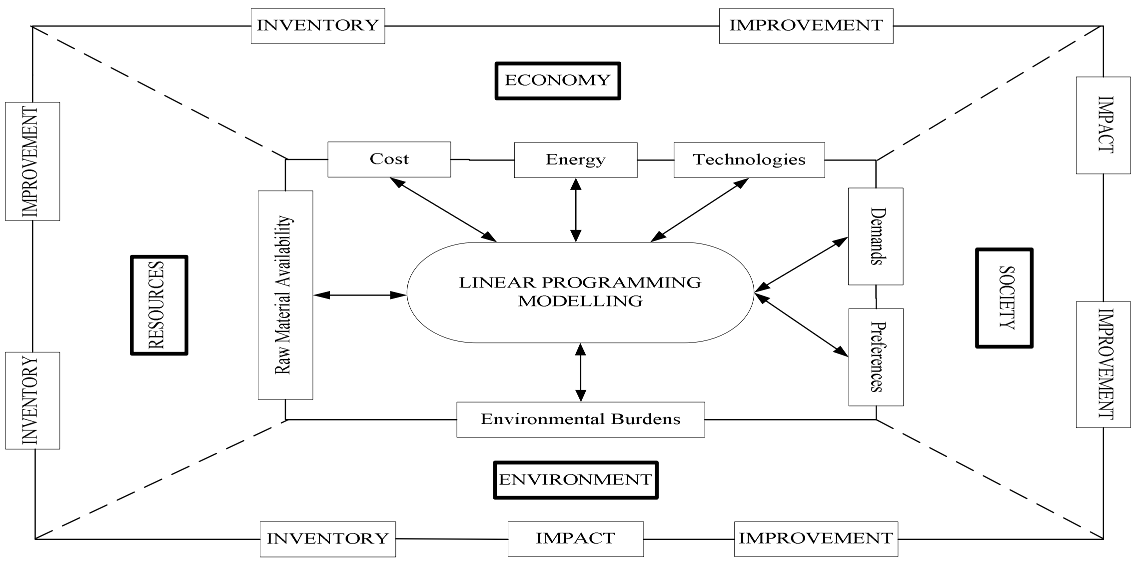


Figure 2.6: Interactions between LCA and LP Modeling (Azapagic, A., 1995)

Azapagic, A. (1999) proposed an optimum LCA performance (OLCAP) methodology which integrates LCA into an optimization system in four steps as shown in Figure 2.7:

1. Prepare the completed LCA study;
2. Formulate the optimization model with LCA information;
3. Perform multi-objective optimization (MO) on environmental and economic criteria;
4. Make decision from multi-criteria decision analysis and choose the best compromise solution.

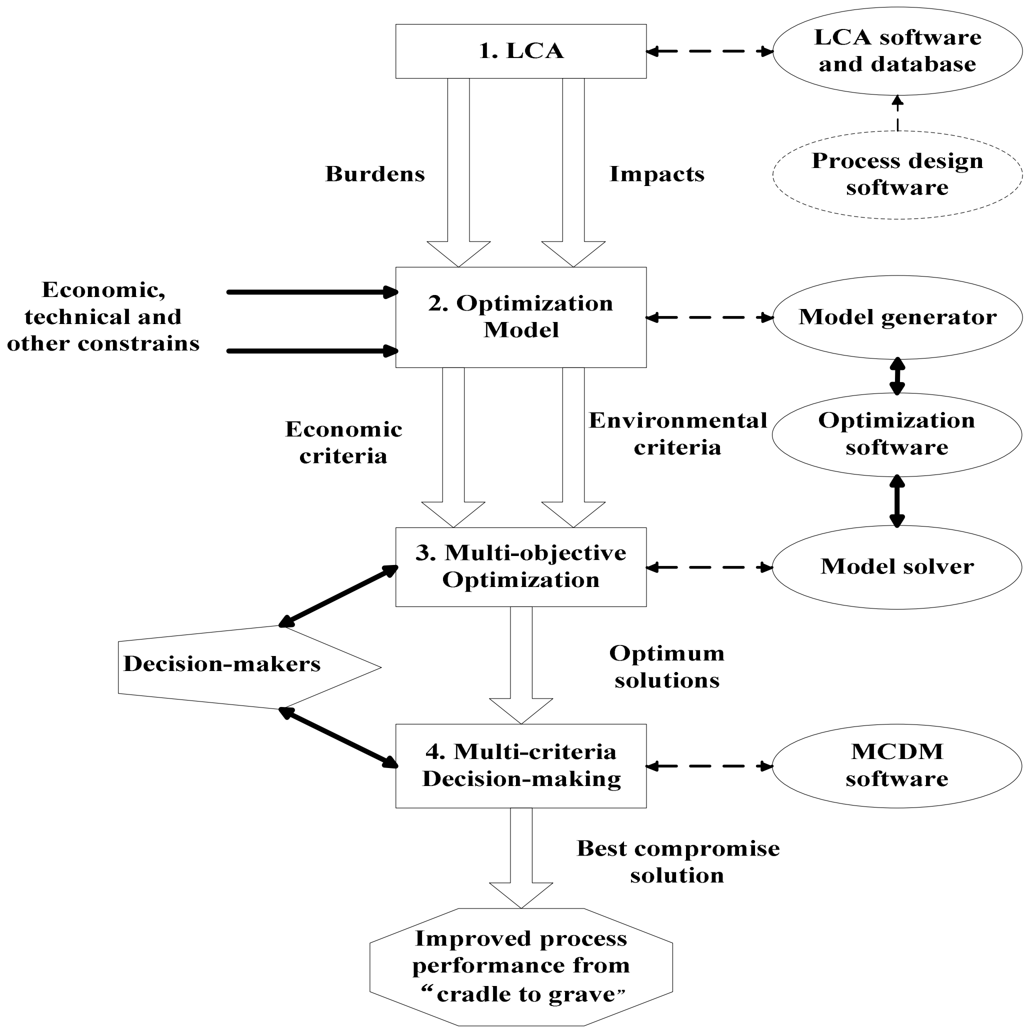


Figure 2.7: The methodological Framework for Optimum LCA Performance (Azapagic, A., 1999)

In Figure 2.7 a multi-objective optimization model with LCA for the step has the following structure:

$$\min f(x,y) = [f_1, f_2, ..., f_p] ....(1)$$
$$s.t.$$
$$h(x,y) = 0 ....(2)$$
$$g(x,y) \leq 0 ....(3)$$
$$x \in X \subseteq R^n ....(4)$$
$$y \in Y \subseteq Z^q ....(5)$$

A linear programming (LP) or a mixed integer non-linear programming (MINLP) is formed in Equations *(1) to (5)* (Azapagic, A., 1999). The objective function *f(x,y)* includes economic and environmental factors. *h(x,y)* represents equality constraints such as material and energy balances, and *g(x,y)* represents inequality constraints such as material availability and system production capacity. A vector of dimension *n* has continuous variables for material and energy flows, while a vector of dimension *q* has integer variables representing alternative processing routes or substitute materials.

$$\min F = c^T y + f(x) ....(6)$$
$$\min B_j = \sum_{n=1}^{N} b_{j,n} x_n ....(7)$$
$$\min E_K = \sum_{j=1}^{J} e_{k,j} B_j ....(8)$$

Other objective functions can be formed as Equations *(6)* to *(8)*. In Equation *(6)*, c is a vector of cost, and F is an economic objective function. In Equation *(7)*, $b_{j,n}$ represents coefficients of emission linked with continuous variables x_n, and B_j is the environmental objective function. In Equation *(8)*, $e_{k,j}$ represents the relative contribution of the environmental burden B_j to impact E_k, and E_k represents the impact function. Take the global warming potential (GWP) as an example, $b_{j,n}$ is the coefficient of transferring mass rate of emission to CO_2 equivalent with linear characteristic, and $e_{k,j}$ is the coefficient of transferring CO_2 equivalent to global warming potential with linear characteristic.

Stefanis, Livingston, and Pistikopoulos (1997) presented a methodology for incorporating environmental considerations in the optimal design and scheduling of batch processes. Stefanis, S. K., (1995,1996) and Pistikopoulos, E. N. (1998) presented methods for minimizing the environmental impact (MEIM) of process systems by embedding LCA principles within a formal process optimization framework.

Process-based LCA method is commonly used for specific processes which have detailed and accurate process flow data for life cycle inventory. Since the life cycle inventory has a linear characteristic for mass and energy balances, linear programming model and optimization method are used as a tool for process-based LCA. Guillen-Gosalbez, G. and Grossmann I.E. (2009), and You, F. and Grossmann, I.E. (2009) perform studies on the uncertainty of supply chains from an LCI perspective in chemical industry. In addition, various applications of optimization-based approaches exist in chemical engineering process synthesis supply, such as heat-exchanger network synthesis, distillation sequencing, mass exchanger networks and reactor network synthesis.

2.2.3 Economic Input Output LCA

Economic input-output model was developed by Leontief, W. (1970), who won the Nobel Prize for its development in 1973. The model utilizes economic transaction data from industry sectors to explore the economic relationships among them. In the EIO model, the production economy is divided into sectors and represented as a table or matrix involving individual economic sectors. Table 2.1 is an example of the input-output transaction table representing purchase flow between sectors.

Table 2.1: Input-Output Table of a National Economy (in physical units) (Leontief, W., 1970),

Into / From	Sector 1 Agriculture	Sector 2 Manufacture	Households	Total Output
Sector 1 Agriculture	25	20	55	100 bushels of wheat
Sector 2 Manufacture	14	6	30	50 yards of cloth

In order to examine the environmental impact based on the economic activity of a product, researchers at Carnegie Mellon University developed an EIO-LCA model (Hendrickson, C., 1998) to combine environmental information and economic input output data for environmental life cycle assessment. EIO-LCA can trace out the emissions of other related processes such as transportation and manufacturing throughout the supply chain.

$$X_{\text{direct suppliers}} = (I + D)F \text{.........................(1)}$$
$$X = (I + D + DD + DDD + ...)F \text{.........(2)}$$
$$X = (I - D)^{-1} F \text{....................................(3)}$$
$$B_i = R_i X = R_i (I - D)^{-1} F \text{.......................(4)}$$

X is the direct supplier process inputs vector and can be obtained from Equation *(1)*. I is an identity matrix. *D* is a direct requirements matrix, and *F* is a desired output vector. In Equation *(2)*, *X* takes all supplier input levels into account. In Equation *(4)*, *B* is a vector of environmental output. i denotes the type of environmental burden, and R_i is a matrix that has diagonal elements representing the environmental impact per dollar of output for each process. Since R_i is a given coefficient from dollar value, the model is linear related with input X and output B. Knowing R_i, B_i can be obtained from Equation *(4)*.

2.2.4 Comparison of Process-Based with EIO-LCA Models

The EIO-LCA model evaluates the impact for an industry sector, which contains several industry types. However, the sectorial aggregation of EIO-LCA is not adequate to model a specific industrial manufacturer. On the other hand, the major limitation for Process-Based LCA is the lack of detailed and accurate process data. Table 2.2 shows the advantages and disadvantages between process-based LCA and EIO-LCA (Hendrickson, C., 2006).

Table 2.2 Process-Based LCA Verses EIO-LCA Method

	Process-based LCA method	Economic Input-output LCA method
Advantages	▪ Detailed and process specific results ▪ Specific product comparisons ▪ Process improvements	▪ Comprehensive assessments for economic usage ▪ Systems-level comparisons ▪ Results publicly available
Disadvantages	▪ Time intensive for LCI ▪ Using confidential or proprietary data ▪ Data availability for environmental impact	▪ Economic boundaries ▪ Difficult for process assessments ▪ Uses aggregated data ▪ Data availability for environmental impact ▪ Timeliness of industrial structure

2.2.5 Life Cycle Assessment for Environmental Decision Making

Life cycle assessment is used widely as a tool for environmental improvement, strategic planning, public policy making, and decision support. There are mainly two applications (Miettinen, P., 1997): public and corporate. The public applications are focused on policy making, for example, to support the development of environmental regulation and legislation. On the other hand, corporations use LCA to analyze products life cycle and to support marketing claims around the environmental performance of products.

From the survey (Smith, J.C., 2006), LCA is commonly used to support business strategy (18%) and research and development (18%), for product or process design (15%), for academia (13%), and for product declarations or labeling (11%).

2.3 Life Cycle Assessment Tools

Many industries and companies have applied the LCA approach to optimize and improve resource management, which leads to a more efficient use of energy and materials. Therefore, LCA is used for comparing different options and as a support tool in decision making. This has led to an increased effort to develop life cycle assessment tools. According to the evaluation of life cycle assessment tools final report by Menke, D.M (1996), 37 life cycle assessment tools existed in 1996. LCA software tools have broad applications in different areas. For instance, the tools are designed for many industries such as plastic materials, building materials and food industry. In addition, as the growth of computer engineering, the graphic user interface (GUI) makes the tools easier to use and can present the results clearly. The criteria for evaluating the LCA tools are: highly detailed and representative life cycle inventory, impact assessment capabilities and flexibility, and extent of use within industry. There are mainly two groups who use the LCA software: researchers and business users. Researchers and scientists have high expectations for LCA tools, because they have a good understanding of the features of the LCA method and need to create their own data to model and compare different complex systems. On the other hand, the business users apply LCA tool to improve their environmental performance, product development, and process optimization. Therefore, analyzing and presenting results and the "easy-to-use" feature are important for decision makers. The primary advanced LCA tools used by both researchers and industry are GaBi 4, SimaPro and TEAM™. These are discussed in more detail below.

GaBi is the popular LCA software developed by PE International in Germany. GaBi has highly sophisticated functions and friendly user interface, which makes it useful for quickly analyzing data-intensive and complex systems for environmental life cycle assessment. GaBi 4 has the function of life cycle assessment (LCA), life cycle engineering (LCE), design for environment (DfE), energy efficiency/benchmark studies, strategic risk management, and carbon footprints. Figure 2.8 shows the GaBi database manager, and Figure 2.9 shows the input of variables of a flow. To design the LCA model of a process or a system in the GaBi 4, plans, processes, flows, parameters, units, and quantities are created and input in the tool. After finishing modeling, the balance of energy and material flow can be calculated and assessed by impact. The tool also can create multiple scenarios to compare impacts of different conditions. The database of GaBi is large and mainly for the use of product manufacturing and specifically the car industry. The clients of GaBi are divided into three groups: industry, university, and government. GaBi has more than 150 users such as Mercedes Benz AG, DuPont, General Motors, Motorola, Nokia, Siemens and Timberland (GaBi, 2009).

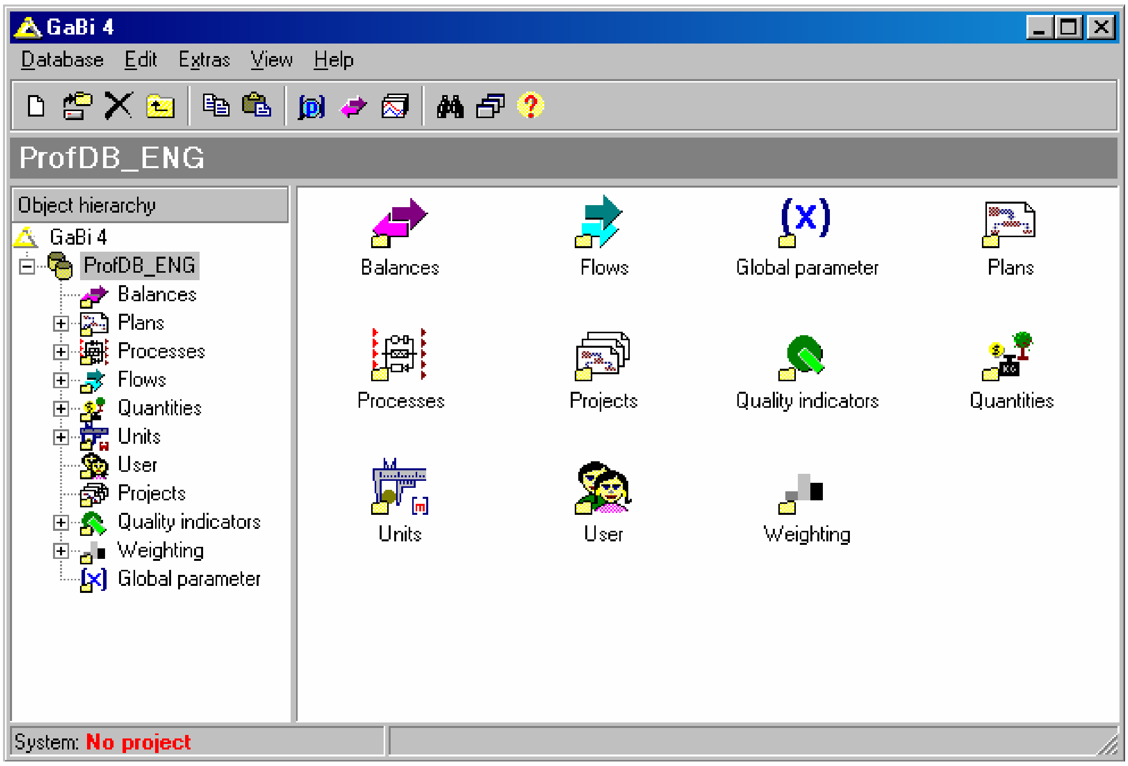


Figure 2.8: GaBi Database Manager (GaBi 4, 2006)

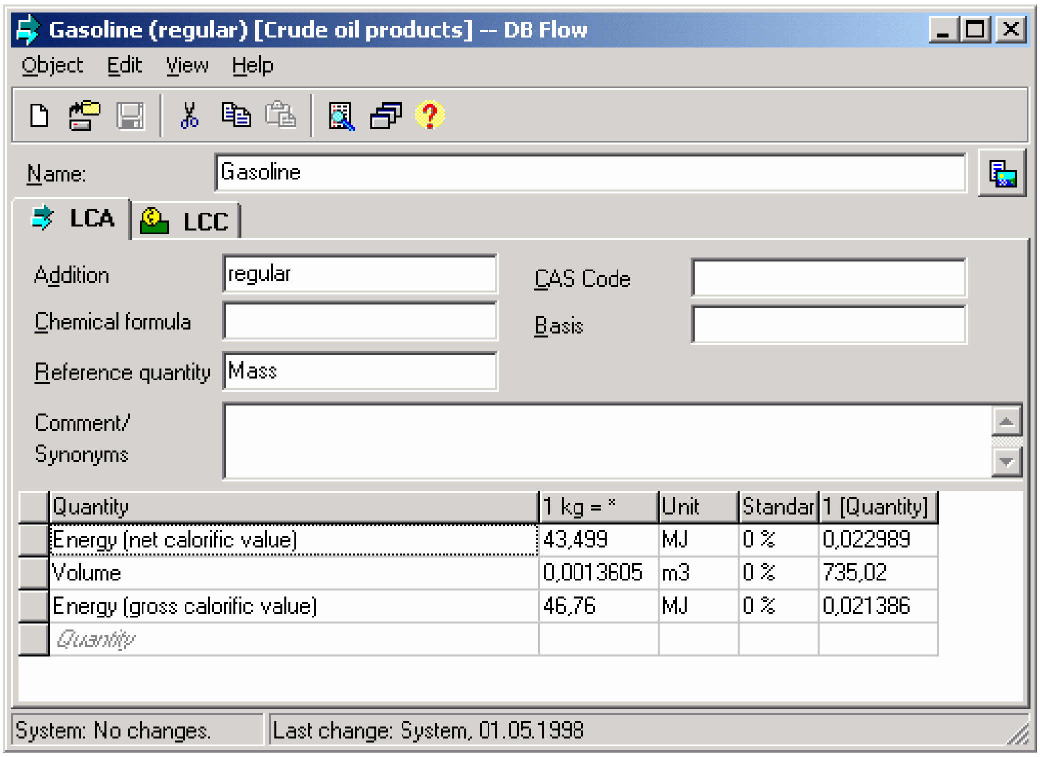


Figure 2.9: Variables of a Flow in GaBi 4 (GaBi 4, 2006)

SimaPro 7 is a life cycle tool to collect, analyze, and monitor the environmental performance of products and services developed by Pre Consultants. SimaPro 7 offers ultimate flexibility of accessing to and unrestricted editing of different database files, parameterized modeling, interactive results analysis and a large included database. Valuable features of SimaPro 7 are the ability to link database entries and access to numeric and visual indications of impact for each stage, process, and material in a product life cycle. Limitations of SimaPro 7 are the lack of sensitivity analysis and the graphical user interface for system development. SimaPro 7 has more than 300 users such as Philips and ABB (SimaPro, 2009).

Tool for Environmental Analysis and Management, TEAM™, is a flexible and powerful life cycle assessment software tool developed by the Ecobilan Group in Paris, France. TEAM™ is a powerful tool used to compile life cycle inventories using different data, including your own data and perform sensitivity analysis. Limitations of TEAM™ are the lack of support for user-defined weighting factors for impact assessment and the comparison of results capabilities. TEAM™ has sophisticated functionality and a large database. TEAM™ has more than 100 users such as BMW (TEAM, 2008).

Building for Economic and Environmental Sustainability (BEES) tool is developed from the National Institute of Standards and Technology's (NIST) BEES program. The BEES model is a publicly available software tool for building designers, architects, and specifiers. The BEES model takes a life cycle approach to building materials and focus on both life cycle environmental and cost data. The BEES model is based on consensus standards including: Life-Cycle Costing (ASTM E917), Building Element Classification (ASTM E1557), Environmental Life-Cycle Assessment (ISO 14040), and Multi-Attribute Decision Analysis (ASTM E1765). Figure 2.10 shows the steps to derive the BEES overall performance score. A total of 23 building elements are represented in BEES 3.0, with 118 generic products and 80 brand-specific products from 14 companies (Review of BEES). The limitations of the BEES are the tool only compares the performance of building products, not permits comparative analysis of entire building components assemblies and ultimately entire buildings. And the BEES overall performance scores do not represent absolute performance. Figure 2.11 shows the user interface of setting BEES analysis parameters. The BEES tool is a software program especially valuable for selecting environmentally friendly building products. The database includes actual environmental and economic performance data for 230 building products. Up to now, over 22,000 copies of BEES 3.0 requested by individuals from more than 80 countries (BEES, 2002).

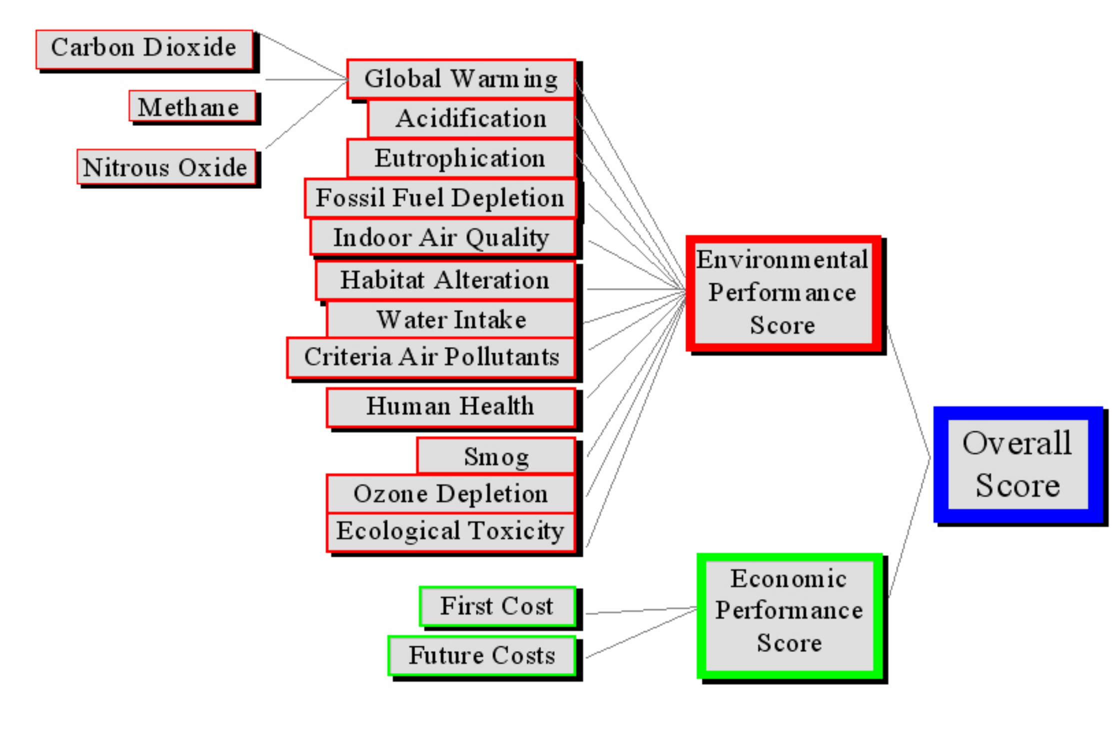


Figure 2.10: Deriving the BEES Overall Performance Score (BEES, 2002)

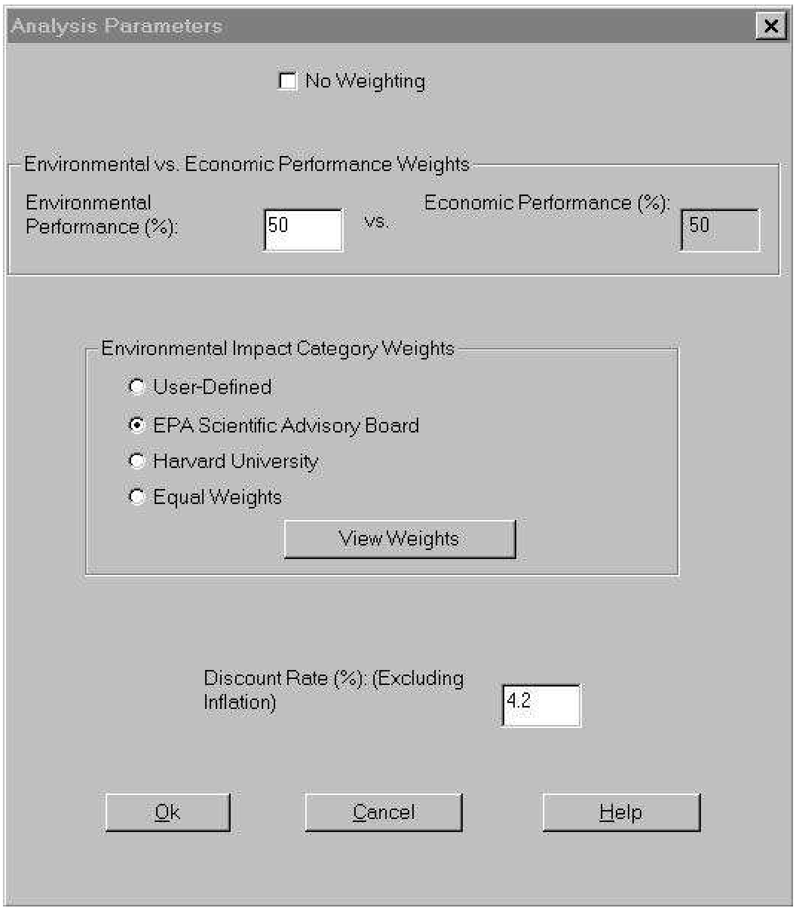


Figure 2.11: Setting BEES Analysis Parameters (Lippiat, B. C., 2001)

Table 2.3 shows a comparison of different LCA tools. The discussed LCA tools have advantages at user interface and graphically presenting the data. The weakness for all existing LCA tools is that lack information for detailed process design.

Table 2.3: Comparison of Major LCA Tools

	GaBi	SimaPro	TEAM	BEES
Domain	Manufacturing, Transportation	Energy, Transportation, Packaging Materials	Chemicals and Plastics	Building Materials
LCI	Extensive, High-Quality GaBi Databases	Detailed Inventory	Primarily European Data	Proprietary Information
LCIA Methods	No	Eco-Indicator 99 EPS 2000,and CML	IPPC, CML, and Eco-99	TRACI
Useability	User friendly	Careful study of examples is needed	Steep Learning Curve	Easy to Use

2.4 Life Cycle Assessment Databases

LCA analysis is data intensive. The demand for LCA databases has increased rapidly in a short amount of time. The quality and accuracy of the LCA based information play a significant role in the study of LCA. The content of database includes which economic sectors to cover, which pollutants are measured. These contents should be consistent as well, for example, they should have the same boundaries and modeling principles. Data in the database should be representative LCI data, up-to-date, clearly defined, and from a reliable source. Last, but not the least, the format of data and if data is exportable are important to users. Generally, the LCI databases are divided into two areas: comprehensive commercial databases such as Ecoinvent, GaBi, and public LCI databases including U.S. life cycle inventory databases, European reference life cycle data system. A list of the well-known existing life cycle inventory databases is shown as follows:

1. The Ecoinvent database is generated by Swiss Center contains up-to-date and consistent life cycle inventory data for more than 2700 industrial processes on material supply, resource extraction, energy, chemicals, metals, agriculture, waste management services, and transport services (Hischier R., 2002 and Frischknecht, R., 2004)). The Ecoinvent database is used by more than 1500 users in more than 40 countries worldwide and is included in various eco-design tools for product design, building, and construction. Main characteristics of the database are its reliable coherent set of LCI data and transparency in reporting to enable individual assessment of data appropriateness. In addition, the Ecoinvent database is an online database with interlinked data which has full access to unit process data and rolled-up data and is open for international collaboration.

2. The GaBi U.S. Extension Database has over 500 cradle-to-gate inventories for energy supplies, commonly used materials, and transportation systems. This is the largest LCI database available on the market focused on LCI information in the U.S. The database includes over 200 cradle-to-gate datasets based on the U.S. LCI database. In addition, the U.S. LCI Basic Database from GaBi is a free database that contains over 180 products and processes gate-to-gate inventories (Spatarb, S., 2001).

3. National renewable energy laboratory (NREL) provides the U.S. life cycle inventory database for researchers to study in the format of Excel. The NREL database is generated from a public/private partnership. In the beginning, Athena Institute started a building LCI project in Canada in 1990s, which caught the U.S. DOE’s attention. Later in

2001, DOE and Athena initiated the U.S. LCI Database project at NREL. The NREL LCI Database has been available since 2003 (NREL, 2004). The non-government organizations involved in the NREL database are Athena Institute, Franklin Associates, Sylvatica, CORRIM, Vehicle Recycling Partnership, American Plastics Council, Portland Cement Association, American Center for Life Cycle Assessment, USGBC, and others. Also, the involved government organizations are DOE, GSA, USDA, EPA, NIST, and the Navy. In addition, government maintains the database and provides common data and industry support with LCI data and some funding to develop the publicly available LCI database for commonly used materials, products, and processes. The common processes are standard transformation processes (stamping, pressing, painting, and other operations), electricity generation, transportation, and energy pre-combustion.

4. The EIO-LCA database involves of aggregate sector-level data quantifying how much environmental impact can be directly attributed to each sector of the economy and how much each sector purchases from other sectors in producing its output. The data in the database are in the format of dollar per physical units. The economic input-output tables in the EIO-LCA database are typically produced by national governments. In the beginning, the EIO-LCA database was based on the 1992 benchmark input-output (IO) commodity tables from the Department of Census, Bureau of Economic Analysis. In addition, national-level data on material or energy resources consumed by industry sectors, and data on industry releases to the environment are included in the database to estimate life cycle impacts (Carnegie Mellon University Green Design Institute, 2008).

Table 2.4 shows the advantages and disadvantages for different LCI databases.

Table 2.4: Advantages and Disadvantages for Different LCI Databases

Database	Advantages	Disadvantages
Ecoinvent Databases	-Interlinked database -Transparent and consistent -Wide breadth of data -User friendly interface -Data in XML format	-Requires purchase of LCA modeling tool -Process data not compatible with certain modeling tools
GaBi Database	-Wide breadth of data -Disaggregated unit process data	-Requires purchase of LCA modeling tool -Process data not compatible with certain modeling tools
NREL Database	-Peer-reviewed, publicly available LCI data -U.S. LCI database -Industry averages -Data in Excel format	-Process data not compatible with certain modeling tools
U.S. EIOLCA Database	-Free and fast -Monetary data -Industry sector data	-Not compatible with certain modeling tools -Product assessments contain aggregate data

Further work on the LCI database may comprise work on the LCI modeling methodology, the database content, for example, new or more detailed information covered in economic sectors, and the structure and features of the database system. Furthermore, building up international co-operations in LCI data collection and supply is the focus of future LCI database activities.

CHAPTER 3

LIFE CYCLE STUDIES FOR CARPET SYSTEM

3.1 Carpet Life Cycle

The United States has the largest carpet industry in the world. The life cycle of a carpet accounts for every impact on the environment from the day the carpet is made until the end of life when it is disposed of or recycled. A carpet’s life cycle impact include chemical emissions from manufacturing, depletion of petroleum and other natural resources, transportation, indoor air quality concerns, and disposal at landfills and recycling processes. A carpet life cycle consists of four basic stages: carpet manufacturing, transportation and installation, use phase, and disposal or recycling. Each stage plays an important role in a carpet's life cycle. Most carpet in use today is made from petroleum based fibers such as nylon, polyester, and polypropylene, whose manufacturing often can contribute to greenhouse gas emissions. Moreover, the economically significant component in carpet products is nylon fibers, which are also environmentally significant in the life cycles of carpet products. Several alternative green fibers exist such as recycled nylon and recycled P.E.T. polyester. Renewable resources also can be accounted for environmental friendly in the manufacturing phase. Like carpet fibers, carpet backing also can be made of recycled content and/or sustainable resources. In the phase of transportation, the majority of the carpet is manufactured in the U.S. in Dalton, Georgia, a town known as the "Carpet Capital of the World." Most of the carpet is transported to its destinations by the use of trucks in the U.S. In terms of transportation, carpet tends to have a much lower carbon footprint than floor coverings like bamboo, because the carpet is significantly lighter than most other types of flooring which consumes less fuel. The use phase for office building carpets is not distinctly different based on the construction: carpets tend to be cleaned on a periodic schedule over the life, and replaced after a certain time period irrespective of the wear. However, there has been heightened interest in recycling of carpet in recent years, driven by a multi-stakeholder agreement between the carpet industry and various government and non-government organizations (NGOs). They signed a memorandum of understanding for carpet stewardship (MOU), a ten-year schedule to increase recycling carpet and reduce carpet to landfills. Hence, one objective is to ensure that the recycling of carpet is beneficial from a life cycle perspective compared to using virgin raw materials.

3.2 Carpet Manufacturing

Most carpet manufactured in the U.S. is made of synthetic materials, especially nylon, polyester, and polypropylene face fibers. A large number of backings are made as a sandwich of polypropylene fabric and latex or PVC. Nearly all commercial carpets are made by bonding a face fiber to a backing fiber. Nylon 6 and nylon 6.6 account for nearly two-thirds of the face fiber market, with polyester as the next most commonly used fiber. 95% of carpet has a tufted structure shows in Figure 3.1. Based on the structure and composition of carpet tile product, a carpet tile is composed of three layers: fiber, primary backing, and secondary backing. Nylon is the most popular fiber for commercial carpet because it is easy to clean and has a better stain-resistance. The backing is used to keep the tufts in place and has three elements: a primary backing, an adhesive, and a secondary backing.

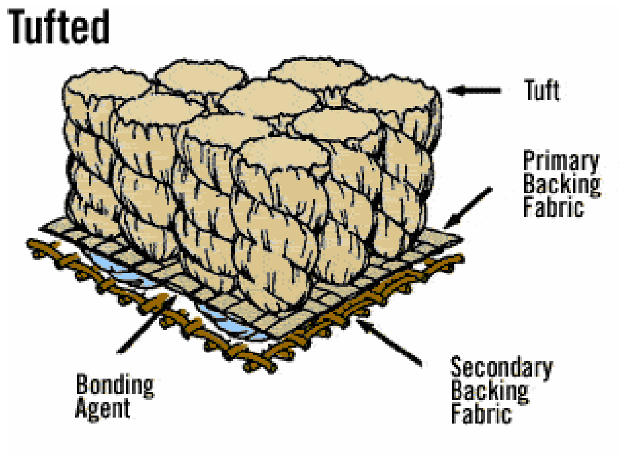


Figure 3.1: General Carpet Structure

Most carpet is made with unsustainable or non–renewable resources such as petroleum. Several types of office carpet materials and structure construction are existed. In this thesis, we focus on one specific construction, a tile, and a specific suite of materials used by a manufacturer, Shaw Industries, to produce EcoWorx^{TM}, whose initial design philosophy and construction was presented by Segars, J.W. (2003). Commercial tiles have three main components of an architecture, face fiber, primary backing fabric, and secondary backing. The secondary backing is often composed of a sandwich of two polymer layers and a layer of glass fiber. The polymer layers are often heavily filled with an inorganic material to reduce the use of expensive polymer and provide mechanical stability. EcoWorx^{TM} tile has a new polyolefin-based secondary backing polymer that replaces the PVC-based backing prevalent in the industry. In addition, the tile can contain recycled materials in various parts of the construction, such as backing polymer, backing fabric, backing filler, and face fiber. For example, Shaw has recently restarted a depolymerization facility in Augusta GA, which can produce limited quantities of nylon 6 from post-consumer carpet, and recovers post-industrial scrap nylon 6. In addition, the polyolefin backing polymer can be recycled as post-consumer EcoWorx^{TM}, and the backing fabric can contain a PET/nylon6 blend with recycled content. There is also a choice in the fillers that make up a substantial fraction of the carpet mass. The fillers can be a recycled glass cullet from post-consumer glass, a fly ash from a coal plant or mined calcium carbonate. Backing fabrics can be produced with or without nylon 6, and the backing from the post-consumer EcoWorx^{TM} carpet is an alternative for the backing polymeric system with backing fillers.

3.2.1 Nylon Carpet Recycling

Through the product life cycle, recycling processes have less environmental impacts, which may save energy consumption, reduce the emission to the environment, and facilitate waste management. The recycling option is applied broadly among many industries such as plastic, glass, paper, metal, and textiles. Our study is focused on the carpet industry. In a carpet, both face fiber and backing materials can contain recycled materials. Figure 3.2 shows the major components and a set of alternative processes for nylon 6 used carpet recycling. There are two primary stages in this system, the first group is physical processes which contains sorting, baling, chopping, fine grinding, and mechanical separation; the second group is chemical processes which is comprised of depolymerization, gasification, and combustion. Baling turns the high volume and different to handle carpet into compact bales; chopping and fine grinding are classified as size reduction (Dahlbo, H., 2005), which cut the carpet into small pieces; face fiber and backing materials are separated, often based on their density differences, and then put to different uses. These operations in group one are nearly always present at the start of the recycling process, and then are followed by one of a number of different options. For example, to obtain caprolactam after depolymerization and purification, to get a new plastic after extrusion and pelletizing, energy recovery through gasification or combustion, or to get new backing material after extrusion and compounding.

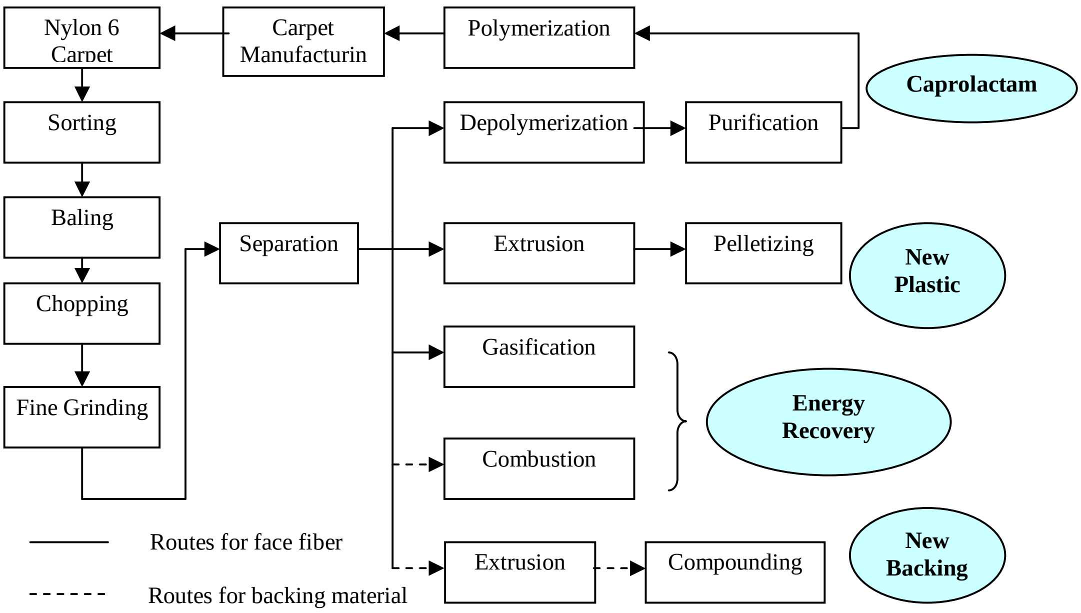


Figure 3.2: Nylon 6 Carpet Recycling Processes

3.3 Transparent and Representative LCI Data

Long term and significant efforts have been invested in developing software tools for the LCI calculation, but the effort is incomplete and unsatisfactory for many products. The problem stems from the nature of LCI results reporting and the overall transparency of the system. Since LCI data describe resource consumption and emissions of products, it may contain proprietary data of the manufacturer or its suppliers. So, the LCI has sensitive information when a business is involved. In addition, LCI has been used frequently to satisfy the needs of regulation and reporting to external stakeholder groups, which does not encourage an open view of the calculations. This has led to “black box” LCI reporting where it is very hard to verify or re-use the results of the studies. Also, it is hard to proceed via a scientific method of repeatable hypothesis testing. As a result, the "black box" LCI reporting has is lack of scientific progress in life cycle inventory studies. However, Kim, S. (2003) proposed two pioneering ideas to enable life cycle science to progress scientifically.

1. Representative GTG blocks. Instead of using an exact process being practiced by a specific company, a representative process flow diagram and stream conditions are constrain from public information. This technique has several benefits for further detailed life cycle studies. These representative process flows are open and communicated as part of the life cycle documentation, and valuable input from engineering are included. The representative GTG blocks serve as a basis to which well understood principles of mass and energy balances and thermodynamics can be applied. The representative GTG blocks make the communication of information more transparent and the LCI database easier to

maintain and update. In addition, a consistent basis to compare different products that have the same functional unit descriptions, but are made in different ways, is provided.

2. Consistent design methodology and calculation. The translation of conditions and unit operations to energy and mass consumption and emissions is done consistently across different blocks of the life cycle. Even though there may be bias and inaccuracy in the calculations, at least it is consistent across the different life cycle blocks. Later on, if new and more accurate methods become available, then the assumptions can be revised, reapplied and consistency maintained across the database. This makes the reuse of information and calculations much easier. This property of clear and unambiguous connection between the description of the process and the life cycle inventory outcomes is referred to as transparency.

In this thesis, all LCI information is calculated using the principles of transparent and representative data.

3.4 LCI Calculation of PET Depolymerization

Most of the chemical processes such as combustion, gasification, and extrusion have been studied by the methods of life cycle inventory through mass and energy balance calculations. The recovery of monomers by depolymerization is a general category of processes that is likely to become increasingly important for carpet recycling. Therefore, a life cycle inventory analysis of depolymerization for polyethylene terephthalate (PET) will be carried out.

The processes of chemical degradation of post-consumer or post-industrial PET are usually divided as follows: 1. Methanolysis. 2. Glycolysis 3. Hydrolysis. The process of methanolysis consists of the depolymerizing PET by methanol at high temperatures and under high pressure conditions. The main products of PET methanolysis are dimethyl terephthalate (DMT) and ethylene glycol (EG), which are raw materials necessary for the production of this copolymer. Currently, there are mainly two methods of methanolysis for PET: at high temperature and 1 atmosphere (atm); or at high temperature and high pressure. The methanolysis of PET at high pressure is commonly used in the chemical industry. Therefore, our LCI is based on this method.

PET methnolysis primary reaction:

$$[OCH2CH2CO\text{-}C6H6\text{-}COO]_n \xrightarrow{2nCH3OH} nHOCH2CH2OH + n\ H3CCO\text{-}C6H6\text{-}COOCH3$$

$$\text{PET (Polyethylene Terephthalate)} \xrightarrow{\text{Methanol}} \text{EG (Ethylene Glycol)} + \text{Dimethyl Terephthalate (DMT)}$$

The process flow diagram of PET methnolysis is shown in Figure 3.3 (Mandoki, (1986), Heisenberg (1962), Naujokas(1991), Smith (1996), and Paszun(1997)). Polyethylene Terephthalate (PET) enters the process at 25 ^oC and is ground and then melted through extrusion to 285 ^oC methanol (combined with the one from recycling) is preheated to 190 ^oC and pumped from 1 atm to 35 atm. Nitrogen is compressed and cooled to 190 ^oC, 35 atm to form an oxygen free atmosphere. All the above three mix in a stirring reactor 1 under 200 ^oC, 35 atm. 80% of PET is depolymerized through excess methanol (the weight ratio of PET to Methanol is about 1 to 4) under high temperature and high pressure. After reactor 1, the stream goes to reactor 2, which is unstirred at 190

^{o}C, 35 atm. In the second stage reaction the conversion of PET reaches 98%. The stream from reactor 2 is cooled to 100 ^{o}C and releases the pressure from 35atm to 3atm by a liquid turbine. To reach the 98% conversion, the stream enters reactor 3. The reactor products are separated by a flash, and a large amount of the methanol and nitrogen are vaporized and get recycled. The liquid mixture of DMT and EG are cooled and separated through a filter. After that, EG is recycled in the process of distillation and the main product DMT goes to centrifuge and dried by a dryer. The bottoms from the distillation contain EG and the tops contain the methanol which can be reused as part of the input of methanol.

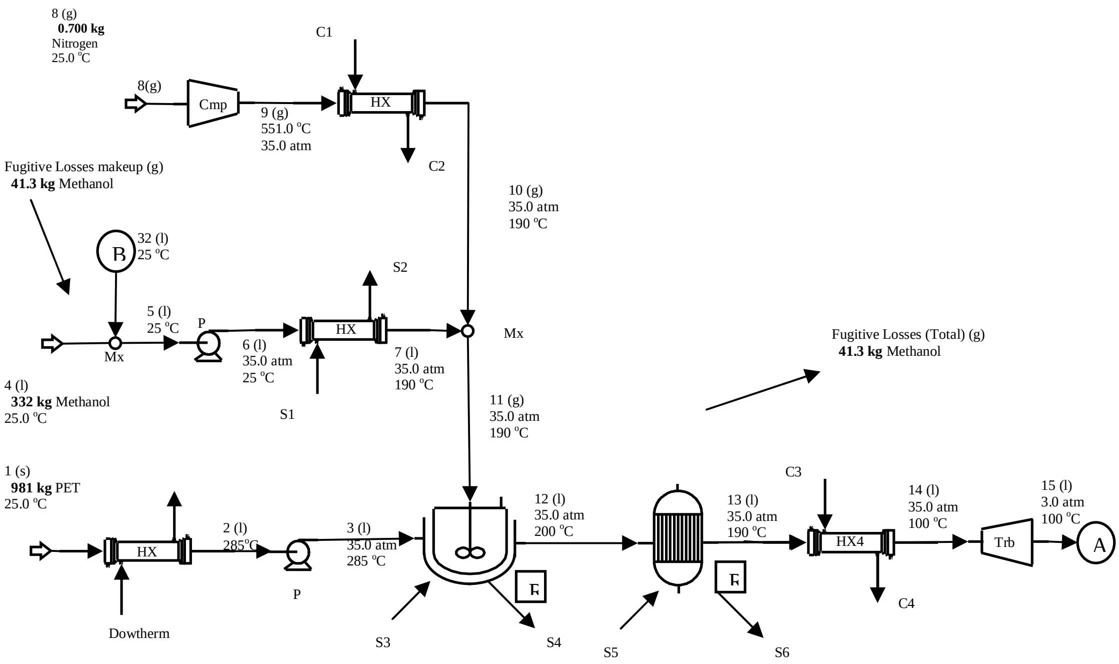


Figure 3.3: PET Depolymerization Process Flow Diagram

Steam enters the process as a gas at 207 ^{o}C and leaves as a liquid at 207 ^{o}C. Cooling water enters at 20^{o}C and leaves at 50 ^{o}C. Unless otherwise indicated, all processes are at 1 atm and 25 ^{o}C.

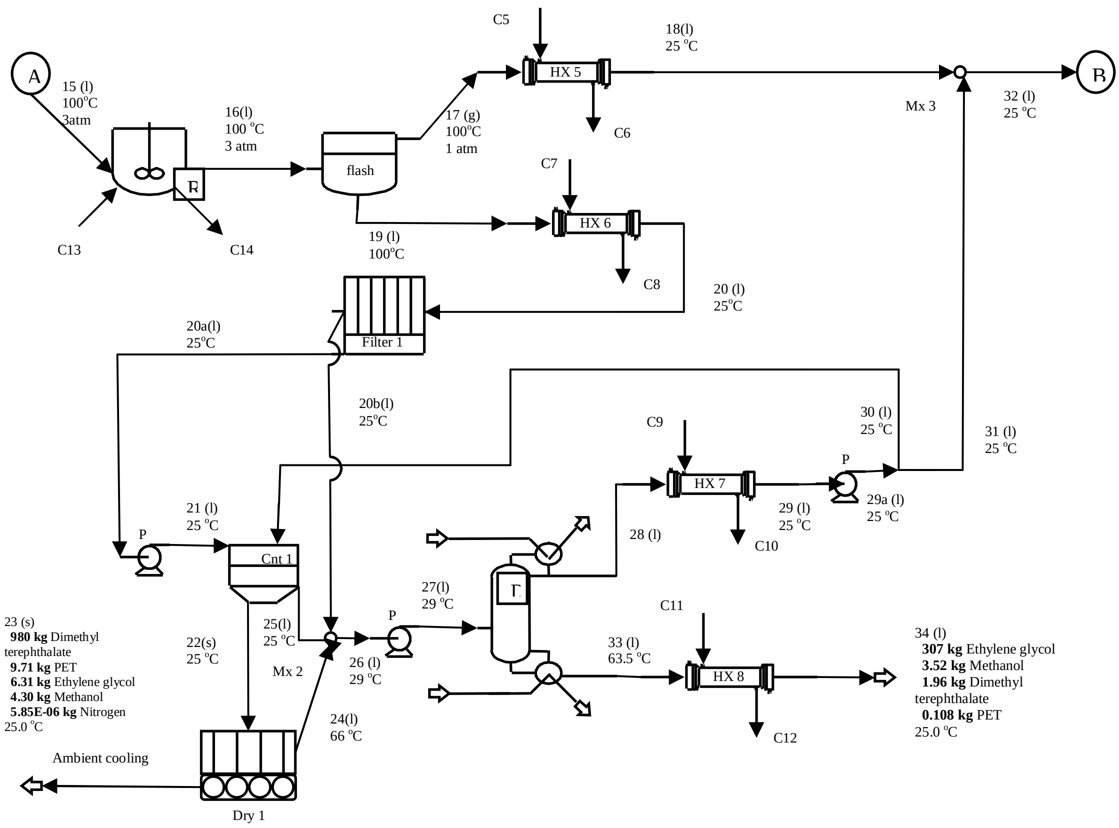


Figure 3.3: PET Depolymerization Process Flow Diagram (continued)

All LCI information for PET depolymerizaion is listed in Tables 3.1, 3.2, and 3.3.

Table 3.1: Inputs of PET Depolymerizaion

Chemical	Amount	Units
Methanol	373	[kg/hr]
PET	981	[kg/hr]
Total	1355	[kg/hr]

Table 3.2: Products of PET Depolymerizaion

Chemical	Amount	Units
Dimethyl terephthalate	1000	[kg/hr]
Ethylene glycol	313	[kg/hr]
Total	1313	[kg/hr]

Table 3.3: Energy Consumption of PET Depolymerizaion

Source	Amount	Units
Electricity	57.1	[MJ/hr]
Dowtherm	531	[MJ/hr]
Heating steam	1.20E+04	[MJ/hr]
Energy input requirement	1.26E+04	[MJ/hr]
Cooling water	-10897	[MJ/hr]
Potential Heat Recovery	-2959	[MJ/hr]
Net energy	9.65E+03	[MJ/hr]

3.5 Life Cycle Impact Assessment

Life cycle impact assessment (LCIA) is the third phase of life cycle assessment. LCIA first classify emissions to proper impact categories, then perform normalization for the effects, and finally assign the importance weights to the impact categories. In the classification and characterization step, all emissions are sorted into categories according to their environmental effects. For example, emissions that contribute to the global warming potential (GWP) or that contribute to acidification are classified into these categories. Emissions can be involved in several categories. For example, NOx is shown in several categories, such as acidification, toxicity, and eutrophication. Furthermore, in each category, there will be an effect score aggregated from different emissions. In the normalization step, normalization is used to understand the relative size of an effect. In the evaluation step, the normalized scores are multiplied by weights which represent the relative importance of the effect.

Mid-points and end-points methods are the two methods for life cycle impact assessment. Mid-points method is also names as problem-oriented method, which measures the environmental damage to several categories: Human toxicity, casualties, noise, photo oxidant formation, ozone depletion, climate change, acidification, eutrophication, and ecotoxicity. On the other hand, end-points method is damaged-oriented approach, which models the environmental damage to ecosystem health, human health or damage to resources. In this dissertation, a mid-points LCIA approach, Tool for the Reduction and Assessment of Chemical and Other Environmental Impacts (TRACI) is applied for the life cycle impact assessment.

CHAPTER 4

A MATHEMATICAL PROGRAMMING TOOL FOR LCI-BASED PRODUCT DESIGN

4.1 Introduction

Chemicals are produced by a series of energy-intensive transformations of raw materials such as crude oil. The life cycle inventory of mass and energy usage in these supply chains is one measure of the overall environmental performance. In this chapter, we present a methodology to examine the life cycle choices available for a product and optimize these based on criteria derived from mass and energy usage. A two-phase framework of path construction followed by optimal path selection was developed. This framework can be applied to improve the overall LCI energy usage of a product when there are different production and recycling options for different product constituents. The approach will be illustrated in a case study of the EcoWorx^{TM} carpet system of Shaw, Inc.

One approach to incorporating environmental objectives into product design and manufacture is to use information provided by a life cycle assessment which gives information along several dimensions of environmental performance. LCA was formalized by the Society of Environmental Toxicology and Chemistry (SETAC) (Fava, J. A., 1991) and later standardized by the International Standardization Organization through ISO 14040 and ISO 14044. A key input to the LCA phase is the inventory of mass and energy usage within the boundary of the analysis. Process-based life cycle inventory approach uses LCI data on individual processes to trace back through the major stages involved within the entire life cycle of a product (from raw materials to ultimate disposal) and to evaluate the environmental burdens at each stage. Commonly used LCI data are available from the LCI database managed by National Renewable Energy Laboratory (NREL) and from the construction materials LCI database from Building for Economic and Environmental Sustainability (BEES) which is maintained by National Institute of Standard and Technology (NIST). However, because of the complicated and extensive nature of the underlying LCI source data, managing the evaluation of the system accurately and efficiently is a challenging task. To help with the LCI data management and to translate between inventories and impacts, LCA software tools have been developed. Two commonly used LCA tools are SimaPro, developed by Pre Consultants in Holland, and GaBi, developed by PE International in Germany.

An alternative to the process-based LCI approach is to leverage economic data about transactions between industry sectors. Environmental input-output life cycle analysis (EIO-LCA) adds environmental outputs to classical economic outputs, apportioned by the dollar amounts involved in the transactions between industry sectors (Leontief, W., 1986, 1970, and Hendrickson, C. T., 1998). EIO-LCA is an efficient way to estimate system performance when an analyst wishes to consider the impact from different sectors of the economy that might be seen far away from the original system boundary (Hendrickson, C. T., 1997, 2006, Hawkins, T., 2007, and Lave, L. B., 1995). However, since the EIO-LCA model contains aggregate industrial sectors of the economy rather than individual operating processes, the aggregation level of most input-output models is too high for detailed product design. Therefore, process level information associated with the production of key chemicals is vital to companies seeking to improve their product performance by substitutions of chemicals or manufacturing methods.

The aim of this chapter is to present a methodology that optimizes LCI measures for products with complex process trees. The methodology is implemented through the explicit construction of alternative production paths that are then selected to meet overall production targets. Rather than looking at an intensive functional unit, we adopt an extensive measure of the product volume over a specified life cycle boundary. This allows the incorporation of the constraints on the absolute amounts of materials available along different process paths involved in the manufacture of products. This constraint appears repeatedly for products that contain recycled materials, either because there are performance specifications that cannot be met without blending recycled and virgin raw materials, or because there is limited availability of recycled materials compared to the overall product volume. In Section 4.2, we describe our approach to modeling the chemical system using a mathematical programming technique that involves a process network construction and a linear programming optimization. In Section 4.3, we illustrate how to employ the tool in the preliminary study of a carpet production system.

4.2 Two-Phase Framework Methodology for Process Synthesize

Our goal is to identify optimal production alternatives given that limited raw materials may impact our ability to use only one path. In addition, we seek to optimize our selections according to different objectives. Our proposed two-phase synthesis optimization framework will divide the whole complex problem into two relatively simple problems. The first problem is to identify the different production paths and the second problem is to select the optimal path(s) among these. The framework uses LCI information (Jiménez-González, C., and Overcash, M., 2000, Jiménez-González, C., and Kim, S., 2000, and Overcash, M., 1994) organized around individual process blocks that is generated independently and hence can be easily extended and maintained. One alternative approach would be to simultaneously synthesize and select the paths, which will lead to a more complex optimization algorithm. We have chosen to avoid this complexity and instead incur the enumeration of the production paths. In addition, the paths themselves contain useful information that would not be revealed by the simultaneous approach.

4.2.1 Overview

We start with definitions of terms used in this work that could have different interpretations in other contexts.

Definitions:

1) A **process** is defined as a chemical or physical process that takes one or more chemicals as input and produces one new chemical or intermediate product while requiring some amount of energy and generating by-products and emissions. Basic inventory information is used to calculate the further life cycle impact for assessment by whatever impact categories are desired. The production of one product from a process means that any co-product allocations have already been made (Curran, M. A., 2007). There is no specific restriction on what allocation method should be used, as long as it is consistently applied for all processes. It is assumed that none of the co-products provide substantial limits on the use of product materials other than those already reflected in product constraints.

2) A **desired product** is the final product that is manufactured and sold. In our analysis, we assume that only one product is being considered.

3) **Raw materials** represent materials that are utilized directly as the input to the system without a preceding manufacturing process. For example, crude oil and air could be categorized as raw materials while benzene and nitrogen could be raw materials in another context. This allows for the boundary of the analysis to be chosen at any point in the supply chain. It is assumed that the LCI of the raw materials is available as an input to the system.

4) **Alternatives** represent processes that differ in some aspect of material and energy usage. For example, there may be two alternatives to producing caprolactam, or two alternatives that can be used to fill a specific product need.

5) A **process tree** represents the manufacture of a desired product from the available raw materials. The desired product is the root of the tree and is the only material not consumed by a process. The raw materials are the leaves of the tree and are only consumed. Intermediates are produced and consumed by processes that lie on a path from raw materials to the desired product.

The basic idea is that the programs will read XML formatted data in the form of the LCI documented blocks. And construct the virtual chemical tree automatically from the blocks on the basis of the target end product. The output matrix will be read into a mathematical programming and then solve for the optimal flows according to the objective function. Consequently, the General Algebraic Modeling System (GAMS) program will find the best overall mix of flows from alternatives for chemicals or alternative routes (such as recycling) to specific materials.

The two-phase approach is illustrated in Figure 4.1: Phase-I is on the left hand side, which consists of a process-library and a process-tree-builder module; Phase-II is on the right hand side, which contains a process-tree-selector module. In Phase-I, all the LCI information that is required to manufacture a desired product is stored in the process library. According to the LCI information stored in the process library, which consists of the desired product and available raw materials, the process-tree-builder module will construct all the possible process trees. In Phase-II, the process-tree-selector module will select the optimal process tree or a combination of possible process trees. The objective can be any of the life cycle inventory measures, such as energy used in various forms, or the mass of certain components. The constraints are the mass balances over the process tree and any limitations on the total flows of materials due to their availability. The bridge between Phase-I and Phase-II are raw materials and a consolidated output matrix of all available process trees generated by the process-tree-builder module. Next, we will explain the overall framework with an abstract example.

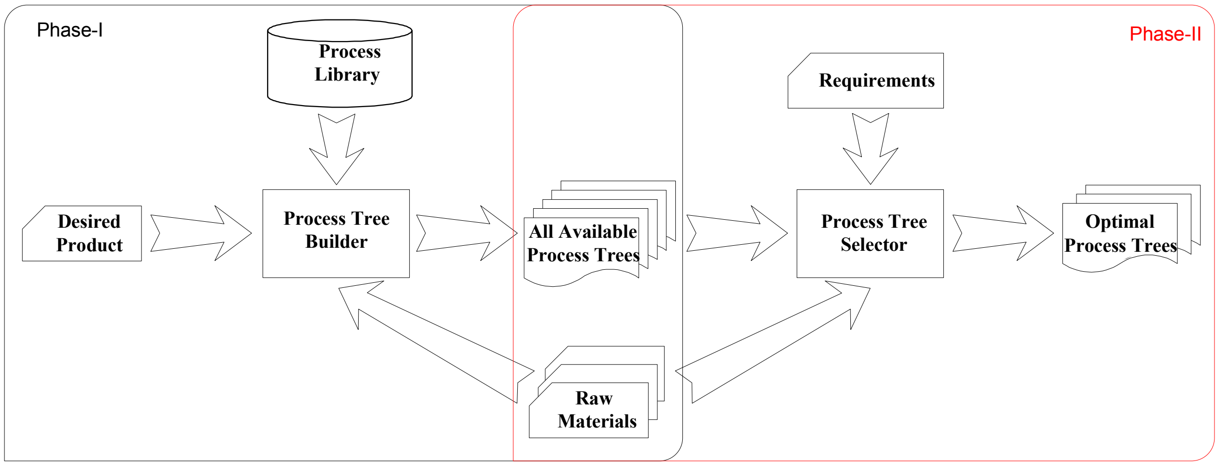


Figure 4.1: The Generic Two-Phase Synthesis Optimization Framework

The framework has been implemented by using Java. Next, we will explain the overall framework with an abstract example.

4.2.2 *Phase-I: Process Tree Building*

Often we have more than one way to manufacture a desired product or intermediate product, thus automatically constructing all the available process trees is a challenge: the algorithm will be described in Section 4.2.3. As an example, consider the process library containing the process trees depicted in Figure 4.2. The tree shown in Figure 4.3 has two alternatives for product *P* and the tree has three levels for illustration.

$$A + 2B \rightarrow P \qquad C + D \rightarrow A \qquad C + E \rightarrow F$$

$$F + G \rightarrow P \qquad C + 2E \rightarrow B \qquad 2D + 4E \rightarrow G$$

Figure 4.2: Simple Illustrative Process Transformations with Molar Units

Assume we need to produce one unit of *P* with enough *C*, *D*, and *E* as raw materials. The process trees would be represented as follows: the root node is *P*, all leaf nodes are raw materials *C*, *D*, and *E*, and the other nodes *(A*, *B*, *F*, and *G)* represent the intermediate products. The number within each node represents the amount. The processes are represented by arrows that the tails are input chemicals, and the head is the directly generated chemical. When we have insufficient raw materials for either one of the single process trees, the circle symbol represents the combination of these two process trees as a new option. For example, if there are limits on the availability of *D*, then the left hand tree may be used in order to complete the demand for *P*.

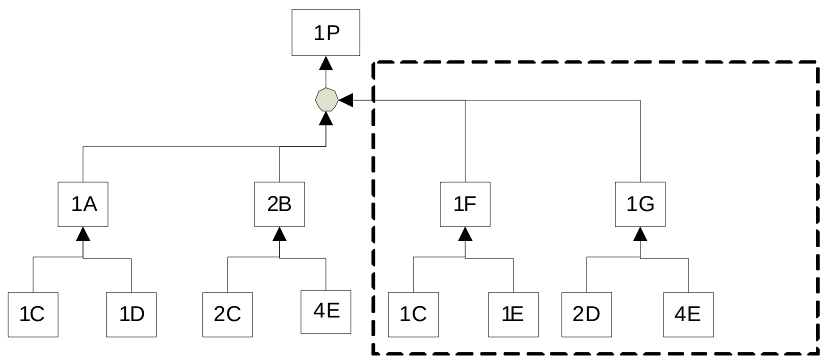


Figure 4.3: Example of a Process Tree for Process Transformation

In our implementation, input files to the process tree builder are written in Extensible Markup Language (XML) format, which creates a straightforward, searchable structure of input LCI information. From the process-tree-builder module, two output files are generated. One contains process emissions, energy consumption, and material requirements for a functional unit of a desired product. The output data are consolidated and stored in the form of a matrix that can be easily imported into optimization software. The other output file contains a list of individual processes that are composed of each entire process tree for the desired product.

XML is a general-purpose specification for creating custom markup languages. The comprehensive XML Schema is used to represent the gate-to-gate life cycle blocks. The following shows an example of XML Schema for reaction $A+2B \rightarrow P$ which including the reaction coefficient, energy type, and energy quantity. As we expand the model into a more general one, emission type, emission quantity, and other characteristics related to the reaction will be added into the XML Schema.

```
<?xml version="1.0" ?>
<reaction-set>
	<!-- A1+A2=G1 -->
	<reaction>
		<reactant-set>
			<reactant quantity="1">A</reactant>
			<reactant quantity="2">B</reactant>
		</reactant-set>
		<resultant quantity="1">P</resultant>
		<energy-set>
			<energy quantity="60">electricity</energy>
		</energy-set>
	</reaction>
</reaction-set>
```

From the process-tree-builder module, two output files are generated. One contains process emissions, energy consumption, and material requirements for a functional unit of a desired product. The output data are consolidated and stored in the form of a matrix shown in Table 4.1 that can be easily imported into optimization software. The other output file contains a list of individual processes that are composed of each entire process tree for the desired product.

Table 4.1: A Matrix of Paths with Raw Materials

	$Material_1$	$Material_2$	……	$Material_n$
$Path_1$	*1.5*	*1*	……	*3*
$Path_2$	*0.5*	*0*	……	*1.5*
……	……	……	……	…
$Path_m$	*0*	*0.5*	……	*1*

The value in each cell shown in Table 4.1 represents the amount of the raw material needed by the specific path in order to generate one functional unit of the desired product. For example, the cell ($Path_1$, $Material_1$) is 1.5, which means that 1.5 unit of $Material_1$ is needed by $Path_1$ in order to generate one unit of the desired product.

4.2.3 Process-Tree-Builder Algorithm

To construct all available process trees from the process library with the obtained raw materials and the desired product, we design an algorithm for the process-tree-builder module. The algorithm starts with the desired product as a seed and produces process trees step by step until all the leaves of the process trees are raw materials. If more than one process for some non-leaf node exists, additional new process trees will be generated. The pseudo-code algorithm "TreeConstruct" is presented as follows in Figure 4.4:

```
Algorithm: TreeConstruct

Input: ma_list: a list of raw materials
       prod: the desired product
       proc_lib: the process library
Output: tr_list: a list of process trees that can generate prod using ma_list
Begin
search proc_lib for all processes that produce prod;
for each found process proc, do {
    create a process tree tr with prod as the root leaf;
    extend the root leaf in tr with proc;
    mark tr as incomplete;
    add tr into tr_list;
}
while (there exist incomplete process trees in tr_list) {
    select one incomplete process tree tr;
    while (there exist leaf materials of tr not in ma_list) {
        select one leaf material l of tr not in ma_list;
        search proc_lib for all processes that produce l;
        if (no process found) {
            mark tr as infeasible;
            break;
        }
        else if (only one process proc found)
            extend l in tr with proc;
        else {
            for each found process proc except the last process l_proc, do {
                create a new process tree new_tr that is the same as tr;
                extend l in new_tr with proc;
                mark new_tr as incomplete;
                add new_tr into tr_list;
            }
            extend l in tr with the last process l_proc;
        }
    }
    if(tr is not infeasible)
        mark tr as complete;
}
for each process tree tr in tr_list, do {
    if (tr is infeasible)
        remove tr from tr_list;
}
End
```

Figure 4.4: The Pseudo-Code Algorithm of the Process Tree Construction

The algorithm’s inputs are a list of raw materials, the desired product, and the process library. The outputs are a list of process trees that can generate the desired product using the list of raw materials. Line 1 invokes a function that can locate all the processes in the process library that can directly produce the desired product. The loop from lines 2 to 7 creates the initial process trees with a process that can directly produce the desired product, marks these as incomplete, and stores these in a list of process trees. The outer “while” loop from lines 8 to 31 “grows” all the “incomplete” process trees, one by one, into either the “complete” or “infeasible” status. Line 9 selects an incomplete process tree from the process-tree list. The inner "while" loop from lines 10 to 28 extend the selected incomplete tree by iteratively extending the non-raw-material leaves into raw-material leaves, and at the same time, create new process trees, if these exist. Line 11 selects a non-raw-material leaf for extension. Line 12 invokes the same function as line 1 and finds all the processes in the process library that can directly produce the selected leaf. To extend a leaf, three possible outcomes are possible: (1) Lines 13 to 16: no process in the process library can directly produce the selected leaf, which shows that the selected incomplete process tree is infeasible. (2) Lines 17 and 18 describe the second situation, in which only one process in the process library can directly produce the selected leaf. In this situation, the algorithm extends the selected leaf in the selected incomplete tree with the only process found. (3) Lines 19 to 27: more than one process in the process library can directly produce the selected leaf. In this situation, the algorithm (lines 20 to 25) first “clones” the selected incomplete process tree for each found process (except the last process) and extends the same leaf of the cloned incomplete trees with the corresponding process (except the last process). For the last process, the algorithm (line

26) simply extends the selected leaf in the selected incomplete tree with the last process. Lines 29 and 30 mark the selected incomplete process tree as complete, if it is feasible. The “for” loop from lines 32 to 35 iterates through the process-tree list and deletes infeasible trees from the list.

4.2.4 Process-Tree-Builder Implementation

Chemical synthesis is a big research area in chemical engineering. Given existing raw materials, one can find numerous routes to produce a product. Here, we define a route as a sequence of chemical or physical processes to generate a final product. Process-Tree-Builder is designed to execute the route finding process. The tool takes input as a library file which contains a set of chemical or physical processes and a capacity file which contains a set of raw materials, executes a predefined route-finding algorithm to search all possible routes, and outputs all found routes and a matrix file which can be used in the succeeding optimization. Process-Tree-Builder is a small handy tool for chemical synthesis analysis. This section briefly introduces Process-Tree-Builder and its technical characteristics.

Programming Language: Process-Tree-Builder is implemented in Java 2 Standard Edition, a programming language of "write once, run everywhere".

Development Tool: Process-Tree-Builder is a graphical user interface (GUI) tool. NetBeans IDE is used as the main development tool because of its GUI design convenience.

Techniques:

Java Swing: Swing is a widget toolkit for Java. It is part of Sun Microsystems' Java Foundation Classes (JFC) - an API for providing a graphical user interface (GUI) for Java programs.

XML DOM： Java2 API provides two ways to handle XML files, SAX (Simple API for XML) and DOM (Document Object Model). Process-Tree-Builder uses DOM to read/write XML files.

4.2.5 Phase-II: Development of LCI Optimization

After Phase-I generates alternative process trees to produce the desired product, process network optimization will choose the optimal process tree or a combination of process trees. We use the process-tree-builder module to explicitly construct production trees because we think these provide useful information about the structure of alternatives. Another approach would be to implicitly embed processes in a superstructure from which the optimal product volumes in each process would be solved by a mathematical programming approach with integer variables representing whether or not a particular process was chosen for inclusion in the process tree. This leads to a smaller problem but more complex structure. The disadvantage of the approach is that some problems might have an overwhelming number of available process trees. However, modern software packages can solve large linear programs (millions of variables and constraints), and hence solving the problem is not predicted to be a major limitation. In addition, information of a specific process tree is useful and allows differentiation of the product volume into different lines with different environmental profiles. These profiles can be screened, and some with unacceptable per unit performance can be eliminated prior to optimization. Because of the output matrix from phase-one, the linear programming model is straightforward:

$$\begin{aligned} &\min \ \sum_i E_i \cdot P_i \\ &s.t. \ \sum_i P_i = D \quad , \\ &\qquad \sum_i a_{ij} P_i < M_j \end{aligned}$$

where D is a parameter that represents the total amount of the product the plant needs to manufacture, P_i is the amount of the desired product that is generated by process tree *(i)*, and M_j is the provided amount of raw material *(j)*, E_i is denoted as the energy consumption for generating one functional unit of the desired product by process tree *(i)*, and coefficients $a_{i,j}$ represent the mass requirements of material *(j)* for generating one functional unit of the desired product by process tree *(i)*. The objective of the optimization module is to minimize energy consumption with two fundamental constraints: the constraint on the amount of manufactured product P should satisfy requirement quantity D, and the usage of certain raw materials should not exceed their availability. This optimization problem can easily be represented by the General Algebraic Modeling System (GAMS) program and solved using CPLEX.

The optimization returns the best overall mix of flows from alternatives for chemicals, or the alternative process trees for the specific materials as an optimal solution based on the appropriate objective function. The optimization model can be created to satisfy different requirements. For example, the objective can be stated as minimizing one particular raw material usage. An insufficient amount of some raw materials will influence optimization results as well. Sometimes we not only need to minimize the total energy consumption, but also desire to minimize fuel usage. Then, the objective function can be posed to $\min \omega_e \cdot \sum_i E_i \cdot P_i + \omega_f \cdot \sum_i F_i \cdot P_i$, in which ω_e, ω_f are the weights between total energy and fuel. This can also be addressed as a multi-objective problem through goal programming (Azapagic, A., 1999). Additional constraints can be incorporated that represent particular problem features. For example, some products cannot incorporate more than a certain recycled content without compromising product performance. Therefore, a constraint represents that only 25% of the desired product *P* can come from trees, *R*, is modeled as $\sum_{r \in R} P_r \leq 25\% * D$, The specific element of *R* can be chosen to include or exclude particular product sub-components or recycling processes.

4.2.6 Summary

To sum up, a system for CTG LCI analysis and synthesis from alternatives has been developed. The approach has three main steps: *1).* Use an XML format input to represent the LCI blocks; *2).* Design an algorithm to traverse the chemical process tree and find all possible routes for the desired product; *3).* Build a matrix to represent the constraints for the LP optimization and based on this matrix, find the optimal solution for different objectives such as minimizing energy consumption or minimizing emissions to the environment. In the next section, a case study of evaluating the alternative carpet production system with different routes will be implemented to demonstrate the approach.

4.3 Case Study

4.3.1 EcoWorxTM Carpet System

To illustrate the methodology, a case study involving an office building carpet product is described. A carpet life cycle consists of four basic stages: supply of materials, carpet manufacturing, use phase, and disposal or recycling. The use phase for office building carpets is not distinctly different based on the construction: carpets tend to be cleaned on a periodic schedule over the life, and replaced after a certain time period irrespective of the wear. However, there has been heightened interest in recycling of carpet in recent years, driven by a multi-stakeholder agreement between the carpet industry and various government and non-government organizations (NGOs). They signed a memorandum of understanding for carpet stewardship (MOU), a ten-year schedule to increase recycling carpet and reduce carpet to landfills. Therefore, one objective of the case study is to ensure that the recycling of carpet is beneficial from a life cycle perspective compared to using virgin raw materials.

There are several types of office carpet construction and materials. In this paper, we focus on one specific construction, a tile, and a specific suite of materials used by a manufacturer, Shaw Industries, to produce EcoWorx^{TM}, whose initial design philosophy and construction was presented by Segars, J.W. (2003). Commercial tiles have three main components of an architecture, face fiber, primary backing fabric, and secondary backing. The secondary backing is often composed of a sandwich of two polymer layers and a layer of glass fiber. The polymer layers are often heavily filled with an inorganic material to reduce the use of expensive polymer and provide mechanical stability. EcoWorx^{TM} tile has a new polyolefin-based secondary backing polymer that replaces the

PVC-based backing prevalent in the industry. In addition, the tile can contain recycled materials in various parts of the construction, such as backing polymer, backing fabric, backing filler, and face fiber. Figure 4.5 shows the structure of EcoWorx^{TM} tile with recycled alternatives. For example, Shaw has recently restarted a depolymerization facility in Augusta GA, which can produce limited quantities of nylon 6 from post-consumer carpet, and recovers post-industrial scrap nylon 6. In addition, the polyolefin backing polymer can be recycled as post-consumer Ecoworx^{TM}, and the backing fabric can contain a PET/nylon6 blend with recycled content. There is also a choice in the fillers that make up a substantial fraction of the carpet mass. The fillers can be a recycled glass cullet from post-consumer glass, a fly ash from a coal plant or mined calcium carbonate. In Figure 4.5, backing fabrics can be produced with or without nylon 6, and the backing from the post-consumer EcoWorx^{TM} carpet is an alternative for the backing polymeric system with backing fillers.

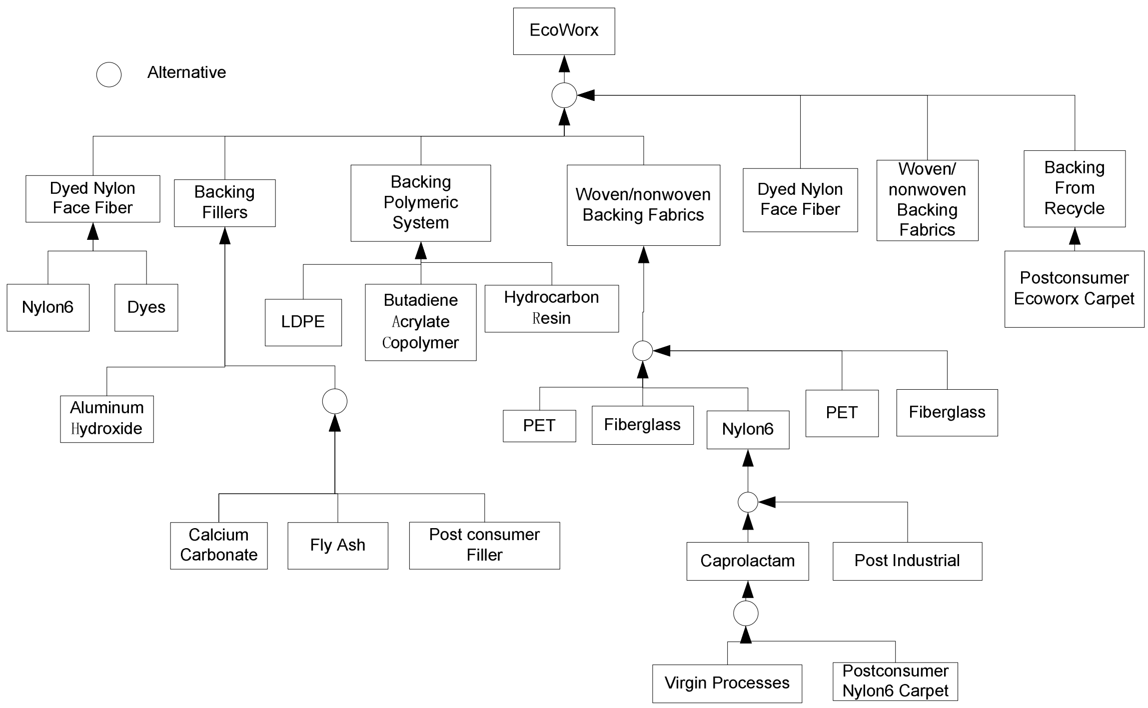


Figure 4.5: The Structure of the EcoWorx™ Tile with Recycled Alternatives.

4.3.2 Input and Output for Process-Tree-Builder Module

The product information was put into the process library in the form of the XML file shown as follows:

```
<?xml version="1.0" ?>
<reaction-set>
    …
        <!-- Dyed nylon  face fiber+ Woven/nonwoven backing fabrics + Backing
polymeric system + Backing fillers + Additives = EcoWorx carpet tile -->
        <reaction>
                <reactant-set>
                        <reactant quantity=" 0.278Kg"> Dyed nylon  face fiber</reactant>
                        <reactant quantity=" 0.071Kg"> Woven/nonwoven backing
fabrics</reactant>
                        <reactant quantity=" 0.274Kg"> Backing polymeric
system</reactant>
                        <reactant quantity=" 0.455Kg"> Backing fillers</reactant>
                        <reactant quantity=" 0.034Kg"> Additives</reactant>
                </reactant-set>
```

```
        <resultant quantity="1Kg"> EcoWorx carpet tile</resultant>
        <energy-set>
            <energy quantity=" 1,383KJ">electricity</energy>
        </energy-set>
    </reaction>
    …
</reaction-set>
```

Table 4.2 shows the input limits of recycled materials based on their availability. Assume the desired output quantity of product to be manufactured is $7.22*10^7$ Kg of the EcoWorx^{TM} carpet, which is representative of the annual EcoWorx^{TM} carpet production rate. This extensive functional unit, rather than an intensive one, such as the resources per square meter of carpet, is needed because certain recycled material availability is limited and it is not known exactly how each recycled material source will be used under different objective functions. It is assumed that 75% recovery of the annual carpet sales ($7.22*10^7$ Kg/year) is feasible, and the material that can be recovered from the carpet tile is 50% of the total tile weight. Therefore, $7.22*10^6$ Kg post-consumer EcoWorx^{TM} carpet could be used as part of the backing system. Since there is a limited availability of the post-consumer nylon 6, we assume that the plant get a yield of 48% of nylon, so the maximum amount of post-consumer caprolactam is about 98% of this. As a result, $3.40*10^7$ Kg post-consumer nylon 6 could be used as part of the face fiber. The post-consumer filler is about 80% of the mass of the rest of the stream that enters the facility, so the limit for post-consumer filler is $3.00*10^7$ Kg annually. The limit for post-industrial material is $4.89*10^6$ kg, which can make 25% of the required nylon 6 (Biehla, M., 2007). Overall, to complete the process tree options to manufacture the EcoWorx^{TM} carpet, materials including natural gas, crude oil, bauxite ore, borax, copper ore, fly ash, limestone, oxygen, calcium carbonate, rutile, silica, water, additives, post-consumer EcoWorx^{TM} carpet, post-consumer nylon 6 carpet, post-industrial material, and recycled fillers are required (Overcash, M., 2008).

Table 4.2: Recycled Materials Availability (kg) of the Case Study

Recycled Materials	Mass (Kg)
Post-Consumer (PC) EcoWorx^{TM}	7.22E+06
Post-Consumer (PC) Nylon6	3.40E+07
Post-Industrial Materials	4.89E+06
Post-Consumer (PC) Filler	3.00E+07

In summary, five main alternatives exist for producing the EcoWorx^{TM} carpet. First, the EcoWorx^{TM} carpet can be constructed either from the backing polymeric system with backing fillers, or from the recycled backing fabrics of the recycled EcoWorx^{TM} carpet. Second, backing fillers can be composed of fly ash, calcium carbonate, or recycled fillers. Third, caprolactam used for the face fiber can be produced either from the recycled nylon 6 carpets, or from the usual virgin materials. Fourth, nylon 6 can be produced either from caprolactam, or from post industrial materials. Last, woven/non-woven backing fabrics can be produced with or without nylon 6. The flow of energy into each manufacturing process was classified as electricity, steam, and direct fuel. When multiple products were produced in a single manufacturing process, energy use and material inputs were allocated by mass (except for caprolactam, which had micro-quasi allocation).

To optimize the material selection of the carpet system, the LCI optimization approach was applied. Given the output from the process-tree-builder module in Figure 4.6 and the significant raw material limits, the optimization formulation was created, and the problem was solved in GAMS.

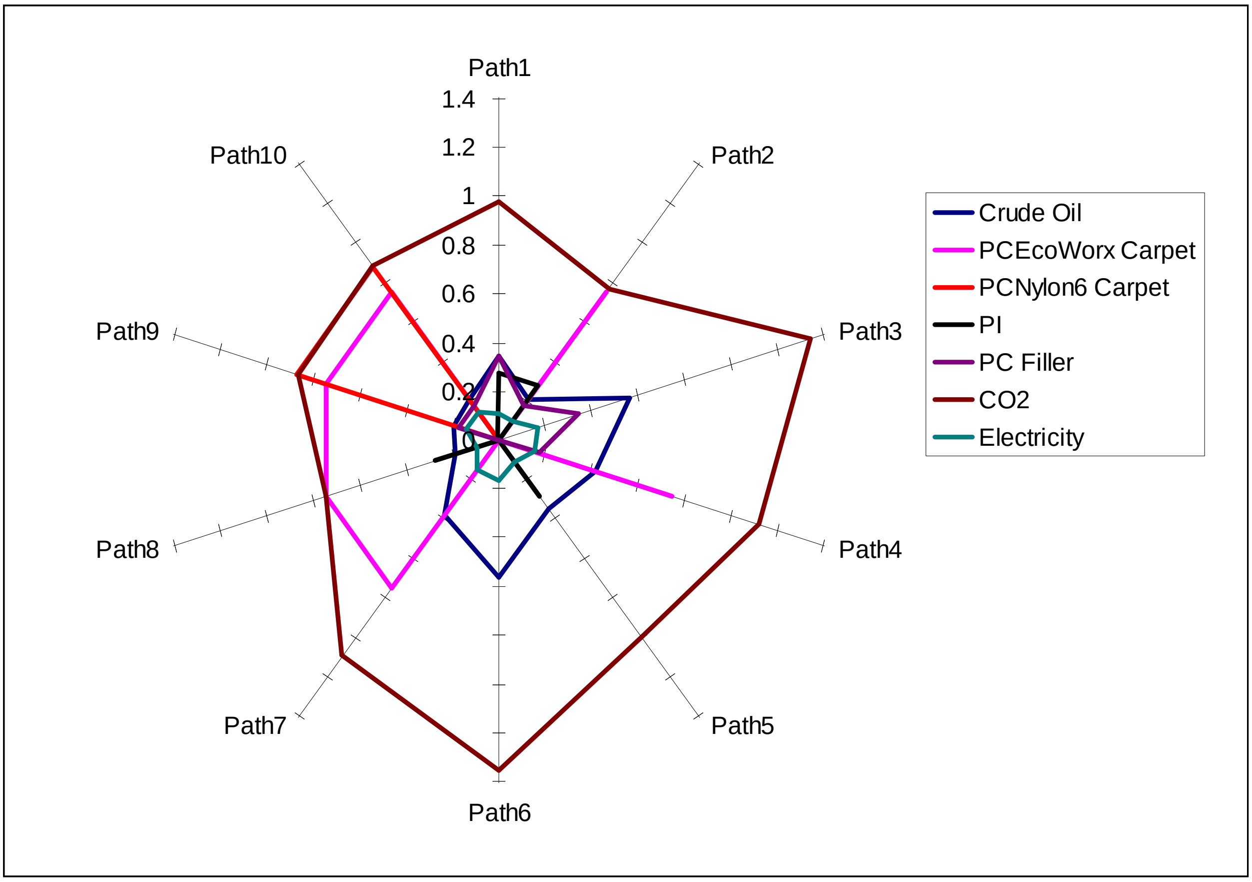
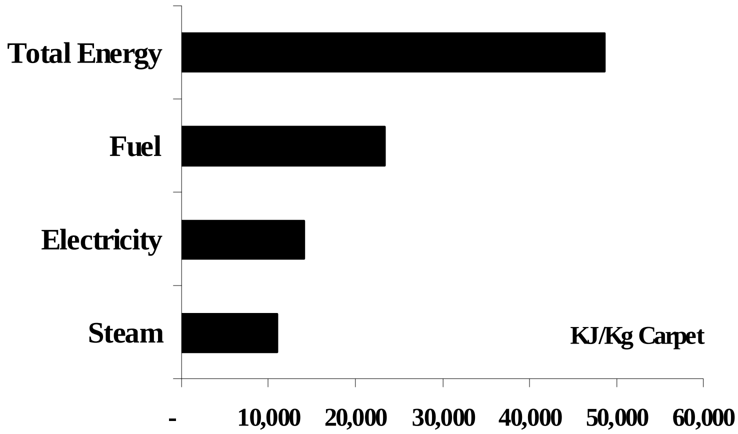


Figure 4.6: Selected Raw Materials [Kg/Kg Carpet], Energy [100MJ/Kg Carpet], and Emissions from Phase-I.

4.4 Results and Discussion

4.4.1 Optimization with Different Energy Type

After the process-tree-builder module is run, various process trees are generated including recycling options. The LCI objectives we chose to explore in this study are based on the consumption of different types of energy. This is to illustrate that different objectives are easily incorporated into the framework and to show that different process trees do have different resource profiles. The LCI data include four different measures of energy consumption, the steam used in the process, electricity, transportation fuel, and high temperature heating often carried out through a furnace. Figures 4.7 to 4.10 show the optimization results of energy and major raw material consumption for minimizing different energy type. In Figure 4.7, post-consumer filler was chosen as alternative to fly ash and calcium carbonate for fillers. Post-consumer nylon 6 was not chosen when minimizing steam in Figure 4.8. In addition, calcium carbonate and fly ash are used for fillers. Figures 4.9 and 4.10 show that minimizing fuel or total energy consumption has similar results for raw material usage which used calcium carbonate for fillers.



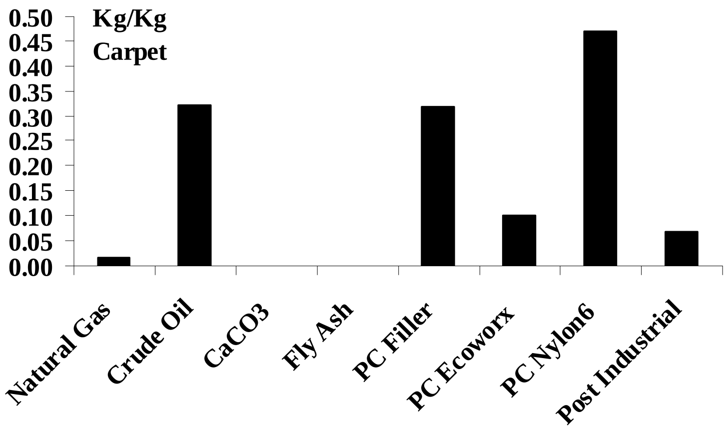
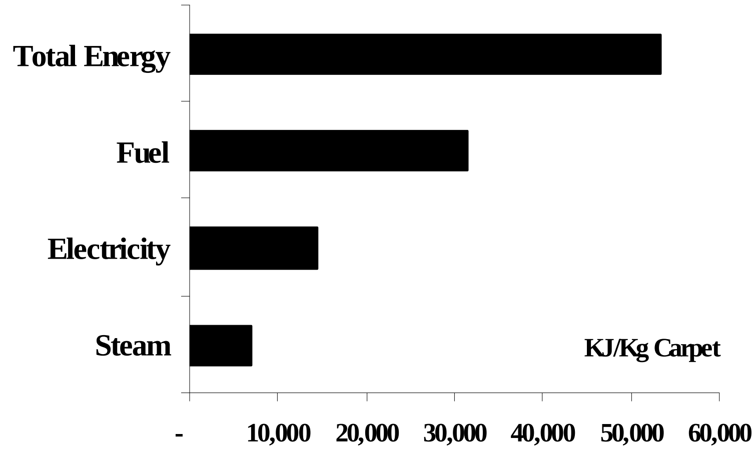


Figure 4.7: Major Raw Materials and Energy Usages for Minimizing Electricity Consumption



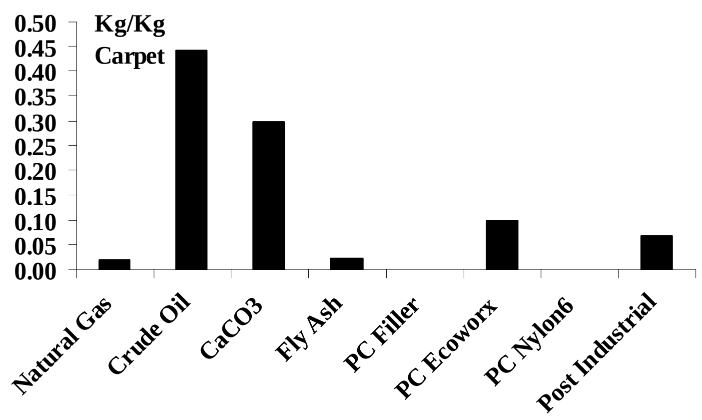
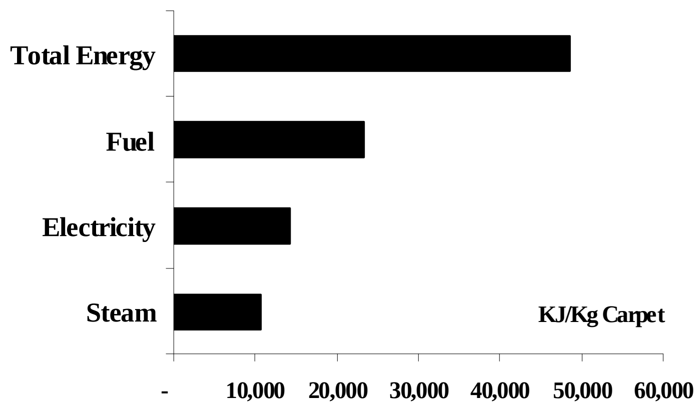


Figure 4.8: Major Raw MaterialS and Energy Usages for Minimizing Steam Consumption



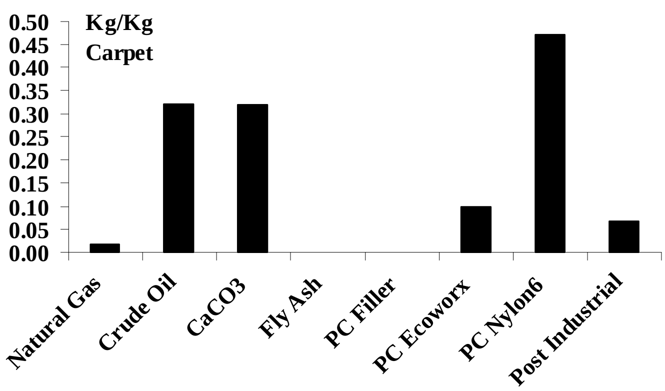
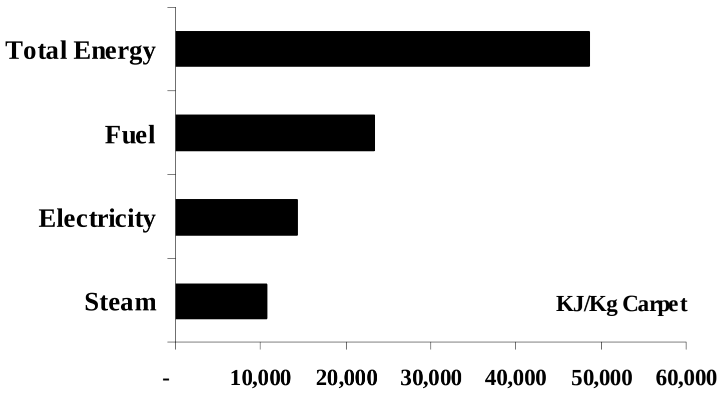


Figure 4.9: Major Raw Materials and Energy Usages for Minimizing Fuel Consumption



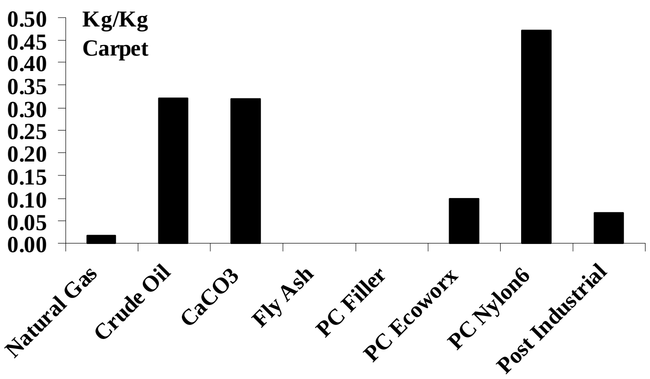


Figure 4.10: Major Raw Materials and Energy Usages for Minimizing Total Energy Consumption

4.4.2 Optimization with the TRACI Method

Energy is part of the life cycle studies, and emissions are important for environmental evaluation as well. In this case study, Tool for the Reduction and Assessment of Chemical and Other Environmental Impacts (TRACI) method (Bare, J.C., 2006) is used for the assessment of emissions. TRACI method is one of the life cycle impact assessment methods for carpets developed by the U.S. Environmental Protection Agency. In addition, TRACI will help to expand the application to pollution prevention and sustainability metrics. In the TRACI method, ten categories including global warming, acidification, eutrophication, photochemical smog, human health, fossil fuel depletion, ecological toxicity, criteria air pollutants, stratospheric ozone depletion, and solid waste that have potential effects to the environment are used to measure the product’s life cycle impact. Table 4.3 shows the unit of calculating TRACI impact for each category. Table 4.4 shows part of the life cycle impact factor value of emissions as assessed by TRACI. Therefore, we can calculate the potential impact by multiplying mass or energy by their corresponding factor value in Table 4.4 for each impact category.

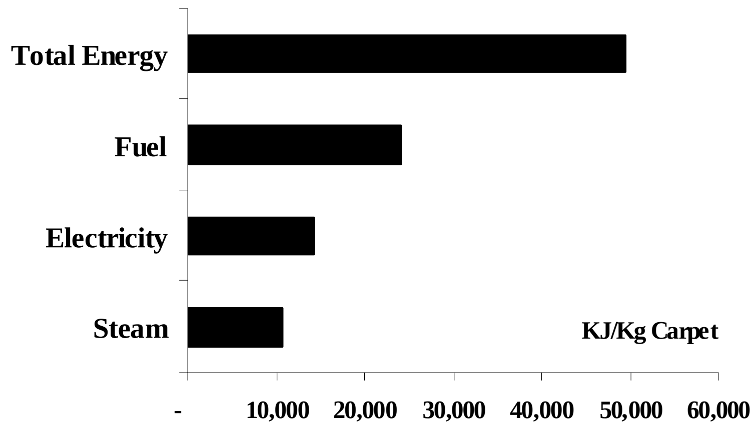
Table 4.3: TRACI Units

Impact Category		**Unit**
Global Warming	CO_2 equivalents	Kg
Fossil Fuel Depletion	MJ surplus	MJ extracted
Eutrophication	Nitrogen equivalents	Kg
Ecotoxicity	2,4-D equivalents	Kg
Acidification	H+ moles equivalent	Kg
Photochemical Smog	g NOx equivalents	Kg
Human Health	benzene equivalents	Kg

Table 4.4: Life Cycle Impact Factor Value for Global Warming and Fossil Fuel Depletion

Global Warming	**Factor Value**	**Fossil Fuel Depletion**	**Factor Value**
Carbon dioxide	1	Crude oil	0.144
Methane	23	Natural gas	0.15
Nitrogen dioxide	296		

First, the objective is to minimize the mass of the emissions such as solid waste. And the results are shown in Figure 4.11.



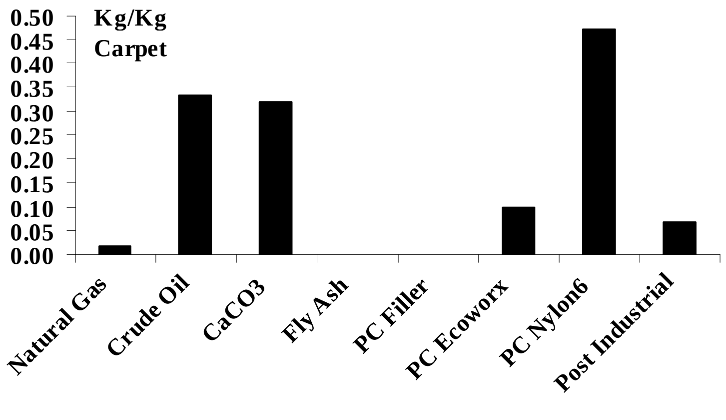


Figure 4.11: Major Raw Materials and Energy Usages for Minimizing Solid Waste Emission

Second, the objective is to minimize the global warming impact or fossil fuel depletion from TRACI. The optimization formulation is changed as follows:

$$
\begin{aligned}
&\min \ \sum_i CO2_i \cdot P_i + 23 * \sum_i Methane_i \cdot P_i + 296 * \sum_i NOx_i \cdot P_i \\
&s.t. \ \sum_i P_i = 7.22 \times 10^7 \\
&\quad \sum_i a_{ij} P_i < M_j \\
&\min \ 0.144 * \sum_i CrudeOil_i \cdot P_i + 0.15 * \sum_i NaturalGas_i \cdot P_i \\
&s.t. \ \sum_i P_i = 7.22 \times 10^7 \\
&\quad \sum_i a_{ij} P_i < M_j
\end{aligned}
$$

The results are shown in Figures 4.12 and 4.13.

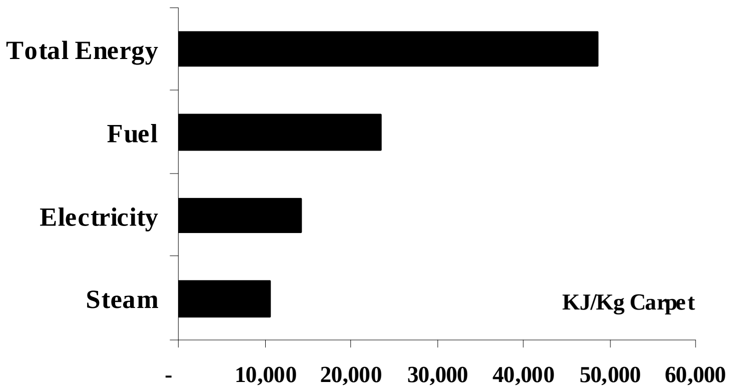


Figure 4.12: Major Raw Materials and Energy Usages for Minimizing Global Warming Impact

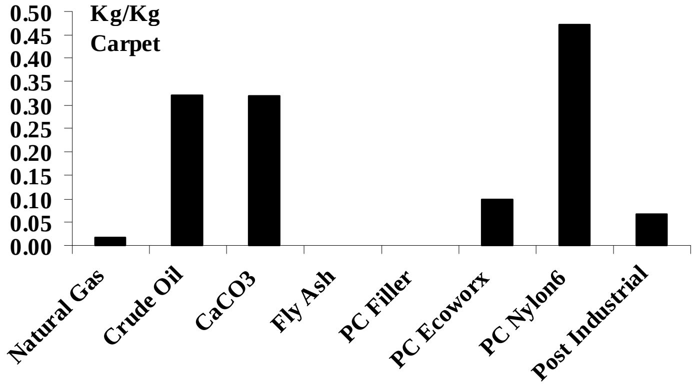


Figure 4.12: Major Raw Materials and Energy Usages for Minimizing Global Warming Impact (continued)

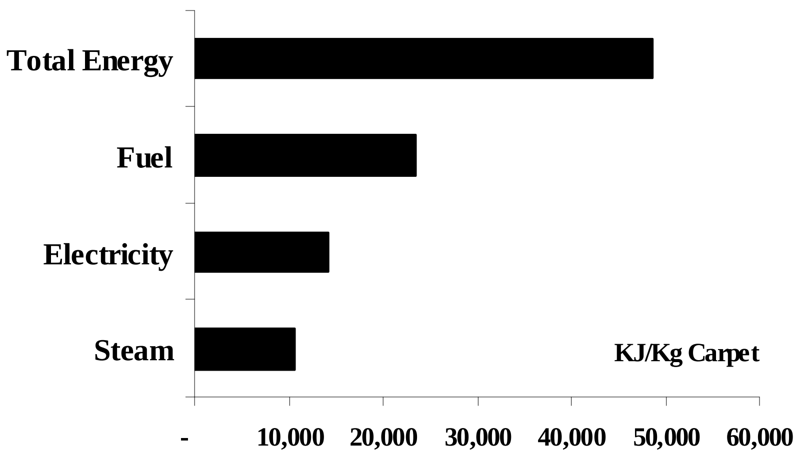


Figure 4.13: Major Raw Materials and Energy Usages for Minimizing Fossil Fuel Depletion Impact

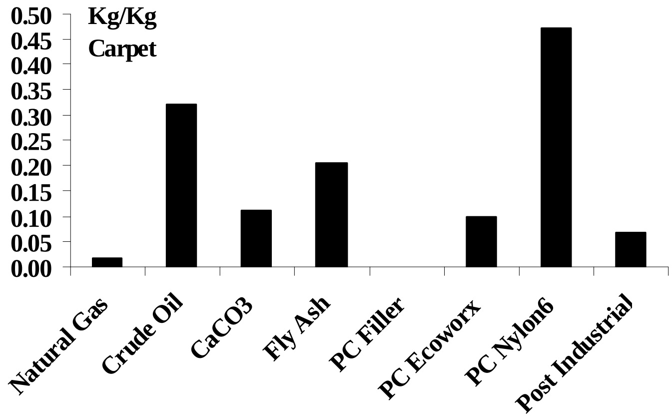


Figure 4.13: Major Raw Materials and Energy Usages for Minimizing Fossil Fuel Depletion Impact (continued)

Tables 4.5 and 4.6 are the summary of energy and major raw materials usage with different objective in the unit of KJ/Kg carpet and Kg/Kg carpet respectively.

Table 4.5: Case Study Summary of Energy Consumption with Different Objective

Optimization	Steam	Electricity	Fuel	Total Energy
Min Electricity	10,953	14,103	23,390	48,786
Min Steam	6,939	14,457	31,425	53,287
Min Fuel	10,647	14,173	23,384	48,547
Min Total Energy	10,647	14,173	23,384	48,547
Min Solid Waste	10,690	14,289	24,142	49,463
Min Global Warming	10,647	14,173	23,384	48,547
Min Fossil Fuel	10,647	14,186	23,452	48,627

Table 4.6: Case Study Summary of Major Raw Material Usage with Different Objective

	Natural Gas	Crude Oil	CaCO3	Fly Ash
Min Electricity	0.016	0.321	0.000	0.000
Min Steam	0.020	0.443	0.296	0.023
Min Fuel	0.016	0.321	0.319	0.000
Min Total Energy	0.016	0.321	0.319	0.000
Min Solid Waste	0.016	0.333	0.319	0.000
Min Global Warming	0.016	0.321	0.319	0.000
Min Fossil Fuel	0.016	0.321	0.111	0.205

Table 4.6: Summary of Major Raw Material Usage with Different Objective (continued)

	PC Filler	PC EcoWorx	PC Nylon6	Post Industrial
Min Electricity	0.319	0.100	0.471	0.068
Min Steam	0.000	0.100	0.000	0.068
Min Fuel	0.000	0.100	0.471	0.068
Min Total Energy	0.000	0.100	0.471	0.068
Min Solid Waste	0.000	0.100	0.471	0.068
Min Global Warming	0.000	0.100	0.471	0.068
Min Fossil Fuel	0.000	0.100	0.471	0.068

4.4.3 Optimization with Different Post-Consumer Material Capacity

Since the recycled materials all reached their capacity for energy saving in the previous experiment, we will increase the available material to see how they will influence the environmental impact. To change the percentage of the recycled material content, we conducted experiments by increasing the percentage of recycling materials as shown in Table 4.7. *Experiment*$_3$ represents essentially unlimited availability of recycled materials, since the allowed percentage is equal to the maximum allowed in the product factoring in the yield of the final product component from the raw material.

Table 4.7: Recycled Content Combination and Percentage of Energy Saving (Compare with Virgin Process) with Different Recycled Content Percentage

Material Availability	*Experiment*$_1$	*Experiment*$_2$	*Experiment*$_3$
PC EcoWorx Carpet	10%	36%	36%
PC Nylon6 Carpet	47%	47%	47%
Post Industrial Material	13%	25%	27.80%
PC Filler	42%	41.60%	45.50%
Electricity	23%	39%	41%
Fuel	48%	58%	59%
Total	37%	59.89%	62.95%

Table 4.7 shows the percentage of energy saving compare with virgin process with different recycled content percentage. The results are consistent with observations of several energy types. The optimal solution explains recycling could save energy. One observation is that as the increase of recycled content, steam and electricity could be saved more than fuel and total energy.

4.4.4 Summary and Conclusions

This chapter has described a methodology to translate product design architectures into material production pathway selections that minimize different life cycle impact objectives. The methodology first synthesizes all the alternative pathways to make the product from the raw materials based on input and output connections of gate-to-gate chemical plants. The life cycle information is organized in this gate-to-gate format and so can conveniently be compiled into a vector of coefficients for each path that represent the life cycle inventory. In the second phase of the method, a subset of the pathways is selected to meet product demand quantities, obey the limits on material availability, and minimizing different life cycle measures. When impact categories are simple functions of the inventory of materials and energy, such as many of the measures in TRACI, these can be incorporated into the optimization and our approach extended to multi-objective studies.

Procedures were illustrated using the EcoWorx™ carpet case study, which compares environmental burdens with and without recycling. The model user can set up the criteria for sustainable development such as minimizing the energy or emissions and alters several of the parameters in the database model to explore which design and material availability constraints are the most important to reducing the overall measures of the product life cycle.

One limitation of this methodology is that it requires that all the processes in the process library have only one output chemical in order to exclude the possibility of a loop in constructing the pathway. This implies that processes with multiple outputs have already been factored into separate gate-to-gate blocks by appropriate allocation of inventory between them. Recycled post-consumer materials do not pose a problem because the source of these materials is not at the same stage in the process tree, and the consumer requires a completely different process chain to recover them. The main issue is if the consumption of one plant output would be dramatically increased or reduced by changing its use in a product, since many commodities are constrained in their ratio of production from a given plant. It is implicitly assumed that the product being examined is not so large a consumer of such commodities that it would alter the overall availability of the commodity in the global marketplace.

The results revealed the importance of recovering materials at the end of the use phase, and designing products to be capable of accepting these recovered materials back into their supply chain. The results also demonstrate that viewing products from a "functional unit" perspective needs to be carefully calibrated. The availability of recycled materials may change the composition of a typical unit as the scale of production is increased. For example, for a new product with unique chemistry there may not be any material available for recycle until a substantial volume of the product has been used and retired. There may be overall limits to the amount of recycled material that a given product component can contain and therefore at small scales certain sources of recycled material may be favored over others, and the composition of a typical functional unit will change with scale. Our methodology is well suited to examine these kinds of issues and can rapidly assess the impacts of changing sources and quantities of materials on the product life cycle.

4.5 Conclusion

This chapter has described a two-phase-framework model to analyze how product designs and situational variables impact the decision-making strategies in terms of life cycle inventory information. Procedures were illustrated in the EcoWorx^{TM} carpet case study, which compares environmental burdens with and without recycling. The results revealed the importance of recovering materials at the end of the use phase, which would be useful to chemical plants because of environmental concerns. In addition, carpet recycling is a promising alternative approach of reducing life cycle impact and can be practiced with a growing scale in the United States. The two primary objectives of this research can be summarized as follows: First, we develop a methodology that integrates LCI information among processes. Then, we employ our methodology to investigate how recycling can influence the environmental performance, and overall contributions will be in the applied domain of the life cycle assessment and its integration with optimization tools and methods.

CHAPTER 5

POINT-BASED STANDARD OPTIMIZATION WITH LIFE CYCLE ASSESSMENT FOR PRODUCT DESIGN

5.1 Introduction

Developing sustainable environmental policies and strategies in government and sustainable environmental processes in industry is evolving towards a more quantitative approach. One essential component is a life cycle inventory, which serves as the input to a number of activities such as process development, design and synthesis, and environmental assessments. The LCI data, such as types and amounts of energy and material consumed, wastes, and emissions, are the fundamental base for the improvement analysis and the life cycle impact assessment. To identify the best environmental option, the life cycle assessment approach provides quantitative measures that are used to compare and assess different design alternatives and process pathways. LCI optimization uses objective functions that reflect environmental life cycle considerations associated with all aspects of a production supply chain in an effort to minimize those burdens while satisfying operational constraints.

LCI optimization shares a similar objective with point-based standards, which aim to minimize environmental impact by maximizing awarded points. Point-based standards have several common features. First, points are earned for undertaking various activities or using certain materials. Second, the points are aggregated to achieve an overall score.

Third, the score is compared to a threshold that determines the rating. An important component in awarding some of the points is the measure of environmental performance within a table having different threshold values. Leadership in energy and environmental design (LEED^{TM}, 2008) and the carpet standard NSF/ANSI 140-2007 (NSF/ ANSI 140-2007, 2007) are two point-based standards developed with substantial life cycle assessment metrics. LEED^{TM} green building rating system is a point-based standard used for evaluating all aspects of commercial building construction. The NSF/ANSI 140-2007 standard is a point-based standard designed for carpet products that provides benchmarks for sustainable carpet improvement and innovation. And the standard is intended to help consumers identify certified carpets with lower environmental impacts.

An implicit assumption in point-based standards is that points earned from different activities or categories are equal in value. For instance, one product that earned N_1 points from category I and N_2 points from category II is evaluated as the same as another product that earned N_2 points from category I and N_1 points from category II. However, the two products could have quite different environmental impacts. This would be the consequence of assigning points to activities or categories without relating them to underlying changes in life cycle inventories. This occurs because at the time the standards were developed, such information was not available to the stakeholder groups. In time, the information to support the standard matures, and the allocation of points to activities can be changed. However, in the meantime, the lack of congruency between life cycle impacts and points creates potential opportunities for production design distortions that maximize the performance against the standard, but have a less than optimal life cycle impact. Scheuer, C.W. (2002) evaluated the LEED^{TM} standard using life cycle assessment methods. This study found that the original LEED™ standard had that comparable outcomes in points did not have comparable outcomes in energy and solid waste generation. They also found that the thresholds for measuring achievement were unrelated to the measured environmental impacts. The studies of Azapagic, A., (1999) and Stefanis, S. K., (1997) have the founding contributions to the LCA optimization field. Azapagic, A., and Clift, R., (1999), described a method of combing LCA method with multi-objective optimization technique to find optimum improvement strategies and choose the best alternative from the environmental standpoint. Stefanis, Livingston, and Pistikopoulos presented a methodology for incorporating environmental considerations in the optimal design and scheduling of batch processes. Lu, D., and Realff, M. (2007) developed a mathematical programming framework that combines LCI and optimization together in a straightforward way. The framework first systematically generates all possible alternatives to be analyzed. Then it evaluates all generated alternatives from an environmental perspective and selects the best or the best combination by optimization. This allows the use of linear programming, rather than integer programming, and hence supports the further development of optimization of points which requires integer structure. In this work, we use optimization methods, coupled with LCI information, to explore how sustainability assessment standards are related to life cycle measures and optimization. The carpet standard, NSF/ANSI 140-2007, is used as a case study to compare life cycle optimization with optimization to earn the maximum number of points in the standard.

The aim of this chapter is to present a methodology that optimizes the point-based standard with LCI measures for products with complex processes. The methodology is implemented through the explicit construction of alternative production paths that are then selected to meet overall production targets and environmental constraints with the point-based standard. In Section 5.2 and 5.3, we describe our approach to modeling the chemical production system using a mathematical programming technique that involves mixed integer linear programming (MILP) optimization and the process network construction. In Section 5.4, we illustrate how to employ the methodology in the preliminary study of a carpet product. In Section 5.5 we analyze the results and present our conclusions. Our studies also can be extended to show how sustainability assessment standards can be re-designed to make them congruent with life cycle measures.

5.2 Methodology

Our goal in this chapter is to identify whether the point-based standards actually promote products that are better from a life cycle perspective, or whether the standards are biased towards certain activities based on a perception that some activities are inherently better than others. Therefore, we seek to optimize our selections according to two different objectives: minimizing energy consumption, or maximizing the awarded points. In addition, our proposed point-based standard optimization modeling will connect the standard with life cycle inventory measures directly.

5.2.1 Point-Based Standards

Generally the points in a point-based standard can be classified into two categories, check-off-points and threshold-points. Check-off-points are earned when a manufacturer, process, or a product complies with some pre-defined rule. They do not play a direct role in life cycle optimization as they are often associated with providing information rather than the product composition. One check-off-point example from the NSF/ANSI 140-2007 standard is as follows,

"A manufacturer shall receive one point for identifying material composition for components present at 1% (10 parts per thousand) or greater of the incoming raw materials, including materials identified as persistent, bio accumulative, and toxic (PBT) as found in Annex B."

Threshold-points are earned according to a pre-defined threshold-point table which specifies the points that a process or a product earns when the results of the activity exceeds a given threshold. Table 5.1 is a threshold-table example from the NSF/ANSI 140-2007 standard, which shows the thresholds and their corresponding points a carpet product can earn when reducing its energy consumption. For example, if the product saves more than 75% energy, it will be awarded 12 points. Table 5.2 has a similar structure as Table 5.1, which shows the thresholds and their corresponding points a carpet product can earn when using bio-based materials or recycled contents, and has a total of 20 points. Table 5.3 shows the thresholds and their corresponding points a carpet product can be awarded for product reclamation, for a maximum of 17 points. In this case the percentage is the volume of reclaimed product compared to the volume of production of the new product. The threshold-points scheme encourages standard users earn more points by achieving higher levels of a given activity, and it is hypothesized these activities will eventually minimize product environmental impacts. Table 5.2 explicitly rewards bio-based and recycled content equally without further assessment of their environmental impacts, which reflected the state of knowledge, and the opinions of the stakeholders, when the standard was developed. The relative maximum number of points earned by the activities, 12, 20 and 17 also reflects the relative weight that stakeholders put on these activities at the time, rather than any explicit knowledge about how much of an impact change the use of renewable energy versus the use of renewable materials or recovery of materials has on the product's overall impact.

Table 5.1: Points Awarded for Manufacture's Use of Renewable Energy and/or Energy Reduction, Adapted from Table 7.1 in the NSF/ANSI 140-2007 Standard

Percent Renewable Energy and/or Energy Reduction of Total Energy Production (T_k)	Points Awarded (N_k)
≥1%	2
≥2%	3
≥5%	4
≥8%	5
≥10%	6
≥15%	7
≥20%	8
≥25%	9
≥35%	10
≥50%	11
≥75%	12

Table 5.2: Points Awarded for Manufacture's Use of Bio-based, Recycled Content, or EPP Materials, Adapted from Table 8.1 in the NSF/ANSI 140-2007 Standard

Bio-Based Content, Recycled Content, or EPP Materials Feedstock Composition (Q_b)	Points Awarded (C_b)
≥5%	2
≥10%	3
≥15%	4
≥20%	5
≥25%	6
……	……
≥90%	19
≥95%	20

Table 5.3: Points Awarded for Product Reclamation, Adapted from Table 10.1 in the NSF/ANSI 140-2007 Standard

Product Reclamation Percentages ($Reclamation_{lu}$)	Points Awarded ($Preclam_{lu}$)
≥2%	1
≥4%	2
≥6%	3
≥8%	4
≥10%	5
≥11%	6
≥15%	7
≥20%	8
≥25%	9
……	……
≥50%	14
≥60%	15
≥70%	16
≥80%	17

5.2.2 NSF/ANSI 140-2007 Sustainability Assessment of Carpet

The purpose of the NSF/ANSI 140-2007 sustainable carpet standard is "to provide a market-based definition for a path to sustainable carpet, to establish performance requirements for public health and environment, and to address the triple bottom line, economic-environmental-social, throughout the supply chain". The NSF/ANSI 140-2007 standard includes a total of 114 points. The points are available in five different categories as shown in Figure 5.1. And there are three sustainable carpet achievement levels: silver, gold, and platinum, regarding awarded points greater than 37, 52, and 60 respectively.

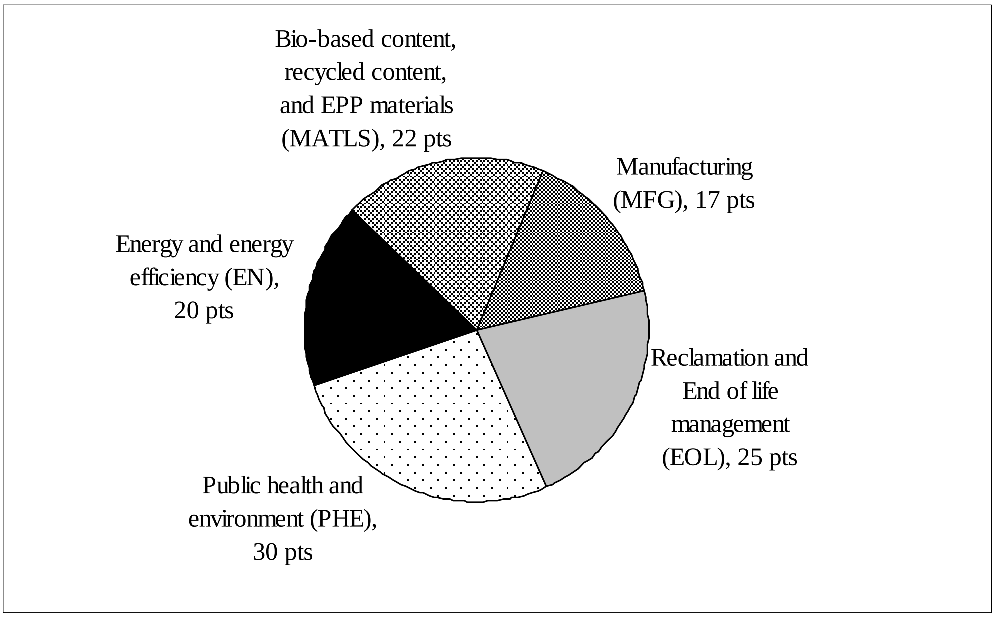


Figure 5.1: Points Distribution in the NSF/ANSI 140–2007 Sustainable Carpet Standard

Our study focused on four major point-based tables in the NSF/ANSI 140-2007 standard. These tables represent 57 out of the total of 114 points, indicating the importance of this mechanism for rewarding the product. The rest of the points are earned for activities that are not directly related to life cycle measures but for environmental quality systems adoption, social indicators, innovation and other aspects of company and product performance related to sustainability assessment.

The "reduction of specified life cycle impact categories (for the years 2000-present)" table is a special point-based table, which represents the life cycle impact categories in Table 5.4. In this table, if more than six and less than ten impact categories are crossed at each range indicated, one point will be awarded accordingly. In addition, another one point will be awarded if all ten impact categories are crossed at each range. In the carpet case study, the manufacturing processes do not have impact on stratospheric ozone depletion, and the major air pollutants is nitrogen oxide, which has already been considered in the categories of global warming and photochemical smog. Therefore, eight impact categories instead of ten were used in our case study. And if more than four and less than eight impact categories are crossed at each range indicated, one point will be awarded accordingly.

Table 5.4: Points Awarded for the Reduction of Specified Life Cycle Impact Categories (for the years 2000-present), Adapted from Table 6.2 in the NSF/ANSI 140-2007 Standard

Percent Reduction (W_L)	Across six (four) Impact Categories	Across Ten (eight) Impact Categories
≥ 10%	1pt	2pts
≥ 25%	1pt	2pts
≥ 50%	1pt	2pts
≥ 75%	1pt	2pts

5.3 Point-Based Standard Optimization

In this chapter, we will focus on optimizing point-based standards mainly based on threshold-point tables, in which stakeholders weigh different environmental impacts. We will re-evaluate the standards by coupling LCA-based mathematical programming techniques, developed in our previous work, with mixed integer representations of the standard. Therefore, the contribution of this work is to develop a normative optimization model that can explore the relationship between standards setting and life cycle inventory calculations, which is important for standards development. We propose a new model to optimize point-based standards with LCA analysis. The major challenges in developing such a model are: how to represent different threshold-point tables, and how to combine LCA optimization with the point-based standard. The model will be used to test the hypothesis that the standard point reward system and life cycle inventory measures are not completely aligned for carpet. The optimal solution will be used to suggest changes to the point allocation scheme that could bring the standard and life cycle assessment into closer agreement.

5.3.1 *Point-Based Standard Optimization Modeling*

The optimization model is shown as follows,

$$Max \sum_k N_k * X_k + \sum_b C_b * Y_b + \sum_{lu} \text{Preclam}_{lu} * Rc_{lu} + \sum_L U_L + \sum_L S_L \text{..(1)}$$

$$\sum_i P_i = D \text{...(2)}$$

$$M_j \geq \sum_i a_{(i,j)} * P_i \text{...(3)}$$

$$\frac{\sum_i (P_i * Percent_i)}{D} \geq \sum_k T_k * X_k \text{..(4)}$$

$$\sum_k X_k \leq 1 \text{...(5)}$$

$$\frac{(D * Benchmark - \sum_i P_i * E_i)}{D * Benchmark} \geq \sum_b Q_b * Y_b \text{..............................(6)}$$

$$\sum_b Y_b \leq 1 \text{...(7)}$$

$$\frac{\sum_i \left(P_i * \sum_{product\ for\ reclamation} a_{(i,product\ for\ reclamation)} \right)}{D} \geq \sum_{lu} \text{Re}\,clamation_{lu} * Rc_{lu} \text{...(8)}$$

$$\sum_{lu} Rc_{lu} \leq 1 \text{...(9)}$$

$$Z * (1 - U_L) + (\sum_{cat} R_{cat,L} - UU) \geq 0 \text{..(10)}$$

$$Z * U_L + (UU - 1 - \sum_{cat} R_{cat,L}) \geq 0 \text{..(11)}$$

$$Z * (1 - S_L) + (\sum_{cat} R_{cat,L} - SS) \geq 0 \text{..(12)}$$

$$Z * S_L + (SS - 1 - \sum_{cat} R_{cat,L}) \geq 0 \text{..(13)}$$

$$\frac{D * Average_{cat} - \sum_i \left(P_i * \sum_f Emission_{(i,f)} * Cat_f \right)}{D * Average_{cat}} \geq W_L * R_{cat,L} \text{...(14)}$$

Nomenclature

Indices:

- ***k*** List of thresholds in the standard table for recycled contents.
- ***b*** List of thresholds in the standard table for energy reduction.
- ***lu*** List of thresholds in the standard table for product reclamation.
- ***L*** List of thresholds in the standard table for cross categories of emissions.
- ***i*** Alternative pathways of manufacturing the product.
- ***f*** Chemicals involved in emissions.
- ***j*** Raw materials.
- ***cat*** Emission categories.

Decision variables:

- P_i The amount of product manufactured through pathway *(i)*.
- X_k Binary variable (0,1): if threshold *(k)* is crossed, X_k=1, otherwise, X_k=0.
- Y_b Binary variable (0,1): if threshold *(b)* is crossed, Y_b=1, otherwise, Y_b=0.
- Rc_{lu} Binary variable (0,1): if threshold *(lu)* is crossed, Rc_{lu}=1, otherwise, Rc_{lu}=0.
- S_L Binary variable (0,1): if SS categories exceed threshold *(L)*, S_L =1, otherwise, S_L =0.
- U_L Binary variable (0,1): if *UU* categories exceed threshold *(L)*, U_L=1, otherwise, U_L=0.
- $R_{(cat,L)}$ Binary variable (0,1): if threshold $w_{(L)}$ is crossed, $R_{(cat,L)}$=1, otherwise, $R_{(cat,L)}$=0.

Parameters:

- ***D*** The production demand.
- $Percent_i$ The recycled percentage of feedstock for each pathway *(i)*.
- M_j The amount of available raw material *(j)*.
- $a_{(i,j)}$ The coefficient of raw material *(j)* to manufacturing one functional unit of product for pathway *(i)*.
- T_k Thresholds value in the recycled content table.
- N_k Awarded points in the recycled content table.
- Q_b Thresholds value in the energy reduction table.
- C_b Awarded points in the energy reduction table.
- $Reclamation_{lu}$ Thresholds value in the product reclamation table.
- $Preclam_{lu}$ Awarded points in the product reclamation table.
- E_i The amount of energy consumption for each pathway *(i)*.
- ***Z*** A big number (For the NSF/ANSI 140-2007 standard, $Z=10$ in the cross categories table).
- Cat_f The environmental potential *(cat)* of chemical *(f)*.
- ***UU*** The lower number of crossed categories (For the NSF/ANSI 140-2007 standard, $UU= 4$ in our case study).
- ***SS*** The higher number of crossed categories (For the NSF/ANSI 140-2007 standard, $SS= 8$ in our case study).
- W_L Thresholds value in cross categories table for emissions.
- ***Benchmark*** Benchmark value of energy consumption.
- $Average_{cat}$ Benchmark value of the environmental impact for the emission category *(cat)*.
- $Emission_{(i,f)}$ The amount of emissions of the chemical *(f)* for each pathway *(i)*.

The above approach applies mixed-integer mathematical modeling techniques to build the optimization model of sustainable production standards with LCI information. In the model, all environmental burdens are expressed as a function of the continuous decision variable P_i and parameters E_i and $Emission_{i,f}$ The binary decision variables X_k, Y_b, $R_{(cat\ ,L)}$, S_L, and U_L denote whether the corresponding threshold is crossed or not, and appear linearly in the objective function and also in the constraints. The inequalities, Equations *(3)* to *(14)*, include raw material limits, which are also linear inequalities. Generally, the representation of emissions constraints may lead to very complex models. Our framework helps to avoid this situation. Instead, specific LCI databases, which contain the inventory of emissions of a wide range of chemical processes, are used to establish the overall emissions for each pathway. And this lumped value is useful in further calculations.

The objective function of the optimization model is to maximize the sum of awarded points in terms of LCI calculations from four perspectives. The first one, which is denoted by $\sum_k N_k * X_k$, is the total points awarded by using recycled content. The second part $\sum_b C_b * Y_b$ represents the total points awarded by reducing energy consumption. The third part $\sum_{lu} \text{Preclam}_{lu} * Rc_{lu}$ represents the total points awarded by product reclamation. The last part $\sum_L U_L + \sum_L S_L$ represents the total points awarded by reducing emissions of the environmental impact. In addition, the constraints are divided into four sub groups. Equations *(2)* and *(3)* are the basic material balances as mentioned in optimization model. Equations *(4)* and *(5)* are incorporated with Table 5.3 of recycled contents, while Equations *(6)* and *(7)* represent Table 5.1 of energy efficiency, and Equations *(8)* and *(9)* represent Table 4.3 of product reclamation. Equations *(10)* to *(14)* deal with Table 4, which evaluate the system from an environmental impact perspective. Among those constraints, constraints *(4)*, *(6)*, *(8)* and *(14)* link LCI calculations with the point-based standard. The model can be solved using the general algebraic modeling system (Brooke. A., 1998) combined with a mixed integer solver such as CPLEX (IBM, 2009).

5.3.2 Life Cycle Assessment Background

Different manufacturers could have different production lines or pathways to produce the same product or deliver the same functional unit. When producing the same amount of the final product, different pathways consume different raw materials and energy, while generating different amounts of wastes and emissions. Therefore, it is valuable to evaluate the performance of each possible pathway from the environmental perspective and choose the pathways that are more energy-efficient, consume fewer raw materials, and release less waste and emissions. In our previous work, (Lu, D., 2007) , we developed a mathematical programming model and related techniques to automatically generate all possible pathways and select pathways based on different environmental objectives. The proposed two-phase synthesis optimization framework breaks the complex problem into two relatively simple sub-problems.

The framework uses LCI information organized around individual process blocks that is generated and validated independently. In Phase-I, all LCI information about the processes that are required to manufacture a desired product is stored in the process library. All possible production alternatives according to available processes and raw materials will be identified in Phase-I through process-tree-builder module. In Phase-II, the process-tree-selector module will select the optimal process tree or a combination of possible process trees in terms of different optimization requirements. The bridge between Phase-I and Phase-II are raw materials and a consolidated output matrix of all available process trees generated by the process-tree-builder module as shown in Figure 5.2. a_{ij} is the coefficient of raw material *(j)* to manufacturing one functional unit of product for pathway *(i)*.

$$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1j} \\ a_{21} & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots \\ a_{i1} & \cdots & \cdots & a_{ij} \end{bmatrix}$$

Figure 5.2: The Output Matrix of the Phase-I

5.4 Case Study-NSF/ANSI 140-2007 Carpet Products

In this case study, a carpet production system was analyzed in terms of life cycle optimization and standard optimization. The evaluated standard is NSF/ANSI 140-2007, which is a point-based standard designed for carpet products that provides sustainability assessment of carpet. As the case study, we will optimize a carpet design according to

NSF/ANSI 140-2007 using the optimization model equations *(1-14).* The carpet design resulting from the maximization of points will be compared to the design minimizing the environmental impact directly from life cycle measures to see whether these two models are consistent. The environmental impact is measured through the tool for the reduction and assessment of chemical and other environmental impact (TRACI) method (Bare, J.C., 2003), which is a reasonable reflection of the current state of the art in LCA methodologies and applications.

5.4.1 The TRACI Method

The TRACI method is one of the life cycle impact assessment methods for carpets developed by the U.S. Environmental Protection Agency. In addition, TRACI will help to expand the application to pollution prevention and sustainability metrics. In the TRACI method (Bare, J.C., 2006), ten categories including global warming, acidification, eutrophication, photochemical smog, human health, fossil fuel depletion, ecological toxicity, criteria air pollutants, stratospheric ozone depletion, and solid waste that have potential effects to the environment are used to measure the product’s life cycle impact. Table 5.5 shows the life cycle impact factor value of emissions as assessed by TRACI.

Table 5.5: Life Cycle Impact Factor Value for Common Emissions in Carpet Products (a)

Photochemical Smog	**Factor Value**	**Human Health**	**Factor Value**
Acetaldehyde	1.79	Acetaldehyde	3.91
Benzene	0.246	Aluminum oxide	30,425
Butane	0.354	Ammonia	3.18
Carbon monoxide	0.017	Benzene	16.58
Cumene	0.612	Copper	17,267
Ethane	0.087	Cumene	0.312
Hexane	0.416	Hexane	0.607
Methane	0.0037	Hydrogen chloride	0.388
Methyl methacrylate	0.968	Hydrogen sulfide	0.051
NOX	1.24	Mercury	18,917,511
Pentane	0.43	Methyl methacrylate	0.139
Phenol	0.915	NOx	0.0101
Propane	0.159	Phenol	0.057
Propylene	3.067	Propylene	0.007
Toluene	1.032	Toluene	1.332
Vinyl acetylene	0.968	Vinyl acetylene	1.927
Xylene	1.916	Xylene	0.234

Table 5.5: Life Cycle Impact Factor Value for Common Emissions in Carpet Products (b)

Global Warming	Factor Value	Fossil Fuel Depletion	Factor Value
Carbon dioxide	1	Crude oil	0.144
Methane	23	Natural gas	0.15
Nitrogen dioxide	296		

Table 5.5: Life Cycle Impact Factor Value for Common Emissions in Carpet Products (c)

Eutrophication	Factor Value	Ecotoxicity	Factor Value	Acidification	Factor Value
Ammonia	0.119	Copper	50	Ammonia	95.5
Ammonium molybdate	1	Mercury	120	Hydrogen chloride	44.7
BOD	0.05	Phenol	0.038	NOx	40
COD	0.05	Toluene	0.0097	SOx	50.8
NO_x	0.0443				

5.4.2 Life Cycle Inventory Optimization and Point-Based Standard Optimization

Given the output matrix from the process-tree-builder module and the recycled material limits in Chapter 4, the optimization formulation was created as follows, and the problem was solved in GAMS. The objective function can be any of the life cycle inventory measures, such as energy used in various forms, or the mass of certain components. To optimize the material selection of the carpet system, the LCI optimization approach will be applied as follows:

$$\min \sum_i E_i \cdot P_i \text{.....................(13)}$$

$$s.t. \quad \sum_i P_i = D \text{...................(14)}$$

$$\sum_i a_{ij} P_i < M_j \text{ ....(15)}$$

where E_i is the amount of energy consumption for each pathway *(i); P_i* is the amount of product manufactured through pathway *(i); M_j* is the amount of available raw material *(j);* $a_{i,j}$ is the coefficient of raw material *(j)* to manufacturing one functional unit of product for pathway *(i);* and D is the parameter of the annual production demand.

In the above LCI optimization model, the objective function in Equation *(13)* is to minimize the total energy consumption for manufacturing the required amount of final product in terms of electricity, fuel, and total energy. The two constraints are the basic material balances: the sum of manufactured product $\sum_i P_i$ should be equal to the required amount D in Equation *(14)*, and the usage of raw materials should be within the limit of available raw materials in Equation *(15).*

5.5 Results and Conclusion

Two sets of optimization programming experiments were conducted in this case study. One is based on life cycle measures with the objective of minimizing energy consumption directly from life cycle inventory information. The other is focused on maximizing the awarded points from the standard point-based tables, which has four sources: using recycled or bio-based content, using reclaimed materials, reducing energy consumption, and reducing emissions to the environment. Energy use is categorized into three types: electricity, fuel, and total energy. In addition, we track various emissions to the environment, such as carbon dioxide, nitrogen oxide, and solid waste. In this case study, five main alternatives exist for producing the EcoWorx^{TM} carpet. First, the EcoWorx^{TM} carpet can be constructed either from the backing polymeric system with backing fillers, or from the recycled backing fabrics of the recycled EcoWorx^{TM} carpet. Second, backing fillers can be composed of fly ash, glass cullet, calcium carbonate, or recycled fillers. Third, caprolactam used for the face fiber can be produced either from the recycled nylon 6 carpets, or from the usual virgin materials. Fourth, nylon 6 can be produced either from caprolactam, or from post industrial materials. Last, woven/non-woven backing fabrics can be produced with or without nylon 6. Among the different alternatives, most of them have recycled contents, which can be awarded points from using recycled materials, using reclaimed materials, and reducing energy consumption. Therefore, recycled materials are favorable not only in LCI optimization models, but also in the point-based standard optimization models. Since a maximum availability of recycled materials is a constraint for the system, the consumption of recycled materials is reached at the upper bound of the constraint. This would not necessarily happen if the recycling processes consumed more energy and resources than virgin material production – although the wisdom of adopting such processes is questionable. If economic objectives or constraints were imposed, this could also cause a reduced adoption of the recycling pathways since they frequently involve expensive logistics and relatively small scale processing of heterogeneous material streams.

Table 5.6 shows the awarded points and energy consumption of the case study: optimizing the LCI uses less energy but gains less points in the standard. The results are consistent across the use of different energy categories as the objective function. Using total energy as an example, maximizing points will get 26 points, while minimizing energy will get 24 points. This indicates that the allocation of points is not solely based on the environmental goal of minimizing energy use, but could be consistent with a different set of objectives that the stakeholders had in mind, such as encouraging recycled content to reduce solid waste. Therefore the results help support analyzing whether the allocation of points to different impact categories reflects the underlying values of the stakeholders.

Table 5.6: Results of the LCI Optimization Verses the Point-Based Standard Optimization

		Points Awarded	Total Energy [KJ/Kg Carpet]	Electricity [KJ/Kg Carpet]	Fuel [KJ/Kg Carpet]
Standard Optimization	Maximizing Total Energy Awarded Points	26	5.10E+04	1.45E+04	2.73E+04
LCI Optimization	Minimizing Total Energy Consumption	24	5.04E+04	1.43E+04	2.69E+04
	Minimizing Electricity Consumption	21	5.02E+04	1.42E+04	2.70E+04
	Minimizing Fuel Consumption	23	5.02E+04	1.43E+04	2.69E+04

The different results from the standard optimization and the LCI optimization can be used to determine if there are legitimate valuation issues underlying and help to justify the point-based system. If the awarded points do not align with the LCA approach as shown in Table 5.7, this could be because the standard embeds values of the stakeholders that are not expressed solely in LCA terms. In particular, the standard has evolved through several generations of stakeholder input to have a certain number of points awarded in different categories of activity, without a systematic understanding of whether the point allocations actually reflect improved environmental performance. However, the difference in the point and energy LCI optimization is relatively small. The accuracy of life cycle inventory data over the complete carpet supply chain is unlikely to lead to overall results that are better than +/- 20%. Hence it would be reasonable to conclude that the differences are not significant. This provides an unbiased way to assess the standard and its alignment with measures of life cycle inventory improvement. The use of life cycle inventory information can therefore help in the construction of the standard and could be useful in guiding the modification of point-based systems to align them with the LCA.

Table 5.7 shows the environmental impact of the case study: the major emissions of the system from the point-based standard optimization model and the LCI optimization model according to energy categories of electricity, fuel, and total energy. Table 5.7 shows the amount of emissions of carbon monoxide, carbon dioxide, toluene, NOx, and SOx from the results of the point-based standard optimization model are more than the ones from the LCI optimization model. Meanwhile, the result from the LCI optimization model has more emissions of solid waste. Overall, the production system from the results of the point-based standard optimization model would have more impact on global warming, photochemical smog, and acidification.

Table 5.7: Major Emissions from the LCI Optimization and the Point-Based Standard Optimization on a Square Yard of Carpet Basis

	[Equivalent Kg/SY carpet]	Carbon Monoxide	Carbon Dioxide	Toluene
LCI Optimization	Minimizing Electricity Consumption	2.08E-02	2.78E+00	1.05E-02
	Minimizing Fuel Consumption	2.50E-02	3.25E+00	3.31E-02
	Minimizing Total Energy Consumption	2.50E-02	3.25E+00	3.31E-02
Standard Optimization	Maximizing Total Energy Awarded Points	2.66E-02	3.28E+00	3.37E-02

Table 5.7: Major Emissions from the LCI Optimization and the Point-Based Standard Optimization on a Square Yard of Carpet Basis (continued)

	[Equivalent Kg/SY carpet]	NOx	SOx	Solid Waste
LCI Optimization	Minimizing Electricity Consumption	1.11E-02	1.06E-02	3.17E-02
	Minimizing Fuel Consumption	2.30E-02	1.21E-02	2.43E-02
	Minimizing Total Energy Consumption	2.30E-02	1.21E-02	2.43E-02
Standard Optimization	Maximizing Total Energy Awarded Points	2.34E-02	1.20E-02	2.55E-02

Table 5.8 shows the major raw materials of the production system from the point-based standard optimization and the LCI optimization according to energy categories of electricity, fuel, and total energy. The production system from the point-based standard optimization model will consume more crude oil and natural gas than the one using the LCI optimization model from the results in Table 5.8, but again the results are not significantly different given the potential inaccuracies of assessing complex chemical supply chains.

Table 5.8: Major Raw Materials from the LCI Optimization and the Point-Based Standard Optimization on a Square Yard of Carpet Basis (a)

	[Kg/SY Carpet]	Bauxite Ore	Borax	Copper Ore	Limestone
LCI Optimization	Minimizing Electricity Consumption	8.42E-01	1.37E-01	3.60E-01	3.18E-01
	Minimizing Fuel Consumption	8.42E-01	1.37E-01	3.60E-01	3.18E-01
	Minimizing Total Energy Consumption	8.42E-01	1.37E-01	3.60E-01	3.18E-01
Standard Optimization	Maximizing Total Energy Awarded Points	8.41E-01	1.37E-01	3.60E-01	3.16E-01

Table 5.8: Major Raw Materials from the LCI Optimization and the Point-Based Standard Optimization on a Square Yard of Carpet Basis (b)

	[Kg/SY carpet]	Rutile	Silica	Water
LCI Optimization	Minimizing Electricity Consumption	8.99E-03	4.40E-01	4.97E-01
	Minimizing Fuel Consumption	8.99E-03	4.40E-01	4.97E-01
	Minimizing Total Energy Consumption	8.99E-03	4.40E-01	4.97E-01
Standard Optimization	Maximizing Total Energy Awarded Points	8.99E-03	4.38E-01	4.99E-01

Table 5.8: Major Raw Materials from the LCI Optimization and the Point-Based Standard Optimization on a Square Yard of Carpet Basis (c)

	[Kg/SY carpet]	Calcium Carbonate	Natural Gas	Oxygen	Crude Oil
LCI Optimization	Minimizing Electricity Consumption	0.00E+00	5.21E-02	9.96E-02	1.07E-00
	Minimizing Fuel Consumption	9.27E-01	5.21E-02	9.96E-02	1.07E-00
	Minimizing Total Energy Consumption	9.27E-01	5.21E-02	9.96E-02	1.07E-00
Standard Optimization	Maximizing Total Energy Awarded Points	8.55E+02	5.23E-02	1.01E-01	1.09E-00

Table 5.8: Major Raw Materials from the LCI Optimization and the Point-Based Standard Optimization on a Square Yard of Carpet Basis (d)

	[Kg/SY carpet]	Post-consumer EcoWorx^{TM} Carpet	Post-consumer Nylon6 Carpet	Post Industrial Nylon6	Recycled Filler
LCI Optimization	Minimizing Electricity Consumption	2.49E-01	6.06E-01	1.96E-01	0.00E+00
	Minimizing Fuel Consumption	2.49E-01	6.06E-01	1.96E-01	0.00E+00
	Minimizing Total Energy Consumption	2.49E-01	6.06E-01	1.96E-01	0.00E+00
Standard Optimization	Maximizing Total Energy Awarded Points	2.49E-01	6.06E-01	1.96E-01	8.41E-01

In this chapter, we described a standard optimization model together with life cycle inventory information to synthesize products earning the maximum number of points in a standard and analyzed how production designs impact the decision making strategies in terms of life cycle inventory information. A number of alternatives of manufacturing the product are examined according to the point-based standard in our model. Procedures were illustrated in the EcoWorx^{TM} carpet case study, which compares environmental burdens according to the results of the point-based standard optimization and the life cycle inventory optimization. The results revealed the importance of allocating points in the standard, which would be useful to standard design. Our proposed method is intended to guide the decision-makers toward the adoption of a sustainable production design from a standard-based perspective, consequently leading to a reduction of the overall environmental impact. In addition, the model user can set up the criteria for sustainable development and alters several of the parameters in the optimization model to discover if the system is preferable when assessed against the standard. The two primary objectives of this research can be summarized as follows: first, we developed a methodology that integrates LCI information with a standards design. Then, we employed our methodology to investigate how point allocation in the standard can influence the decisions of chemical company's preference of their environmental performance to reflect the goals of the stakeholders. The overall contributions are in the applied domain of the life cycle assessment and its integration with optimization tools and methods. In the future we intend to study re-allocating the awarded points of the point-based standard to ensure congruency of life cycle impact and points.

CHAPTER 6

STANDARD DESIGN USING LCI INFORMATION

6.1 Introduction

The previous chapters have outlined two important advances. First, how a product architecture that minimizes life cycle measures can be implemented by material production routes. Second, how to evaluate a points-based standard against life cycle impact minimization to assess how congruent the standard is with life cycle impact reduction. The second advance allows someone to analyze how well a particular standard design works to align life cycle and points, but does not shed any light on the design of the standard in the first place. This chapter will address the systematic derivation of points-based standard components based on life cycle inventory and assessment.

From an environmental perspective, emissions and energy consumption are the major evaluation subjects when conducting the life cycle assessment. Therefore, standards related to the life cycle studies often contains tables with threshold values for life cycle measures or improvements and corresponding credits, we term these category-based tables. Another type of table in points-based standards usually have thresholds with certain percentage of decrease or increase with respect to different activities, for example energy consumption, emissions, bio-based content, or recycled content, we term these activity-based tables.

The current carpet sustainability assessment standard, in its first version, was developed with substantial insights from the Joint Committee on what product changes might lead to sustainability improvement. In general, these potential product changes were simply intuitive concepts by which points were subsequently awarded. Some of the sustainability improvements (and points) were related to organizational level categories (such as for environmental management systems) which are vital to achieve change. The other improvements (and points) were directed at material and energy improvements (such as for bio-based materials). Other national standards such as LEED™ also began as intuitive point systems for change. However these organizations then recognized that a science-based approach was ultimately needed for the improvements related to material and energy changes for sustainability. The carpet industry has a national leadership position in the science-based information systems for their products from their investment in a life cycle database. The use of this database for material route selection and evaluation of the NSF 140 standard has been demonstrated in earlier chapters. Thus the NSF 140 standard is well-positioned to transition to a science-based point system for material and energy issues.

6.1.1 General Issues in Standards' Design

Standards are tools to measure and calibrate product or system performance and are often used to regulate and certify them. An emerging area for standards development is sustainability assessment. Standards in this area have several features that are common to many products and some which play a more prominent role. First, as with many standards, the stakeholders interested in the standard come from diverse groups with different values and interests. Second, the dimensions along which the product or system has to be measured are numerous. However, unlike many standards, the underlying metrics for sustainability are not well understood, agreed upon, or defined. The metrics encompass technical product performance, often for reasons of safety and longevity, company or facility performance, such as social metrics of corporate responsibility or use of environmental management systems, and production process performance, such as energy, resource use, and waste.

The diversity of product, process and company performance metrics creates unique problems in how to balance the metrics and how to synthesize a single measure of performance. This latter point, the conversion of a set of categories into a single multi-category measure, is a feature of the sustainability standards such as LEED™ and the NSF-140 Carpet Sustainability Assessment Standard. These two standards resolve this by using points awarded for performance along each dimension and then adding the points to give a total score. This creates an interesting challenge for the development of this kind of points-based standard: how best to determine the point allocations across the performance dimensions?

We start with the basic assumption that overall products with lower life cycle impact should be rewarded with more points in the life cycle component of the standard than a product with a higher life cycle impact, given all other things being equal. This does not mean that overall the product with a lower impact will achieve a higher point total – since there are often many factors outside the impact that are considered.

The ideal approach for points-based standards setting can be summarized as follows. The stakeholder group agrees on a category set that they feel reflects the sustainability of the system. For example, the toxicity of the materials, the amount of waste, the energy use in manufacturing, the safety and health of workers and the social and financial performance of the company. The group then decides how many points in total that the standard will have. Then they divide up the points between the categories, reflecting the importance they assign to them. After that they decide how many points a given attribute level should receive and allocate the points to the different levels of achievement. Unfortunately this is very difficult to do. Often the division or allocation is implicit, arrived at by developing a set of activities that can be taken to improve a category, and then allocating points to the activities. The points are then totaled for the activities.

6.1.2 Principles and Requirements in Standards' Design

Two formal principles should be enforced in the design of the point-based standard to assure our method of standard design is consistent with the notion that we prefer products with overall lower life cycle impacts.

Principle1:

If an activity a_i causes the same or better improvement in each category compared to activity a_i', activity a_i should be awarded the same or more points in the standard.

If this principle is not enforced then it is possible for a product that improves the life cycle of a product the same or more in every category than another to have a worse point total. This implies that certain relationships between activity tables must be implicitly obeyed within activity-based standards. An issue with point-based standards is the assumption that points earning from different categories are equal based on which those earned points are summed up. According to the point-based standards, one activity earning *N1* points from Category I and *N2* points from Category II is evaluated as the same as another activity earning *N2* points from Category I and *N1* points from Category II, this could cause an undesirable outcome, according to Principle1, when two activities have different environmental impacts. This issue leaves potential opportunities for production design distortions to maximize the performance against the standards but have a less than optimal life cycle impact. Therefore, the tables must be designed a certain way in order to avoid a contradiction of Principle 1.

Principle 2:

> An agreed upon reference state LCI for each product platform. This would only be necessary in the case of the percentage reduction from the baseline, or where an absolute standard is used where the baseline plays a role in defining the minimum or maximum values of the impact.

If the standard allows for companies to make improvements relative to their own products rather those of the entire industry, then it is possible to have products which have higher impacts to earn more points in the standard. This demonstrates that agreed product platform baselines for a company are insufficient to guarantee that lower LCI products are preferred in a standard.

In summary, the minimum information required to design LCIA category-based standard is as follows:

Requirement 1: Impact category set I_j, $j=1,2\ldots\ldots n$.

Requirement 2: Relative weights on categories W_j, $j=1,2\ldots\ldots n$.

Requirement 3: Total number of LCIA-based points.

If it is required to use percentage reductions, then in addition:

Requirement 4: Baseline/reference LCIA values.

If we want to use an LCI based frameworks, then we will also need:

Requirement 5: Relationships between LCIA and LCI measures, for example, $C_{q,j}$, in equation $I_j = \sum_q C_{qj} * m_{e,q}$ where q represents the emissions and j represents the impact categories, $q=1,2......m$, $j=1,2......n$.

6.1.3 *Definitions*

We start with definitions of terms used in this chapter that could have different interpretations in other contexts.

1). An **activity** is defined as a chemical or physical process that has certain materials such as bio-based materials, post consumer, and post industrial material, or an operation that uses renewable energy or has reclamation of end of life materials.

2). A **category** is the environmental influence such as global warming, acidification, and hazard waste. In our analysis, we assume that the overall environmental impact is being considered.

3). **Total points** represents the total points that can be allocated for all the tables with different activity.

The threshold and tabular threshold types of points are reasonably easily represented in mixed integer form (see Chapter 5).

$$\alpha_p \geq \tau_{ip} x_{ip}$$
$$\sum_i x_{ip} \leq 1 \quad ,$$

where α represents a property of interest, τ_{ip}, represents the i_{th} threshold value, and x_{ip} represents a binary variable that indicates whether the threshold has been crossed. Note that only one of the binary variables will be 1, and the highest one of these will be selected because the objective function $Max \sum_{i,p} Num_{ip} X_{ip}$ will be to maximize the number of points awarded, where Num_{ip} represents the cumulative number of points awarded for reaching the i_{th} threshold for the property p.

The overall approach is to examine the quantitative life cycle inventory link between carpet sustainability change and environmental improvement. That is, if 2 points are awarded for some increment of bio-based material and if 2 points are awarded for some increment of recycled content, what are the comparative environmental improvements from these changes? If there are different improvements in such things as energy use, CTG mass efficiency for the same 2 points, then the life cycle would suggest different points that should be awarded.

The life cycle approach should be as simple and as transparent as possible. We proposed a approach to evaluate potential material and energy changes from a life cycle perspective using

- Life cycle inventory data as

  The simplest expression of the product improvement

  The most directly related to plant manufacturing information

  The most directly related to cost

- Natural resource energy (total fuel from natural resources to implement change) including the energy utilized prior to the point of energy use (delivery)
- Natural resource mass requirements (total materials from nature, such as fossil fuel, mined materials, etc.)

The proposed mechanism has two-step procedures to construct the table for each category. The product manufacturing system will be evaluated both on the environmental impact level and the activity level. The proposed method is used to allocate points fairly among different categories and keep the threshold structure of tables. In addition, the proposed approach can be applied to the system with combination of different substitutable production routes.

6.1.4 Activity-Based Verses Category-Based Standard

A point-based standard can be classified as activity-based or category-based standard. A category-based standard is one that maps points to life cycle impact categories, such as global warming potential, acidification, eutrophication etc. In the category-based standard, the points are awarded based on categories which may be contributed by different activities. On the contract, in the activity-based standard, the points are awarded based on activities instead of categories. An activity-based standard takes the mapping one step further to consider the activities themselves that lead to the life cycle impacts. There are different activity tables with corresponding threshold values and points for improvements. The difference between the activity-based standard and the category-based standard is how to map the activity to the category. Generally, the mapping is generated from the LCI to the LCIA. Overall, it will be seen that category-based standards are easier to design and maintain, but that this places a high burden on the producer to map their "natural" way of approaching improving products, through activities, on to the more abstract space of life cycle impact categories.

6.1.5 From LCI to LCIA in the Standard Design

First, we give a formal definition of a LCI. Figure 6.1 shows all information included in the LCI, where m_e is the amount of emission; m_p is the final product *P*; m_{raw} is the amount of raw material; m_{by} is the amount of by product; *E* is the amount of energy consumption.

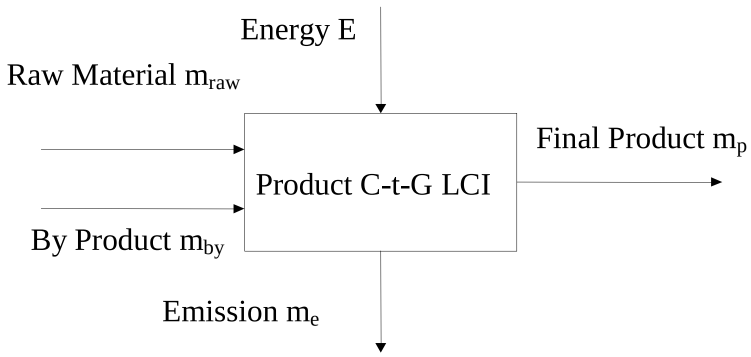


Figure 6.1: General Product Cradle-to-Gate LCI Block

We propose the use of a linear relationship between LCI and LCIA. If the impact category *(j)* has a linear relationship with certain function of emission $m_{e,q}$ in mass, then the impact can be expressed in equation $I_j = \sum_q C_{qj} * m_{e,q}$, given the coefficient C_{qj} transforming the LCI to LCIA, where I_j is the value of impact category *j*; C_{qj} is the characterization factor for impact category *j* for emission *q*; $m_{e,q}$ is the amount of emission *q*.

For example, the LCIA approach of TRACI has the similar linear relationship such as $NV_{(j)} = \sum_{x,s} CF(j)_{x,s} * e_{x,s}$, where *NV(j)* is the normalized value for impact category *(j)*; $e_{x,s}$ is the emission or resource depletion of stressor *(x)* for the spatial scale *(s)*; $CF(j)_{x,s}$ is the characterization factor for impact category *(j)* for stressor *(x)* within spatial scale *(s)*.

The rest of this chapter will focus on how to design the standard tables using LCI information. Category-based standard and activity-based standard will be discussed in section 6.2 and 6.3 respectively. How to employ the mechanism in the preliminary study of the NSF-140 carpet standard will be illustrated in section 6.4. Then a discussion and conclusion is given in section 6.5.

6.2 Category-Based Standard Design

Category-based standard design is based on the stakeholders view on the relative importance of LCIA categories such as $w_1, w_2, \ldots\ldots, w_n$. It is expected that the stakeholders will be able to agree on a set of weights, although arriving at this agreement may require significant effort. The threshold tables will be generated given the total points in the standard. Figure 6.2 shows the category-based standard framework.

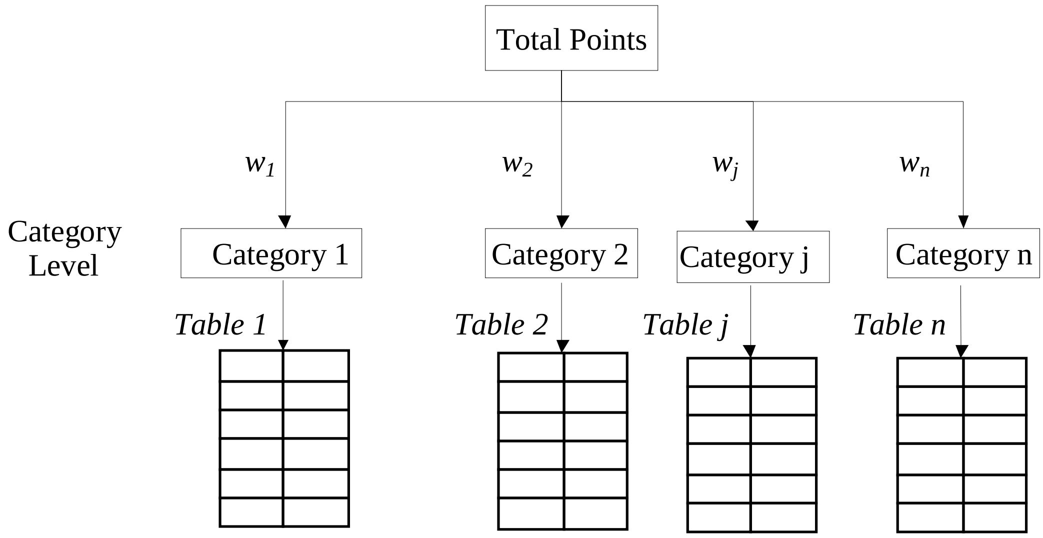


Figure 6.2: Category-Based Standard Frameworks

For each impact category *j*, a weight w_j is given from stakeholders. Each impact category will be allocated to certain points according to the given total points and weights w_j. Then, the standard tables with the structure like Table 6.1 will be formed linearly with percentage of improvement in each impact category.

Table 6.1: A Standard Table Structure in the Standard Framework

Impact Improvement % for Category 1	Point awarded
0~~5%	1
5%~~10%	2
……	……
95%~~100%	20

LCI impact can be expressed as $I_j = \sum_q C_{qj} * m_{e,q}$, given the coefficient C_{qj} transforming the LCI to LCIA, specified $m_{e,q}$ from LCI information, and weights w_j from the stakehbolders perspective. A category-based standard can be designed straightforwardly – given an absolute range of values that the impact category can take $[I_{min}, I_{max}]$. Essentially, the life cycle inventory can be found for a product and then the value for each impact category computed. The stakeholders will have assigned points to each category, and the fraction of those points awarded to the product will be based on:

$$Percentage = \frac{I_j - I_{\min}}{I_{\max} - I_{\min}} \quad \text{…….(2)}$$

The difficulty with this absolute basis for the points is that finding the appropriate values for the minimum and maximum impacts is challenging. Zero could be taken for the minimum and then one approach would be use a baseline product to define the maximum, this would then lead to a standard based on the fraction of impact of the baseline product. Another alternative design for a category-based standard is to reward the percentage of improvement from a baseline. A baseline or reference state (Θ) for category j, I_j^{Θ}, is shown in Equation (3).

$$I_j^{\Theta} = \sum_q C_{qj} * m_{e,q}^{\Theta} \quad \text{……………………..…………………………(3)}$$

After a series of transformations from Equation (4), the standard with incentive for improvement can be designed given the baseline.

$$\frac{I_j^{\Theta} - I_j}{I_j^{\Theta}} = \frac{\sum_q C_{qj} * m_{e,q}^{\Theta} - \sum_q C_{qj} * m_{e,q}}{\sum_q C_{qj} * m_{e,q}^{\Theta}} \quad \text{……………….……………….(4)}$$

Category-based standards are relatively straightforward to stakeholders but less transparent to manufacturers. When considering the improvement of the standard for continuous development, the category-based standard is easy to expand with a new category, while the activity-based standard may have difficulties with introducing new activities. However, the activity-based standard and the category-based standard can be transformed between one another, when the connection from LCI to LCIA is well characterized and obeys the linearity relationship.

6.3 Activity-Based Standard Design

This section addresses two aspects of activity-based standards design. First, the problems of design these standards are highlighted. Then, despite these problems, it demonstrated that it is possible to design standards according to the principles laid out in section 6.1.2.

There are at least two significant problems that arise from the generation of points-based standards by an activity-based procedure. First, allocating points to activities shifts the focus from improving the categories to rewarding specific activities. These activities may actually improve (or worsen) several of the categories that were originally of interest to the stakeholders, but this will not be transparent to the standard because the activity receives the points – not the improvement of the category. In other words, an activity-based standard mixes the rewards for improving categories together in the rewards for the activities, which may then be much harder to interpret. For example, recycling may lower material resource use, energy consumption and landfill waste, but may receive points that do not reflect the original concern of the stakeholders for each of these categories. Second, new activities that could improve the original categories, such as reducing the material use of the product, may receive no points at all because this activity was not considered as part of the original stakeholder discussion. Recycling of the product may not change the recycled content of the product itself, if the material is used in some other secondary stream, yet the recycling is saving material resources overall. However, the standard may reward only the activity of increasing the recycled content of the product, hence the recycling activity would not be rewarded in this context.

In general it seems unlikely that we will think of all the activities that might be taken to improve categories. Thus it will be difficult to avoid constant adjustment of the standard and to make sure that activities are rewarded appropriately, because new activities may require adjustments to the existing activity rewards, to avoid inflating the total number of points available in the standard.

The goal of this section is to develop a more scientific approach to the generation of activity-based standards that address these two concerns. First, the approach keeps the focus on rewarding product category improvement that reflects the original values of the stakeholders. Second, it admits many different forms of activity, and constructs the points reward scheme to ensure that different activities are rewarded proportionately to their improvement of product categories, as opposed to a more arbitrary view of how good it is to do something. The focus will be on those components of life cycle assessment that are directly related to life cycle inventory measures, such as global warming potential, and other emission or resource use categories. From Section 6.3.1 to 6.3.3, we describe our approach to allocating the point-based standard from three different scenarios that involves simple category, multi-category, and uncertainty with introducing a new activity. In Section 6.4, we illustrate how to employ the mechanism in the preliminary study of the NSF-140 carpet standard.

6.3.1 Case 1 – Single Category Activity-Based Design

For a standard to be consistent with Principle1, the same amount of points earned by each activity should reflect an equivalent environmental impact. To achieve this goal, two assumptions are made: the awarded points should have a linear characteristic within the same category and the relations among different categories are known. Assume there are $n+1$ activities. Given the relations of reduction among different activities for the same impact as shown in Table 6.2, the coefficient of $a_1, a_2 \dots a_m$ that represent the improvement percentage of each activity i compare with activity 0. For example, using 5% recycled materials is equal to 1% of electricity reduction from an environmental perspective. This ratio can be established through the life cycle information as explained later.

Table 6.2: Algorithm of Awarded Points According to Equivalent Percentage Reduction among Different Activities

Activity	0	1	…..	m
% of Reduction	1	a_1	……	a_m
% of Reduction to Gain 1 point	x	a_{1*} x	……	a_{m*} x
Maximum Achievable %	b_0	b_1	……	b_m

Take category 0 as the baseline: x% of reduction from activity 0 will earn 1 point. Therefore, a_1*x% of reduction from activity 1 will earn 1 point as well. Therefore, from Equation (1), the points of each activity n will be allocated as follows:

$$\frac{b_0}{a_0 * x} + \frac{b_1}{a_1 * x} + \frac{b_2}{a_2 * x} + ... + \frac{b_m}{a_m * x} = \text{Total Points} ....(1)$$

where b_i represents the maximum percentage of an activity can achieve. For example, activity 1 stands for using recycling materials, in some system the maximum percentage of recycling materials being used can not exceed 25%. Therefore, b_1 is equal to 25% and the upper bound of the threshold in the recycling materials table is 25%. The constructed table will have the same structure as the existing standard as shown in Table 6.3 and Table 6.4.

Table 6.3: Activity 0's Standard Table Structure

Threshold	Point awarded
0~~x	1
x~~2*x	2
……	……
$(b_0$-x)~~b_0	b_0/x

Table 6.4: Activity i's Standard Table Structure 0<i<=m

Threshold	Point awarded
0~~a_m*x	1
a_m*x~~2*a_m*x	2
……	……
(b_i- a_m*x)~~ b_i	b_i/(a_m*x)

The coefficients a_i are considered known and are determined from stakeholders' experience. However, because of the development of LCA, LCI information can be used to determine the relation coefficients a_i for those categories for which relationships between LCI and LCA are known and for which activities LCI values are known. b_i are based on the product system's condition which means only b_i of the limit can be reached. The b_i*'s* are typically determined by manufacturer performance specification for material content, or can be set as goals for the system to reach. These can be adjusted with time as the ability of manufacturers to meet the current goals increases.

Once the tables have been set up, we can use it to evaluate the system by getting the total points from the standard. The point-based table structure is especially useful for the system when having a combination of different activities that are substitutable. Figure 6.3 shows processes with multiple recycling methods. If the production system is performed only on one recycling method, the awarded points will be read through Table 6.5. However, if the system is a combination of two or three different recycling methods, for example, 20% of product from using the recycling method 1, 30% of product from using the recycling method 2, and 50% of product from using the recycling method 3 as shown in Table 6.6, then we need some means of combining them. Also, each recycling method has certain energy reduction: 20%, 15% and 25%. As a result, the system performance for combination of different methods can be calculated.

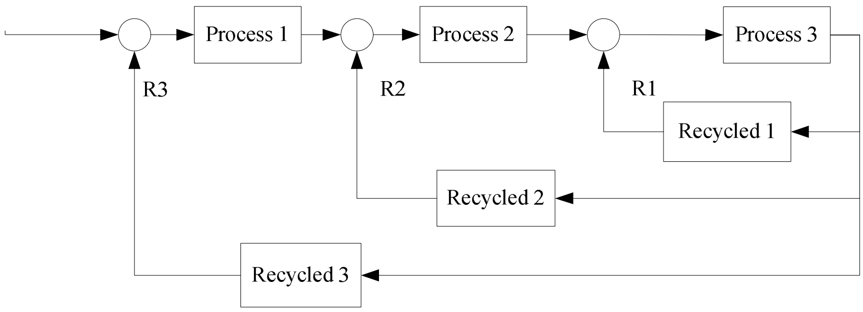


Figure 6.3: An Example of Multiple Recycling Process System

Table 6.5: An Example of Energy Reduction Table

Energy Reduction %	Point Awarded
10%~~15%	1
15%~~20%	2
20%~~25%	3

Table 6.6: Percentage Combination of Multiple Recycling Process System

	R1	R2	R3
% of Combination	20%	30%	50%
% of Energy Reduction	20%	15%	25%
Point Awarded Based on 100% of this Activity Type	2	1	3

The combined percentage energy reduction of the system is 20%*20%+30%*15%+50%*25%=21%. Therefore, the combined system will get 3 points by looking up the threshold value from Table 6.6.

6.3.2 Case 2 – Multiple Category Activity-Based Design

Case 1 represents the single category standard, which can have different activities but within the same category. However, normally one activity affects has different impact categories instead of just one. This raises the issue of how to construct multi-category tables in the standard. To normalize the process of creating standard, a four step procedures based on impact level and activity level are proposed as shown in Figure 6.4.

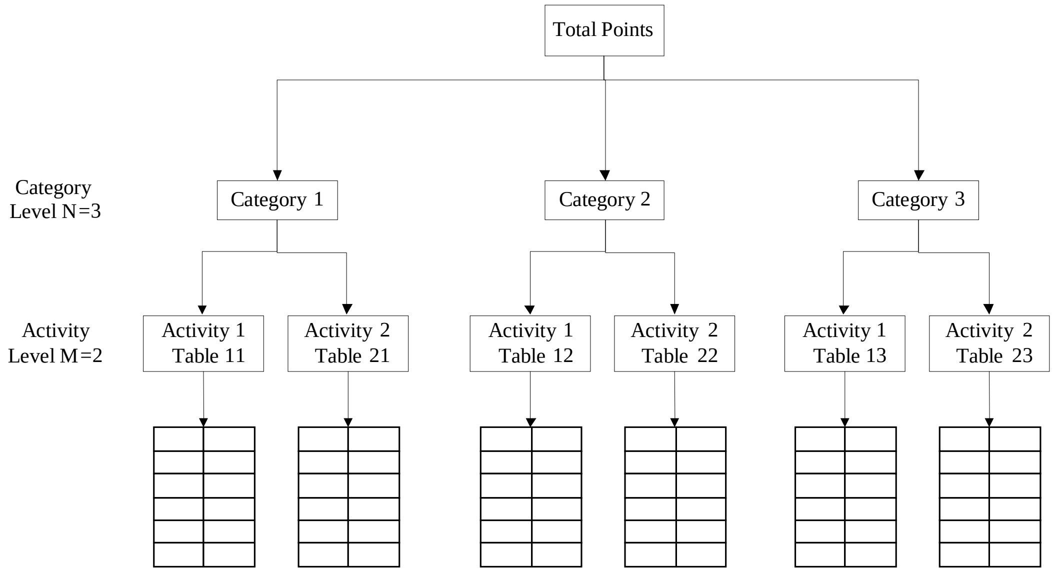


Figure 6.4: Multiple Category-Based Standard Frameworks

The first step is to generate the matrix having the categories (the number of impacts is n) as column and the activity (the number of activities is m) as row.

	$Category_1$	$Category_2$	......	$Category_n$
$Activity_1$	$Table_{11}$	$Table_{12}$	......	$Table_{1n}$
$Activity_2$	$Table_{21}$	$Table_{22}$	......	$Table_{2n}$
......	......	......	......	......
$Activity_m$	$Table_{m1}$	$Table_{m2}$	......	$Table_{mn}$

The second step is to get the impact weights from stakeholders and allocate the total points to each impact category. For example, assume three impact categories are included in the standard with weights w_1, w_2, and w_3 respectively. Given the total points as T, each impact category will get points $T*w_1$, $T*w_2$, and $T*w_3$ respectively.

The third step is to allocate points within each impact category. After knowing how many points gained for each impact category, points within the same impact category will be allocated through different activities as shown in section 6.3.1 for single category activity-based design.

Then, we have $m*n$ tables with respect to each impact and each activity. Finally, we will integrate the $m*n$ tables into m activity tables. And each table has the following structure in Table 6.7.

Table 6.7: Activity i's Standard Table Structure 0<i<=m

Impact Improvement % for Activity i	Point Awarded
0~~5%	1
5%~~10%	2
……	……
95%~~100%	20

The following shows how to integrate two impact category tables into one activity table as an example. Assume activity1 can contribute to impact category 1 and 2. And the two impact category tables for activity1 has been formed as Table 6.8 and Table 6.9.

Table 6.8: Impact Category 1 Standard Table for Activity 1

Category 1 Impact Improvement % for Activity 1	Point Awarded
0~~20%	1
20%~~40%	2
……	……
80%~~100%	5

Table 6.9: Impact Category 2 Standard Table for Activity 1

Category 2 Impact Improvement % for Activity 1	Point Awarded
0~~10%	1
10%~~15%	2
……	……
90%~~100%	10

The above two tables can be integrated into Table 6.10 for activity1.

Table 6.10: Integrated Activity Standard Table

Overall Impact Improvement % for Activity 1	Point Awarded
0~~10%	2
10%~~20%	3
20%~~30%	5
30%~~40%	6
40%~~50%	8
50%~~60%	9
60%~~70%	11
70%~~80%	12
80%~~90%	14
90%~~100%	15

The sequence of allocation also can be changed. For instance, the activity level can be allocated first and then assign the points for impact level. The advantage of this procedure is that we can use the LCI information on the activity level to get the weights which will have more support content from the calculation. Also, this is a useful interpretation of how the LCI can help us from standard point view.

6.3.3 Case 3 – Dealing with Uncertainty in Activity Impact

Often, it is difficult to get the exact values for a_i. Instead, we know the range of the weights, characterized by an upper bound and lower bound. The range will introduce uncertainty into the system and make it more difficult to specify the standard threshold value. However, we can use the interval arithmetic operations as shown in Equations (1) to (4). Assume there are three activities, activity 0 where the percentage of improvement will gain one point is x known from pervious studies, and activity 1 to n with lower bound and upper bound of their activities improvement ($a_1 \in [\underline{a_1}, \overline{a_1}], a_2 \in [\underline{a_2}, \overline{a_2}]$) compared to activity 0. After a few steps of calculation from Equation (5), we could solve and find the interval of x as shown in Equation (6). Therefore, the new percentage of improvement for getting one point for activity 0 can be estimated as in a range $[\underline{x}, \overline{x}]$.

$$
\begin{aligned}
&\textit{Assume}:\\
&a_1 \in [\underline{a_1}, \overline{a_1}], a_2 \in [\underline{a_2}, \overline{a_2}]\\
&[\underline{a_1}, \overline{a_1}] + [\underline{a_2}, \overline{a_2}] = [(\underline{a_1} + \underline{a_2}), (\overline{a_1} + \overline{a_2})] \ldots\ldots\ldots(1)\\
&[\underline{a_1}, \overline{a_1}] - [\underline{a_2}, \overline{a_2}] = [(\underline{a_1} - \underline{a_2}), (\overline{a_1} - \overline{a_2})] \ldots\ldots\ldots(2)\\
&[\underline{a_1}, \overline{a_1}] * [\underline{a_2}, \overline{a_2}] = [(\underline{a_1} * \underline{a_2}), (\overline{a_1} * \overline{a_2})] \ldots\ldots\ldots(3)\\
&\frac{[\underline{a_1}, \overline{a_1}]}{[\underline{a_2}, \overline{a_2}]} = [\underline{a_1}, \overline{a_1}] * [\frac{1}{\overline{a_2}}, \frac{1}{\underline{a_2}},] \ldots\ldots if\ \underline{a_2} \neq 0, \overline{a_2} \neq 0 \ldots\ldots\ldots(4)
\end{aligned}
$$

$$
\begin{aligned}
&\textit{Then}\\
&\frac{b_0}{a_0 * x} + \frac{b_1}{a_1 * x} + \ldots\ldots + \frac{b_n}{a_n * x} = Total \ldots\ldots\ldots(5)\\
&[\underline{x}, \overline{x}] = \left[\frac{1}{Total} * (\frac{b_0}{a_0} + \sum_{i=1}^{n} \frac{b_i}{\overline{a_i}}), \frac{1}{Total} * (\frac{b_0}{a_0} + \sum_{i=1}^{n} \frac{b_i}{\underline{a_i}}) \right] \ldots\ldots\ldots(6)
\end{aligned}
$$

Then the percentage of activity 0 reduction to gain one point is in the range below:

$$
[\underline{x}, \overline{x}] = \left[\frac{1}{Total} * (\frac{b_0}{a_0} + \sum_{i=1}^{n} \frac{b_i}{\overline{a_i}}), \frac{1}{Total} * (\frac{b_0}{a_0} + \sum_{i=1}^{n} \frac{b_i}{\underline{a_i}}) \right].
$$

The next step is for stakeholders to choose the percentage improvement value x' from the above range $[\underline{x}, \overline{x}]$ for activity 0 to get one point, where the maximum amount of points for activity 0 to gain is $\frac{b_0}{x_0'}$. And the standard table for activity 0 will be constructed in Table 6.11.

Table 6.11: Activity 0 Standard Table

Impact Improvement % for Activity 0	Point Awarded
$0 \sim\sim x_0'$	1
$x_0' \sim\sim 2*x_0'$	2
……	……
$(b_0 - x_0') \sim\sim b_0$	$\frac{b_0}{x_0'}$

Activity 1 and 2 will have the same standard table structure as Table 6.11. Take activity 1 as an example, $[\underline{a_1} * x_0', \overline{a_1} * x_0']$ will be the percentage improvement range of activity 1 to get one point. Therefore, stakeholders need to choose the percentage improvement x_1' for activity 1 to get one point. After knowing x_0' for activity 0 and x_i' for activity i from 1 to n-1, x_n' for activity n-1 can be calculated through the equation $\frac{b_0}{x_0'} + \frac{b_1}{x_1'} + ... + \frac{b_n}{x_n'} = Total$.

An abstract example is given in the following to illustrate the above machinery. Assume there are three activities 0, 1, and 2; the total points for allocation is 30; x of reduction for activity 0 can gain one point; a_1 is in the range [2%, 5%], and a_2 is in the range [5%, 8%].

After calculation, the percentage reduction range for activity 0 is [4.42%, 5.67%]. Then we choose x_0' of activity 0 to be 5%, which means 5% of reduction will gain one point for activity 0. And activity 0 will gain 20 points maximum. Subsequently activity 1 will have the percentage reduction range [10%, 25%]. We choose 20% of activity 1 to get one point, so activity 1 can get 5 points in total. According to the equation $\frac{100\%}{5\%} + \frac{100\%}{20\%} + \frac{100\%}{x_2'} = 30$, x_2'is 20% as a result.

Overall, Table 6.12, Table 6.13 and Table 6.14 will be constructed as the standard.

Table 6.12: Example of Activity 0 Standard Table

Impact Improvement % for Activity 0	Point Awarded
0~~5%	1
5%~~10%	2
……	……
95%~~100%	20

Table 6.13: Example of Activity 1 Standard Table

Impact Improvement % for Activity 0	Point Awarded
0~~20%	1
20%~~40%	2
……	……
80%~~100%	5

Table 6.14: Example of Activity 2 Standard Table

Impact Improvement % for Activity 2	Point Awarded
0~~20%	1
20%~~40%	2
……	……
80%~~100%	5

6.4 Case Study

The NSF-140 standard is an example of a points-based standard with activities and with categories. The standard awards points in several different ways.

1. Process/Documentation – the standard awards points for following certain processes in documenting product activities and in managing the product, such as using an environmental quality control system.

2. Threshold properties – the standard awards points for crossing certain thresholds, such as eliminating toxics from the product. Once the specific threshold is crossed no more points can be earned in the category.

3. Tabular threshold properties – the standard awards points on the basis of crossing thresholds but an increasing number of points are awarded according to the highest threshold crossed. This is typically applied to materials and energy usage in the product. Higher amounts of using desirable materials and energy and lower overall energy usage will be rewarded. However, the NSF-140 standard mixes both category and

activity tables, which in general is not a good idea, because it will lead to double counting of LCI improvements and may make it difficult to have a consistent standard.

From an optimization perspective, the points in category 1 are not really significant as they do not interact significantly with other decisions and are focused more around company policy than the actual materials and energy content of the product. The points in category 2 can be calculated through the optimization model of Chapter 5 and may interact with other product life cycle decisions. To achieve a threshold in category 2, you may increase or decrease the inclusion of specific materials in the product. The points in category 3 are the most interesting one from an optimization perspective. In the NSF-140 standard these points are earned in three major categories, product reclamation, recycled or bio-based content, and renewable energy and energy efficiency. A substantial number of points are distributed in these categories, and they are awarded for increasing performance.

In the NSF-140 standard, the total awarded points are 114, among which 32 points are awarded by direct material and energy improvement from LCI perspective. Our focus is on the 32 points awarded with threshold values in Table 6.15 and 6.16.

Table 6.15: Manufacturer's Use of Renewable Energy and/or Energy Reduction

Percentage of Energy Reduction	Points Awarded
≥1%	2
≥2%	3
≥5%	4
≥8%	5
≥10%	6
≥15%	7
≥20%	8
≥25%	9
≥35%	10
≥50%	11
≥75%	12

Table 6.15 is not consistent with a linear relationship between renewable energy and impact categories especially under 10% use of renewable energy or energy reduction. The reason that more points are distributed at the beginning of the energy percentage reduction in Table 6.15 is to encourage manufacture to take on changes from energy perspective. Moreover, since the last two points are hard or never going to be earned, 35% probably represents the b value for this table.

Table 6.16: Points Awarded for Manufacturer's Use of Bio-Based, Recycled Content, or EPP

Percentage of Recycled Content	Points Awarded
≥5%	2
≥10%	3
≥15%	4
……	……
≥95%	20

Table 6.16 is much more consistent than Table 6.15. Manufactures can earn 1 point per 5% of recycled content. However, manufactures cannot get a point below using 5% of recycled content, because manufacturers genuinely believe that they could get to 100% recycled, bio-based or EPP materials.

With a life cycle approach, the algorithm of point allocation shown in Table 6.2, threshold value and awarded point will be allocated automatically through Equation (1). $a_1 \ldots a_n$ represents the reduction equivalent relations between each activity (for example a 15% use of biomaterials or a 10% use of renewable energy). b_i is the maximum extent that each activity can achieve. x is the extent of activity 0 reduction that will get one point for activity 0, and activity 1 will get one point for the reduction of $a_1 * x$. Assume there are $m+1$ activities and x of activity 0 reduction will gain one point.

From the mathematical programming tool for LCI based process design, all possible production process flow pathways were recorded as an output file with mass and energy information. Data were sorted and compared based on different process options: using bio-based material, using recycled material, and using energy efficient method. And the equivalent percentages from different options were generated as the first row in Table 6.17 with three different options: using post industrial material, using post consumer backing material, and using post consumer face fiber material. Therefore, in the proposed standard, three tables will be created instead of just two tables.

Table 6.17: Case study of Awarded Points According to Equivalent Percentage Reduction among Different Activities

Activity	PC Face Fiber	PC Backing	Post Industrial
Coefficient	1	0.537	0.064
Use of material to gain 1 point	x	0.537* x	0.064* x%
Maximum use of material	0.894	1.32	0.278

$$\frac{0.894}{x} + \frac{1.32}{0.537 * x} + \frac{0.278}{0.064 * x\%} = 32 \qquad (2)$$

Solving Equation (2) for *x*, we get *x*=0.239 kg. Therefore, Tables 6.18 to 6.20 are created, and total points allocated are 32.

Table 6.18: The Post Industrial Materials Table

Usage of Post Industrial Material (kg per 1 kg product)	Awarded Points
≥0.015	1
≥0.031	2
≥0.046	3
≥0.062	4
≥0.077	5
≥0.093	6
≥0.108	7
≥0.124	8
≥0.139	9
≥0.154	10
≥0.170	11
≥0.185	12
≥0.201	13
≥0.216	14
≥0.232	15
≥0.247	16
≥0.263	17
≥0.278	18

Table 6.19: The Post Consumer Backing Materials Table

Usage of PC Backing (kg per 1 kg product)	Awarded Points
≥0.13	1
≥0.26	2
≥0.39	3
≥0.52	4
≥0.64	5
≥0.77	6
≥0.90	7
≥1.03	8
≥1.16	9
≥1.29	10

Table 6.20: The Post Consumer Face Fiber Materials Table

Usage of PC Face Fiber (kg per 1 kg product)	Awarded Points
≥0.24	1
≥0.48	2
≥0.72	3
≥0.95	4

The case study reveals several important features of redesigning tables according to the goal of rewarding life cycle impact equally across different activities. First, reducing the actual energy consumption of the product manufacturing earns a very high percentage of the overall points, whereas recycling material earns a relatively small number of points. The relative improvement for different activities is captured in the a_i values. This reflects the fact that recycling takes a significant amount of energy and transportation and therefore its benefit is not as high as directly reducing energy consumption, particularly electrical energy. Second, the maximum reduction that can be achieved by the activity does play an important role in the assignment of points. Two activities with similar relative impacts will be assigned different points if one can only be undertaken at a rate half that of another.

6.5 Discussion and Conclusion

Standards are a general tool to measure a product or a system performance and are used to drive industry towards superior outcomes. For the chemical industry, energy and emissions are the most important issues. And environmental impact is a significant session that reflects both the energy and emissions of a chemical product system. Therefore, major points of the chemical industry standard will be allocated to the environmental side which including energy, recycling and bio-based materials. The standard settings of point allocation across different categories are mostly based on the stakeholders' previous experiences and often lack empirical evidence as to the impacts of different product activities.

The stakeholders' experiences are indeed valuable; however, there is a desire to have a more scientifically based standard that aligns the standard with environmental impacts, particularly when points are assigned to undertaking different activities. Moreover, since these points are rewarded cumulatively according to corresponding threshold, how to award the point equally among different category for the same impact such as using recycling or bio-based material for the same impact is a key issue. Therefore, a standard generating mechanism for point allocation has been developed and could be utilized broadly for many points-based standards. Consequently, we focus on creating the mechanism of setting up the standard scientifically and build in the stakeholder experience and values through specific weightings of impact categories.

Therefore, a standard generating mechanism for point allocation was proposed and can be utilized broadly among many industries.

From the standard design point of view, activity-based standard and category-based standard have their own advantages and disadvantages. For instance, manufacturers may prefer activity-based standards, because they can most easily map their day-to-day decisions to activities. And it is clear for manufacturers to earn points by improving their activities directly. However, if the category-based standard is used, the manufacturer would have to do extra work, such as LCI and LCIA analysis, to translate their activities to each environmental category to get points. On the contrast, there are other stakeholders who participate in standards design who would prefer the category-based standard, because they understand the categories better than the specific activities of a given industry.

An advantage for category-based standards is that it is relatively straightforward and practicable to expand the standard when including a new category in the standard. But for the activity-based standards, introducing a new activity to the standard will dilute the points awarded for other activities. If the points are maintained as before, then adding new activities increases the ways to earn points and may dilute the standard. Overall, the major difference between the two kinds of standard is that either manufacturers or the standards developer performs the transformation from LCI to LCIA measures. However, since the transformation is feasible for mature areas where well accepted LCI and LCIA measures exist, then category-based activity is relatively simple. In developing/understanding areas for LCI and LCIA method, then activity-based standard is relatively simple. In addition, it is recommended that the stakeholders either create activity only standard or category only standard since a mixture will incur the issue of points double counting for improvements in the same category.

Another issue from the standard design is that linear relationship is required between points and percentage of improvement to ensure the equal points allocation of the standard. Nevertheless, the stakeholders would like to deviate from this linear design. For two reasons, concave points-awarded structure is to encourage early adoption of the standard, while convex points-awarded structure is to promote for greater improvement later on.

There is an existing standard, NSF-140, to evaluate the carpet production system. A case study for NSF-140 carpet standard was carried out to demonstrate the ability to reconstruct tables based on life cycle information. In the NSF-140 standard, two tables (manufacturer's use of renewable energy and/or energy reduction and manufacturer's use of bio-based, recycled content, or EPP materials) with 32 points were reconstructed. In the case study, three tables (using post industrial material, using post consumer backing material, and using post consumer face fiber material) instead of two were created with linear characteristic. The set of new tables enable the manufacture to use the standard straightforwardly and encourage them to earn points clearly by performing process improvement.

CHAPTER 7

CONTRIBUTIONS AND FUTURE WORK

7.1 Contributions

The objective of this thesis was to develop a general methodology for the selection of product chemical production systems using LCI information that can identify optimal process pathways. This objective was extended to examine the design of products in the context of sustainability assessment standards that incorporated significant life cycle assessment measures. Finally, the design of the standards themselves to be congruent with life cycle measures was considered. Each of these objectives was met.

First, we developed a two-stage approach to select the optimal production strategy (that is defined by a process tree) considering the life cycle impact (measured in terms of emissions or energy usage) of alternative product strategies that are implicitly defined for a product. The first stage enumerates all feasible process trees taking important constraints (e.g., material availability and/or recycled material content requirements) into account for the product. Using the output of the first stage, the second stage uses a linear programming model to select the optimal process tree with the objective of minimizing total energy/fuel/electricity usage while ensuring that the total demand for the product is satisfied and respecting the availability of recycled materials. This avoids problems that intensive life cycle functional units incur: they may not be capable of being scaled up to production volumes because of the unavailability of the input material mix.

The approach was illustrated for a carpet system. The numerical results from the case study illustrate how the proposed approach can be used to evaluate the energy use impact of increasing the recycled material content of the product. The key advantage of this approach is that rather than embedding the alternatives into a mixed integer linear programming optimization that can be difficult to solve, we de-couple the generation of alternatives from their selection. The framework easily extends to other products and the addition of alternative ways to produce chemicals that form part of the tree that leads from raw materials to the final product.

Overall, Chapter 4 presented a novel approach to product design combining LCI information and mathematical optimization with appropriate physical constraints and sustainability objectives. The systematic framework is coupled to an optimization algorithm that is a simple linear program. This enables choices of product compositions and routes that can be evaluated against different objectives based on the inventories of mass, energy and emissions. Therefore, the first contribution of this work lies in the development and implementation of the process-tree-builder module and the implementation of a linear programming model for the selection of the optimal process-tree among all the alternatives presented.

Second, we introduced an optimization model coupled with life cycle inventory information to explore whether sustainability assessment standards actually promote products that are better from a life cycle perspective, or whether the standards are biased towards certain activities based on a perception that some activities are inherently better than others. This enables choices of product compositions and routes that can be evaluated against life cycle optimization and point-based standard optimization based on the inventories of mass, energy and emissions. The model is used to test the hypothesis that the standard point reward system and life cycle inventory measures are not completely aligned for carpet. The optimal solution is used to suggest changes to the point allocation scheme that could bring the standard and life cycle assessment into closer agreement. The key advantage of this approach is that we connect LCA with the point-based standard in optimization. Our work was extended to show how sustainability assessment standards can be re-designed to make them congruent with life cycle measures in Chapter 6.

In general, Chapter 5 compared points-based and LCA-based approaches for product design, with application to carpets. Points-based standards have become quite popular, but there is a perception that they are based on subjective criteria that may not be better from a life cycle point of view. This work is useful for guiding decisions toward sustainable engineering and enabling the modification of point-based systems to align them more closely with LCA principles. As a result, the second contribution of this work is to develop a normative optimization model that can explore the relationship between standards setting and life cycle inventory calculations, which is important for standards development. This provides an unbiased way to assess the standard and its alignment with measures of life cycle inventory improvement. The use of life cycle inventory information can therefore help in the construction of the standard and could be useful in guiding the modification of point-based systems to align them with the LCA.

Third, this work developed a methodology for designing a standard using LCI information, which is another application of using the framework described in Chapter 4. Chapter 6 discusses the activity-based and category based standard design from life cycle analysis perspectives. This contributes to establish the design strategy of a standard from life cycle knowledge.

In conclusion, this work addressed some critical issues such as optimization and modeling in the design of product systems using LCI information and developed a standard design strategy from LCI/LCIA perspective. This work contributes to simplifying the optimization process, the use of life cycle information to help design early in the product life cycle, and identification of regulatory needs to address public concerns for chemical industry.

7.2 Future Work

Future work on the optimization, modeling and standard design that could have the most impact includes the following subjects.

7.2.1 Product Portfolio Design

One extension for LCI optimization would be to look at multiple products simultaneously – a portfolio, where we still have the same limited resources that we would have to spread over multiple products with certain constraints on the product compositions (such as having a minimum of 10% recycled content). This would mirror the problem faced by companies who want to have the maximum amounts of different product lines that meet certain environmental performance criteria. Assume the company plan to produce a series product *(A,B,C……N)* with the same kind of raw materials (M_j) but different compositions

($Percent_{(A,recycled\ material)}$, $Percent_{(B,recycled\ material)}$ …… $Percent_{(N,recycled\ material)}$) for recycled material. The objective is to minimize energy consumption with different products. The optimization formulation would have the structure as follows:

$$
\begin{aligned}
\min\ & \sum_{Ai} E_{Ai} \cdot A_{Ai} + \sum_{Bi} E_{Bi} \cdot B_{Bi} + \sum_{Ci} E_{Ci} \cdot C_{Ci} + ... + \sum_{Ni} E_{Ni} \cdot N_{Ni} \\
s.t.\ & \sum_{Ai} A_{Ai} = D_A \\
& \frac{\sum_{Ai} \left(A_{Ai} * a_{(Ai,recycled\ \text{material})}\right)}{D_A} \geq Percent_{(A,recycled\ material)} \\
& \sum_{Bi} B_{Bi} = D_B \\
& \frac{\sum_{Bi} \left(A_{Bi} * a_{(Bi,recycled\ \text{material})}\right)}{D_B} \geq Percent_{(B,recycled\ material)} \\
& \sum_{Ci} C_{Ci} = D_C \\
& \frac{\sum_{Ci} \left(A_{Ai} * a_{(Ci,recycled\ \text{material})}\right)}{D_C} \geq Percent_{(C,recycled\ material)} \\
& .... \\
& \sum_{Ni} N_{Ni} = D_N \\
& \frac{\sum_{Ni} \left(N_{Ni} * a_{(Ni,recycled\ \text{material})}\right)}{D_N} \geq Percent_{(N,recycled\ material)} \\
& \sum_{Ai} a_{Ai,j} A_{Ai} + \sum_{Bi} a_{Bi,j} B_{Bi} + \sum_{Ci} a_{Ci,j} C_{Ci} + ... + \sum_{Ni} a_{Ni,j} N_{Ni} \leq M_j
\end{aligned}
,
$$

where Ai is the set of pathways to produce product A; j is the set of raw materials; A_{Ai} is the amount of product A manufactured by pathway Ai; E_{Ai} is energy consumption for product A from pathway Ai; D_A is the demand for product A given by manufacture; $a_{(Ai,j)}$ is the coefficient of material j for product A from the process pathway Ai; $a_{(Ai,recycled\ material)}$ is the coefficient of "recycled material" for product A from the process pathway Ai. The objective is to minimize energy consumption. And three sets of constraints are included:

(1) The amount of A produced from pathway Ai should meet the demand D_A ($\sum_{Ai} A_{Ai} = D_A$);

(2) The composition of product A should at least have certain percentage of recycled material ($\frac{\sum_{Ai}\left(A_{Ai} * a_{(Ai,recycled\ \text{material})}\right)}{D_A} \geq Percent_{(A,recycled\ material)}$);

(3) The usage of raw materials should be within the raw material availabilities ($\sum_{Ai} a_{Ai,j} A_{Ai} + \sum_{Bi} a_{Bi,j} B_{Bi} + \sum_{Ci} a_{Ci,j} C_{Ci} + ... + \sum_{Ni} a_{Ni,j} N_{Ni} \leq M_j$).

In addition, given a product portfolio demand profile, optimization models could be used to discover the best way to meet that demand from a material selection perspective. The objective is to minimize the material consumption such as crude oil.

$$
\begin{aligned}
\min \ & \sum_{Ai} a_{Ai,Crude\,Oil} A_{Ai} + \sum_{Bi} a_{Bi,Crude\,Oil} B_{Bi} + \sum_{Ci} a_{Ci,Crude\,Oil} C_{Ci} + ... + \sum_{Ni} a_{Ni,Crude\,Oil} N_{Ni} \\
s.t. \ & \sum_{Ai} A_{Ai} = D_A \\
& \sum_{Ai} a_{Ai,Aj} A_{Ai} \leq M_{Aj} \\
& \sum_{Bi} B_{Bi} = D_B \\
& \sum_{Bi} a_{Bi,Bj} B_{Bi} \leq M_{Bj} \\
& \sum_{Ci} C_{Ci} = D_C \\
& \sum_{Ci} a_{Ci,Cj} C_{Ci} \leq M_{Cj} \\
& \quad .... \\
& \sum_{Ni} N_{Ni} = D_N \\
& \sum_{Ni} a_{Ni,Nj} N_{Ni} \leq M_{Nj}
\end{aligned}
,
$$

where $a_{(Ai,Crude\,Oil)}$ is the coefficient of crude oil for product A from the process pathway Ai ; M_{Aj} is the raw material limit for product A. In this optimization model, the objective is to minimize the total crude oil usage to meet different product demand. The above optimization models could be implemented straightforwardly given enough information or requirements from the manufacture.

7.2.2 Standards Design

Some new issues arise and need further study in the design of standards.

One of the concerns in the standard design is what product range is allowed within a certification? This has typically manifested itself in the definition of the product platform undergoes certification. The competing concerns for the product platform are:

1. The cost of certification for a product. Not every product can be put through certification. Instead manufacturers seek to certify platforms that will give them the broadest set of products that meet certification standards.

2. The integrity of the standard. If we define a platform as a group of products then we have to come up with a definition of the platform. If this is too broad then we will certify products that do not earn a sufficient number of points for the certification level. Therefore it is important to come up with a platform definition that does not allow the system to be gamed in this way.

The naïve approach to ensuring the integrity of the standard is to define the worst possible product that can be in a given platform and then ensure that this product meets the minimum point threshold. This is obviously highly conservative and many products within the platform may exceed the threshold by a substantial margin. If it is assumed that we value the integrity of the standard above all else, we would want to ensure that every product within the platform meets a given level in the standard. This would define combinations of properties that the platform would have to meet. We can think of this as an optimization problem where the goal is to find a set of relationships between the product qualities such that if one quality is reduced others must be increased by sufficient amounts to compensate. The activity tables that are constructed to ensure that points are appropriately awarded implicitly contain the ratios between activities. It might be possible to leverage this idea to design a procedure for defining product platforms. In addition to the problem of ensuring fairness in the point thresholds, we will have certain physical constraints that we would want to respect such as not allowing product platforms to span across different backing types for the carpet system.

7.2.3 Standard Design and Mapping LCI to LCIA

Another interesting subject for future exploration is to expand the transformation from LCI to LCIA. As discussed in Chapter 6, the linear relationship between LCI and LCIA $(I_j = \sum_i C_{ij} * f_j(m_{e,i}))$ is a core assumption in our standard design. The overall environmental impact could be expressed in the form of the following equation: $\sum_j \omega_j * I_j = \sum_j \omega_j * \sum_i C_{ij} * f_j(m_{e,i}) = \sum_i (\sum_j \omega_j * C_{ij}) * f_j(m_{e,i})$. And given the reference state $I_j^{\Theta} = \sum_i C_{ij} * f_j(m_{e,i}^{\Theta})$, the expression for percentage improvement is shown as follows:

$$\sum_j \omega_j * \frac{I_j^{\Theta} - I_j}{I_j^{\Theta}} = \frac{\sum_j \omega_j \sum_i C_{ij} * (f_j(m_{e,i}^{\Theta}) - f_j(m_{e,i}))}{I_j^{\Theta}} = \frac{\sum_i (\sum_j \omega_j C_{ij}) * (f_j(m_{e,i}^{\Theta}) - f_j(m_{e,i}))}{I_j^{\Theta}}.$$

The question of whether or not the standard design method will work if there are other forms of function for LCIA could be addressed as follows. Another generalization of the transformation from LCI to LCIA (Soares, S.R., 2006) is $I_j = \sum_i C_{ij} * f_j(E_i^2)$.

The overall environmental impact could be expressed in the form of the following equation: $\sum_j \omega_j * I_j = \sum_j \omega_j * \sum_i C_{ij} * f_j(E_i^2) = \sum_i (\sum_j \omega_j * C_{ij}) * f_j(E_i^2)$. And given the reference state $I_j^{\Theta} = \sum_i C_{ij} * f_j(E_i^{\Theta 2})$, the expression for percentage improvement is shown as follows:

$$\sum_j \omega_j * \frac{I_j^{\Theta} - I_j}{I_j^{\Theta}} = \frac{\sum_j \omega_j \sum_i C_{ij} * (f_j(E_i^{\Theta 2}) - f_j(E_i^2))}{I_j^{\Theta}} = \frac{\sum_i (\sum_j \omega_j C_{ij}) * (f_j(E_i^{\Theta 2}) - f_j(E_i^2))}{I_j^{\Theta}}.$$

The above expression is a non-linear equation with corresponding to Ei, which could require some adjustment to the standard design method. Overall, if the mathematical conversion between LCI and LCIA is available, more environment influence can be incorporated into the standard design.

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