Product Design: Accounting for Government Policy, Corporate Social Responsibility, Supply Chain, Sustainability, and Human Senses

By

ZHANG, Xiang

A Thesis Submitted to

The Hong Kong University of Science and Technology

in Partial Fulfillment of the Requirements for

the Degree of Doctor of Philosophy

in the Department of Chemical and Biological Engineering

June 2019, Hong Kong

Authorization

I hereby declare that I am the sole author of the thesis.

I authorize the Hong Kong University of Science and Technology to lend this thesis to other institutions or individuals for the purpose of scholarly research.

I further authorize the Hong Kong University of Science and Technology to reproduce the thesis by photocopying or by other means, in total or in part, at the request of other institutions or individuals for the purpose of scholarly research.

ZHANG, Xiang

June, 2019

Product Design: Accounting for Government Policy, Corporate Social Responsibility, Supply Chain, Sustainability, and Human Senses

By

ZHANG, Xiang

This is to certify that I have examined the above PhD thesis
and have found that it is complete and satisfactory in all respects,
and that any and all revisions required by
the thesis examination committee have been made.

Prof. Henry H N LAM, Supervisor

Prof. Ka Ming NG, Co-Supervisor

Prof. I-Ming HSING, Head

Department of Chemical and Biological Engineering
June, 2019

Acknowledgements

Looking back on the past 4-year PhD study in HKUST, it is a treasurable and memorable experience in my life. I would like to take this opportunity to express my deepest gratitude to all people who have been helping me during the journey.

First of all, I would like to thank my supervisor Prof. Herry LAM and co-supervisor Prof. Ka Ming Ng for the consistent inspiration, support, and great guidance throughout these years. The rigorous and scientific thinking methods and hardworking attitude showed by them will greatly influence my entire career. Thank you for setting a high-quality standard and level of innovation for my research work from the very beginning. Thank you for providing me with the great freedom to generate new ideas. It is really a great privilege and honor to have worked with you.

Moreover, I appreciate the valuable supports from Dr. Fung Ka Yip Kelvin during the entire PhD study. We worked closely on the every research project. Without the critical comments and suggestions, I cannot make the achievements today. In addition, I owe my deep gratitude to Dr. ZHANG Lei who was a postdoc in our group. We gave me a lot of insightful advices to open my mind. The constructive ideas from him really pushed my work up to a higher level.

I would like to thank all the colleges in my research group: Dr. Yang Li, Dr. Wei Zhang, Dr. Dou Qianqian, Mr. Faheem Mushtaq, Mr. Tianpeng Gao, Mr. Khak Ho Lim, Mr. Quan Li, Mr. Lie Cai, Ms. Shengnan Liu, Mr. Jiayu Tang, Mr. Kaiqi Yan, Ms. Ting Lin, Mr. Lingda Xu, etc. Thank you for the valuable discussions. Thank you also for spending your time with me, which I will never forget.

Finally, I want to express my deepest gratitude to my family, especially my dear grandparents and parents. Nothing would have been done without their support, love, and encouragement. The

only wish of my grandpapa in his last few years was I can become the first Doctor of Philosophy in our big family. Now I finished his last wish. He will be proud of me in the heaven.

List of Publications

1. **Zhang X**, Zhang L, Fung KY, Rangaiah GP, Ng KM. Product design: Impact of government policy and consumer preference on company profit and corporate social responsibility. Computers & Chemical Engineering. 2018;118:118-131.
2. Zhang L, Fung KY, **Zhang X**, Fung HK, Ng KM. An integrated framework for designing formulated products. Computers & Chemical Engineering. 2017;107:61-76.
3. **Zhang X**, Zhang L, Fung KY, Ng KM. Product design: Incorporating make-or-buy analysis and supplier selection. Chemical Engineering Science. 2019;202:357-372.
4. **Zhang X**, Zhang L, Fung KY, Bakshi BR, Ng KM. Sustainable product design: A life-cycle approach. (under revision)
5. **Zhang X**, Zhou T, Zhang L, Fung KY, Ng KM. Food product design: A hybrid machine learning and mechanistic modeling approach. (under review)

Table of Contents

List of Figures

List of Tables

Product Design: Accounting for Government Policy, Corporate social Responsibility, Supply Chain, Sustainability, and Human Senses

ZHANG, Xiang

Department of Chemical and Biological Engineering

The Hong Kong University of Science and Technology

Abstract

Chemical processing industry has been expanding its focus from primarily business-to-business products (B2B) to business-to-consumer (B2C) products. The production of B2B products generally emphasizes on process design and optimization, whereas the production of B2C products focuses on product quality, ingredient selection, and product structure. Product pricing, costing, and competitive analysis must be considered as well. By far, these considerations have already been accounted for in the Grand Product Design Model, which consists of a process model, a property model, a quality model, a cost model, a pricing model, an economic model.[1,2] Despite the advances of the previous Grand Product Design Model, many issues have still not been fully understood and incorporated into. Thus, another evolvements and improvements are highly desired to further improve the previous Grand Product Design Model and thus promote the efficiency of new product development. In this thesis, the influences of the business and management issues (i.e., government policy, corporate social responsibility, supply chain, sustainability, and human senses) on product design and development are concerned.

Four extensions on the Grand Product Design Model have been explicitly made. In Chapter 2, the impact of government policy on company profit and corporate social responsibility is studied. The interactions of government-company-consumer are elaborated and a multi-objective optimization framework is proposed to account for these interactions. In Chapter 3, an integrative design procedure is developed where two important issues in supply chain (i.e., make-or-buy analysis and supplier selection) are explicitly incorporated into product design for generating more profitable products. In Chapter 4, product sustainability is concerned. A systematic framework is proposed for sustainable chemical product design where life cycle sustainability, rule-based methods, and general sustainable product design principles and knowledge are properly integrated. In Chapter 5, the Grand Product Design model is expanded as a generic approach to food product design where the influence of human senses on food quality is considered. A hybrid machine learning and mechanistic modeling approach, formulated as a grey-box optimization problem, is proposed to expedite new food product design. Finally, Chapter 6 summarizes the major contributions and the future work.

Chapter 1: Introduction

1.1.Background

1.1.1. Emergence of Chemical Product Design in Chemical Engineering

Many chemical products are utilized in the modern society for its survival and prosperity, such as fuels for transportation; fertilizers for agriculture; medicines for healthcare; detergents for cleaning. The development and evolution of modern society greatly depends on the continuous availability of these products and the introduction of new and better products. Figure 1.1 represents a product tree that covers all the types of chemical products.[3] Typically, a product can be obtained from resources placed lower than it on the product tree. For instance, the basic chemicals are produced from the natural resources such as petroleum, natural gas, air, etc. Basic chemicals are used to synthesis intermediate products such as methanol, urea, acetic acid, etc. Additionally, acting as root, basic and intermediate chemicals are utilized to manufacture different consumer products.

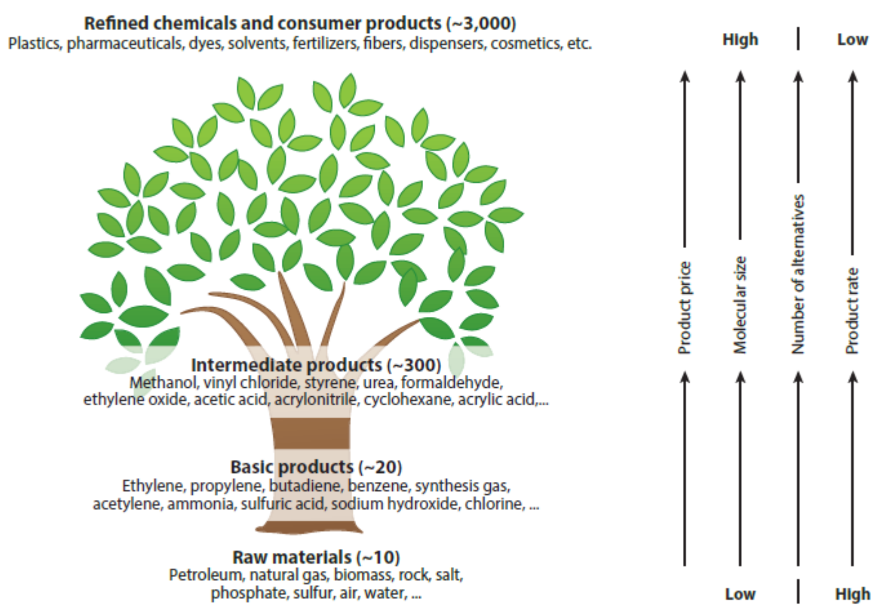


Figure 1.1 Chemical product tree[3]

In general, the basic and intermediate products are the so-called 'commodity products'. They are often produced in amounts of over 10000 tons annually. Over the past 50 years, the chemical industry has been dominated by the production of commodity products. Most research in the chemical engineering discipline focused on the synthesis, design, optimization, operation, and control of processes for producing commodity chemicals. Ideally, they should be produced as cheap, pure, and in a large-quantity as possible. In fact, through all the efforts made within the chemical industry, significant achievements have already been made to improve the performances of commodity production processes. For instance, chemical engineers already changed the clothes on human backs and increased the food on human tablets.[4]

Currently, the chemical industry is changing dramatically. On the one hand, it is not easy to significantly enhance the production processes for commodities, especially reduce the production cost. On the other hand, consumers are no longer satisfied by only using a limited number of products. The increasing needs for better and more versatile chemical products should be met as soon as possible. Thus, since the year 2000, chemical product design or chemical product engineering has already been recognized as the third paradigm of chemical engineering.[5,6] Many researchers approved that in addition to commodity products, consumer products such as detergent, paint, smart window, etc. should be emphasized in academic research and teaching.

Despite the early enthusiasm and substantial efforts, it was felt by many that research activities on chemical product design have been flagging and there are many challenges in pushing chemical product design forward.[7] One of the major challenges is that consumer products are so diverse that it is hard to define the scope of chemical product design. Gani and Ng[7] classified the diverse consumer products into three types:

- Formulated product: a mixture of selected components together to get the desired product attributes such as hand lotion, liquid detergent, shampoo, etc.
- Functional product: those products made up of materials in a certain structure to perform a desired function such as controlled-release herbicide granule, moisture absorber, etc.
- Device: perform a certain function often to an input stream so that the output stream has some desired characteristics such as indoor air purifier, water filter, wine aerator, etc.

Each type of chemical product is manufactured by different processes and has different ingredients and structures. In addition, each type of chemical product has different prices, costs, supply chains, etc. Clearly, the issues in chemical product design are multidisciplinary in nature.[1] The success of chemical product design depends on product quality, product manufacturing, product pricing, product cost, supply chain, government policy, etc. Thus, it is hard to develop a general approach for chemical product design.

For any new product development project, there are four broad questions to be answered:

1. What product to make?
2. How to make the desired product?
3. Do we want to make the identified product?
4. If the above is affirmative, how do we come up with such a product efficiently and profitably?

In answering the first question, market study should be conducted to identify the consumer needs. Meanwhile, new product conceptualizations are generated so that several product alternatives can be obtained. Then, we have to perform prototyping, process design, feasibility study, and engineering design so that the desired product alternative can be manufactured in a large quantity.

For the third question, we need to consider the business decision making to arrive at a successful product. The product must be profitable, environmental friendly, sustainable, etc. Last but not least, when we answer the above questions, we need to consider how the projects can be performed in an efficient manner. This requires clear understandings on every task in new product design. Therefore, a generic and multidisciplinary design framework or model is highly desired to manage new product development projects efficiently.[1,7]

1.1.2. The Evolution of Grand Product Design Model

1.1.2.1.From Ingredients and Process Design to Product Quality in 2002

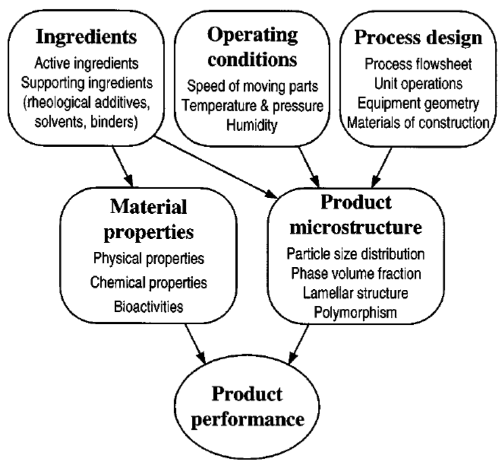


Figure 1.2 Factors determining product performance (from Wibowo and Ng[8])

Since the year 2000, Ng and his students have started to study product-centered processing. Systematic framework has been developed for designing new products with desired quality and the corresponding manufacturing processes, such as creams and pastes, dry toner, cosmetics, and pharmaceutical tablets and granules.[8-10] At that time, Figure 1.2 was proposed to account for the conceptual relationships from ingredients and processes to product performances. The arrows among different boxes were represented by mathematical models and heuristics. To design a new product, the selection of active and supporting ingredients is concerned. Each ingredient has different properties (i.e., physical, chemical and biological properties). In addition, process flowsheet and operating conditions should be properly designed to generate the desired product structure. Then, the technical performances of products can be decided based on the ingredient properties and product structure.

Clearly, such a framework in Figure 1.2 only aims to design a product with desired quality. In other words, only the first two questions were answered: what to make and how to make? However, whether the product is profitable and how the product can be commercialized efficiently were not concerned at that time (i.e., before the year 2003). Moreover, only mathematical models and heuristics were utilized. Nevertheless, it has been gradually found that for designing many new chemical products, a limited number of models and heuristics are available. In this case, how the arrows should be represented is not clear yet. Therefore, with these limitations, substantial improvement on Figure 1.2 is required.

1.1.2.2.Extensions to Product costing, Pricing, and Economic Analysis in 2015

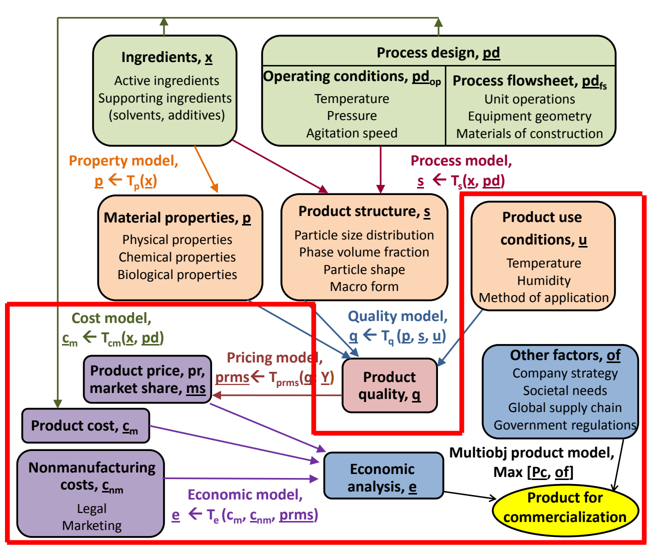


Figure 1.3 Grand Product Design model (adapted from Fung et al.[2])

As the research on chemical product design progressed, it has been gradually recognized that the success of chemical product design does not simply depend on product quality. Many other issues can have significant impact such as pricing, product cost, government policy, supply chain, etc. Bagajewicz[11] proposed a new pricing model which accounts for consumer awareness and preferences for the new product in comparison to competing products. This model leads to a way relating product quality to product price and demand and has been applied to the design of wine,[12] carpet deodorizers,[13] and lotion.[14] Cheng et al.[15] developed an integrative framework that covers marketing, product design and prototyping, process design and manufacturing, cost estimation, and economic analysis. Additionally, Bernardo and Saraiva[16] proposed a conceptual model which firstly considered the influence of product use conditions on product quality. Later on, based on these progresses, the Grand Product Design Model in Figure 1.3 was developed in the year 2015. Compared with Figure 1.2, the boxes highlighted within the red envelop were added which includes product price and market share, product cost, nonmanufacturing cost, economic analysis, and product for commercialization. Additionally, the model was formulated as an optimization problem in Eq. 1.1-1.8. Note that this was also the first time that the 'Grand Product Design Model' appeared.

$$\max\left[\underline{e}, \underline{of}\right] \tag{1.1}$$

Subject to
$$\underline{s} \leftarrow T_s(\underline{x}, \underline{pd}) \quad \text{(process model)} \tag{1.2}$$

$$\underline{p} \leftarrow T_p(\underline{x}) \quad \text{(property model)} \tag{1.3}$$

$$\underline{q} \leftarrow T_q(\underline{p}, \underline{s}, \underline{u}) \quad \text{(quality model)} \tag{1.4}$$

$$\underline{c}_m \leftarrow T_{cm}(\underline{x}, \underline{pd}) \quad \text{(cost model)} \tag{1.5}$$

$$\underline{P}_{prms} \leftarrow T_{prms}(\underline{q}; \underline{Y}) \quad \text{(pricing model)} \tag{1.6}$$

$$\underline{e} \leftarrow T_e(\underline{c}_m, \underline{c}_{nm}, \underline{P}_{prms}) \quad \text{(economic model)} \quad (1.7)$$

$$\underline{c}^L \leq f\left(\underline{p}, \underline{s}, \underline{u}, \underline{x}, \underline{pd}, \underline{q}, \underline{c}_m, \underline{c}_{nm}, \underline{P}_{prms}\right) \leq \underline{c}^U \text{(constraint)} \quad (1.8)$$

Moreover, since only using mathematical models and heuristics cannot perform chemical product design effectively, the usage of other methods or tools are necessary. Conte et al.[17,18] developed a systematic methodology which integrates computer-aided tools and experimental testing for designing liquid formulated products such as water-based insect repellent and waterproof sunscreen. Mattei et al.[19] expanded the methodology to emulsion-based formulated product. In addition, Korichi et al.[20] presented a multi-level molecular knowledge framework where various databases were utilized to generate new ingredients. Based on these studies, it can be found that in addition to mathematical models and heuristics, databases, experiment, and tools can still be applied for different product design activities (i.e., correlating the boxes in Figure 1.3). Thus, upon the Grand Product Design model proposed, the arrows which are described as relationship models (i.e., arrows in Eq. 1.1-1.8) were considered to include mathematical model, heuristics, databases, tools, and experiments. Moreover, all the design activities are generally inter-correlated directly or indirectly. From this perspective, there is no need to add arrows. However, considering the messy interactions, it is impractical to cover all the possible interactions simultaneously for designing new products. Typically, the importance of certain arrow varies for different products. For instance, the arrow from microstructure to quality is critical for die attached adhesive, instead of detergent. Since the quality of the adhesive greatly depends on the microstructure of metal particles in the polymeric matrix. However, the quality of detergent is significantly by ingredient properties. In this case, the identification of the most critical design activities and most important interactions are highly desired. Thus, the arrows added in the Grand Product Design model should account for the direct and significant interconnections among various design activities. For designing a specific product, some arrows are definitely worth to consider while others are not influential.

Despite the great improvement of the Grand Product Design Model in the year 2015, it is worth to noting that the box 'other factors' was added to emphasize that other factors (e.g., sustainability, government policy, supply chain, etc.) still have great impacts on product design and development. The variable '$\underline{of}$' in Eq. 1.1 was temporarily used as an objective function to denote their impacts. However, at that time the exact impacts of these factors were not clear yet. It was suggested that their influences should be explicitly studied in the future. Therefore, another extensions for the Grand Product Design Model are highly desired.

1.2.Motivations and Thesis Structure

This thesis aims to investigate how the five business and management factors (i.e., government policy, corporate social responsibility, supply chain, sustainability, and human senses) can affect the product design and development. In other words, based on the original Grand Product Design Model published in 2015, this thesis should properly integrate the five boxes into the original model. Arrows should be added to represent how each new box can be correlated to others. Moreover, appropriate methods must be developed to tell when and how these factors can be explicitly considered for new product design.

In chapter 2, a multi-objective optimization framework that considers the influence of government policy on product design is presented. The government policy affects product design in the form of financial and non-financial incentives, and regulations. The consumers affect product design by their purchase behavior that is in turn influenced by price, product quality, and the presence of competing products. The company responds to these influencing factors to design a product with as high a profit as possible while satisfying corporate social responsibility. Different models as well as rule-based methods –quality, consumer utility, product demand, product cost, capital budgeting, social indices, and government policy –are presented. A solar photovoltaic case study is used to illustrate the framework.

In chapter 3, a new product design framework is presented with the simultaneous consideration of make-or-buy analysis and supplier selection. Consumer preferences are first identified. Product ingredients are classified into different types based on their functionalities. For each ingredient type, potential ingredient candidates are generated from material databases or predictions using computer-aided tools. Heuristics and models (e.g., statistical, empirical, and mechanistic) are used to screen the ingredients and to design a process to manufacture a product with the desired product quality. Then, product price and market demand are determined by using a pricing model. After this, make-or-buy decisions are made through heuristics and suppliers are selected to maximize the profit. Two case studies consisting of light duty liquid detergent and controlled release granular herbicide are provided to illustrate the framework.

In chapter 4, a systematic framework is proposed for sustainable chemical product design. The product technical requirements are first identified as design constraints. Then, a base-case product is generated as a reference on top of which a more sustainable product is designed. To do so, the life cycle of base-case product (in particular, whether and how it should be recycled) is decided by using life cycle sustainability assessment (LCSA) or rule-based methods depending on the availability of life cycle inventory data. In addition, the hotspots (i.e., life cycle stages with major impact) are identified. Afterwards, to reduce the impact on hotspots, product design targets and design alternatives are generated using knowledge-base and heuristics. Lastly, LCSA or rule-based methods is applied to decide the most sustainable product from the generated product design alternatives. Two case studies – composite bumper beam and lithium ion battery – are provided to illustrate the framework.

In chapter 5, the Grand Product Design model is expanded as a generic approach to food product design and the influence of human senses on food product quality is studied. To expedite the development of new food products, a hybrid machine learning and mechanistic modeling approach is proposed. Sensorial ratings are predicted using a machine learning model trained with historical data for the food under consideration. The approach starts by identifying a set of food ingredient candidates and the key operating conditions in food processing based on heuristics, databases, etc. Food characteristics such as color, crispness, and flavors are related to these ingredients and processing conditions (which are design variables) using mechanistic models. The desired food characteristics are optimized by varying the design variables to obtain the highest sensorial ratings. To solve this grey-box optimization problem, genetic algorithm is utilized where the design constraints (representing the desired food characteristics) are handled as penalty functions. A chocolate chip cookie example is provided to illustrate the applicability of the hybrid modeling framework and solution strategy.

Finally, a brief summary of this work is provided and a few recommendations for future work is represented.

Chapter 2: Product Design: Impact of Government Policy and Consumer Preference on Company Profit and Corporate Social Responsibility

2.1.Introduction

Due to increasing global competition, it is a constant struggle for chemical companies engaging in commodity chemicals to maintain a sufficiently high profit margin.[21] In response to this challenge, the chemical processing industry as a whole has been expanding from a primarily process-centric industry towards a more product-centric one.[22,23] Although this shift has slowed down recently because of the availability of shale gas, different types of product development projects are currently being implemented by many companies.[3] According to the DuPont Data Book,[24] 1643 new products were commercialized in the year 2015 and 31% of sales were derived from products launched in the previous four years. To succeed in product development, the collaboration of personnel from R&D, engineering, marketing, finance, and business development is crucial.[1,4,25]

Product development involves different tasks such as project management, marketing, research and design, and so on spread out in three phases: product conceptualization, detailed design & prototyping, and product manufacturing and commercialization.[26,27] After over two decades of research on chemical product design, much is known for handling these tasks effectively. For instance, Smith and Ierapepritou[23] used conjoint analysis to select product composition and process operating conditions so that consumer utility is maximized. For a similar objective, Lee et al.[28] proposed a knowledge-based ingredient formulation system to facilitate the communication between the sales personnel and formulators so that the most popular formulations are offered to the consumers. The methods for formulating a wide variety of chemical products ranging from fuel additives to refrigerants have been developed.[16,29-32] The integration of product and process design has also attracted much interest.[8-10,33,34] An interesting example is the approach proposed by Bernardo and Sarariva[16] that treats a product design problem as the inversion of three design functions: quality, property, and process functions. Product pricing is an important task in product commercialization. Bagajewicz[11] derived a pricing model that relates product price to product quality, the consumers' familiarity of the product, and the price and quality of competing products on the market. This model has been applied in the design of various products such as disinfectant, wine, and skin lotion.[12-14,35] Based on this pricing model, Chan et al.[36] proposed a new framework to systematically determine the model parameters for a completely new or an existing but improved chemical product. Recently, Fung et al.[2] proposed the Grand Product Design Model which shows how the key issues in product development (e.g., ingredient selection, process design, product quality, product cost, and the economics of a product development project, etc.) are interconnected. It was pointed out that government policies and corporate social responsibility should be considered alongside profit analysis. However, how these two factors influence product development has not been elaborated. Thus, these two issues are explicitly considered in this work.

The impact of government policies, in the form of regulations and incentives, on product development is shown in the expanded Grand Product Design Model (Figure 2.1). The 'Government policy' icon and the 'Policy model' have been newly added. Government regulations can prohibit the use of certain chemicals because of environmental and safety concerns. This is captured by the policy model on the top-left corner of Figure 2.1. The ban on DDT (dichloro-diphenyl-trichloroethane) as a pesticide and the phasing out of phosphates in detergents are classic examples. Regulations can also influence plant design. For example, regulations can dictate how a waste stream should be treated in a chemical plant. The incorporation of regulatory requirements into product design drives the implementation of eco-design and shortens the time to market.[37]

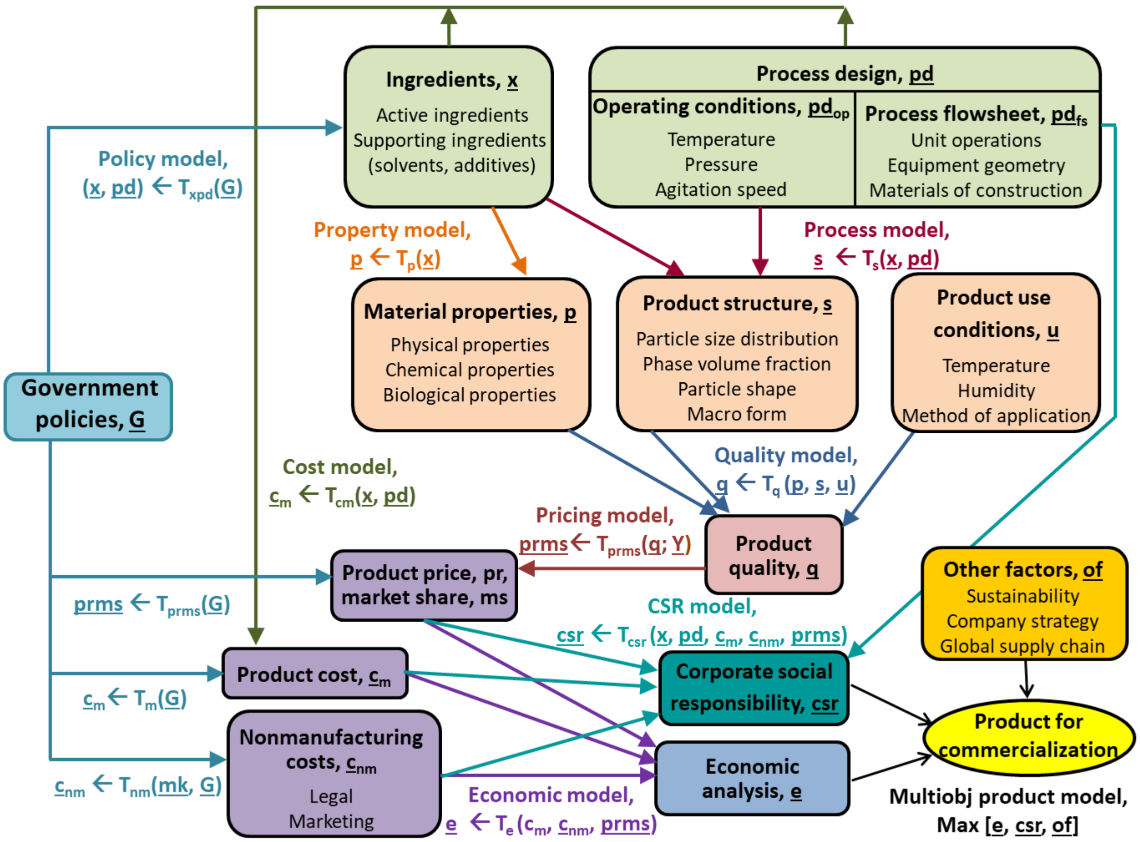


Figure 2.1 An expanded Grand Product Design Model for decision making in product development

Government incentives can provide the required financial or non-financial resources (such as subsidy, information, product promotion, etc.) for product development.[38] These are captured by the three relationships linked to the Government policies icon at the bottom-left of Figure 2.1. Most of these incentives are designed to invigorate the local economy.[39] For instance, the US government would procure solar panels manufactured in the US for local job creation. You et al.[40] considered the impact of government production and construction incentives on choosing the location for the development of cellulosic biofuel. Moreover, another influencing factor on product development is the increasing adoption of corporate social responsibility (CSR) with which a firm advances social good that goes beyond the firm's financial interest and what is required by law.[41,42] Thus, as shown in Figure 2.1, another icon 'Corporate social responsibility' and the 'CSR' model have been newly added. Clearly, whether the targets of CSR are achieved depends on the various decisions made during product development.

In this study, the impact of government policy on product development is explicitly considered from the company's perspective. In developing a new product, ingredients and processes are identified to provide a product with the desired quality. In addition, decisions on product price, marketing strategy, labor force, etc. should be made. The problem we aim to solve as follows. Given different government policies how decisions should be made for the company to make profit and achieve CSR. Note that as CSR covers very broad environmental and social performance, only certain key aspects are considered in this study.

The chapter is organized as follows. First, the way in which the government, company, and consumer interact is elucidated. Then, various models for product design such as product quality, consumer utility, and demand that account for these interactions are presented. Based on these models, a multi-objective optimization framework is developed to quantify the trade-off between profitability and CSR for a given set of government regulations and incentives. Finally, a solar photovoltaic case study is discussed to illustrate the application of the developed framework.

2.2. Government-Company-Consumer Interactions

Three stakeholders, namely government, company, and consumer, interact with one another in product development as shown in Figure 2.2. Government launches various incentives and regulations to improve the quality of life, to keep the society competitive, and to ensure the safety of its citizens. Company aims to carry out product development projects to satisfy the needs and wants of consumers at a profit, while being socially responsible. Consumers primarily look for products that meet their needs and wants at the lowest price. These behaviors are detailed below.

2.2.1. Government Policy

Government incentives can be broadly classified into two groups: Product Creation (PC) and Market Creation (MC). The former are the incentives that are used for developing new products or upgrading existing ones. The latter are used to open up market for the product being developed. The incentives can also be classified as financial or non-financial. The financial incentives can be

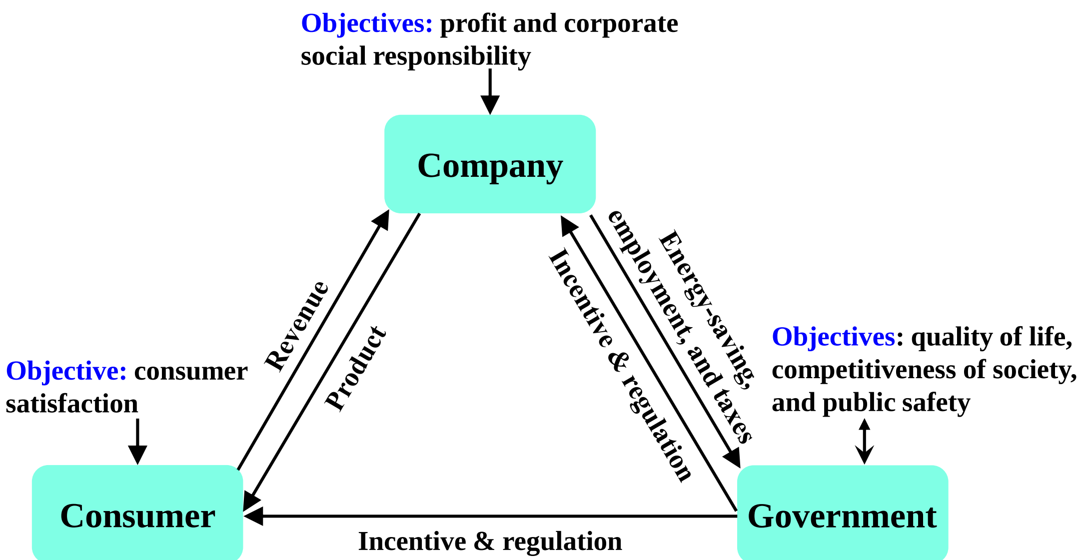


Figure 2.2: The government-company-consumer relationship triangle

given to the company or consumer through direct payment or tax reduction. All financial incentives are countable in monetary terms. Non-financial incentives are hard to count in monetary terms and include the provision of free information, technical expertise, and network to the company to spur product development. Table 2.1 shows several examples of government incentive programs thus classified. For example, a government can offer an R&D grant to a company to develop a new product. Alternatively, a government can train workers for a specific industrial sector so that companies can benefit from the availability of a suitable workforce in a timely manner.

In general, only firms benefit from PC incentives. The impacts of various PC incentives on product development are given in the top two rows in Table 2.2. For instance, R&D funding, seed capital, funding for purchasing technology and equipment, and availability of a technical

Table 2.1 The classification of various government incentive programs

	Financial	Non-financial
Product Creation	• R&D grant and tax rebate • Seed capital • Funds for purchasing technology & equipment	• Provision of land, professionals by immigration and education, etc. • Cooperation and consultation with public research centers and universities • IP protection
Market Creation	• Consumer subsidy and tax rebate • Government procurement	• Product promotion, information exchange, tradeshow, and advertisement • Public guarantee • Government sponsored worker training • Infrastructure development

community for consultation and cooperation are all conducive to the development of high-quality and low-cost products. Non-financial PC incentives such as provision of land and channels for professional immigration can help reduce manufacturing as well as nonmanufacturing costs.

MC incentives can be given to company or consumer to open up the market so as to accelerate the achievement of economies of scale. The impacts of different MC incentives are given in the bottom two rows of Table 2.2. For example, government procurement can lead to a substantial increase in product demand. The government can also provide subsidy to consumers to buy a type of product it favors. Similarly, many non-financial MC incentives such as free promotion, public guarantee, and worker training can help reduce nonmanufacturing costs (e.g., marketing expenses) and increase product demand.

Such incentive schemes are available in almost all the economies in the world. Example schemes in Germany, Hong Kong, Singapore, and the United States are listed in Table 2.3. Table A2.1-A2.4 in the Appendix offer a brief description of these government incentive programs to validate the incentive classification scheme and impact analysis in Table 2.1 and 2.2, respectively. For example, the feed-in tariff (FIT) in Germany was launched to kick-start the adoption of solar photovoltaic (PV) as a means to replace fossil fuels by renewable energy (Table A2.1). In the past decade, about 1.5 million PV systems have been installed in Germany and the price has dropped by more than 70%. Another example is the Innovation & Technology Fund (ITF) set up by the Hong Kong government in 1999 to provide research funding to companies and universities to conduct R&D (Table A2.2). With the government funding, the companies can reduce the R&D expenses and develop new technologies to upgrade the products. The Singapore government launched the TradeXchange initiatives through which businesses can efficiently exchange the supply-demand information to facilitate product logistics (Table A2.3). This program can increase product demand by avoiding unnecessary out-of-stock or shortage and reduce supply chain costs.

Table 2.2 Impact of each government incentive listed in the Table 2.1

	Government incentives	product quality	product utility	product demand	manufacturing cost	nonmanufacturing cost
Product creation financial	R&D grant and tax rebate	↑				↓
	Seed capital	↑			↓	↓
	Funds for purchasing technology & equipment	↑			↓	
Product creation non-financial	Provision of land, professionals, etc.				↓	↓
	Cooperation & consultation	↑				
	IP protection				↓	
Market creation financial	Consumer subsidy and tax rebate		↑	↑		
	Government procurement			↑		
Market creation non-financial	Promotion, information exchange, tradeshow, and advertisement			↑		↓
	Public guarantee			↑		
	Government sponsored worker training					↓
	Infrastructure development					↓

↑: upward arrow means increase; ↓: downward arrow means decrease

Table 2.3 Government incentive programs in various economies

		Germany	Hong Kong	Singapore	United States
Product creation	Financial	ERP	ITF	RISC	SBIR
	Non-financial	PG	R&D centers	WSQ	CRADA
Market creation	Financial	FIT	GSP	DTD	CPG
	Non-financial	BAFA	BDP	TXC	FEMP

Lastly, the Cooperative Research & Development Agreements (CRADA) program developed by the United States government provided joint collaborations between government agencies and private companies to speed up the commercialization of high-quality products (Table A2.4). Note that different economies may provide the same type of incentive albeit to different extents. The information is of interest to companies interested in choosing a production site in different countries and can be obtained from the government official documents and websites. For instance, as listed in Table A2.1, the details of Germany's feed-in tariff program is available on the website labelled a3. China offers a similar program and the tariff rate can be found on the Chinese official website.[43]

In addition to incentives, the development of new products can be initiated by regulations. For instance, to replace the phosphate-based materials to handle hard water, detergent manufacturers have introduced zeolite A-polycarboxylate and sodium citrate, which are not fertilizers.[44]

2.2.2. *Company Decision Making*

A firm's main objective is to earn profit for its shareholders. This requires the participation of stakeholders at all organizational levels.[27] The R&D department is responsible for identifying new products and processes. The business unit formulates a business plan that includes product specifications, estimated product cost, projected product demand, necessary financial and human resources, and considerations of government incentives and regulations. Then, decision makers at the corporate level decide whether and how to implement the product development project to maximize profit, and how to fulfill CSR. To date, firms, either initiated by management voluntarily or nudged along by the government and consumers, are more likely to devote considerable time, effort, and money to serve society. These can include donation to charities, and building a plant at a certain location to provide job opportunities to the locals.

2.2.3. Consumer Decision Making

Consumers make purchase decisions to meet their needs based on their preferences and product price. In microeconomics, this consumer behavior is captured by the maximization of a utility function in which a rational consumer buys the product that offers maximum satisfaction from a set of alternatives subject to a limited consumer budget. Government incentives such as reduced sales tax and cash payment can significantly influence consumers' purchase decision. For instance, the California's Clean Vehicle Rebate Project offered an over $2000 subsidy in the form of tax rebate to electric vehicle buyers. The impact on sales can be very significant. Consider the tax credit and sales of Tesla in Hong Kong. With the tax exemption provided by the Hong Kong government, consumers only need to pay the effective price of HK$72,900 for the Model S. However, after the tax credit was stopped in April 2017, consumer must pay the effective price of HK$118,400 for the same Model S. After the cancellation of tax credit, the Tesla first-time registration fell from 2939 in March to zero in April.[45] A similar drop in sales occurred in the U.S. The end of a $5,000 Georgia state tax credit sent EV sales down 90% over the course of a year.[46]

2.3. Multi-objective Optimization Formulation

A multi-objective optimization model for product development that accounts for the government, company, and consumer interactions, which is a subset of the Grand Product Design Model, is presented below. A company maximizes its profit for a new product development project in terms of the net present value (*NPV*) and CSR in terms of a composite social index (*SI*) in Eq.

2.1. This optimization model has nine supporting models. *NPV* is calculated in capital budgeting in Eq. 2.2. *SI* is evaluated in Eq. 2.3 based on the decisions on the ingredients ($\underline{x}$), the manufacturing process ($\underline{pd}$), labor ($\underline{la}$), waste treatment ($\underline{wt}$), marketing activities ($\underline{mk}$), product price ($\underline{pr}$), and R&D activities ($\underline{rd}$). Note that the price can be considered as a vector because price may vary in different geographical regions and demographics based on the pricing strategy.[36] Moreover, government policy ($\underline{G}$) is given and Eq. 2.4 shows how company management should consider the utilization of known government incentives for product and market creation ($\underline{IC}_{PC}$ and $\underline{IC}_{MC}$) and comply with government regulations ($\underline{G}_r$). Meanwhile, Figure 2.3 is a refined version of Figure 2.1 focusing on the impact of government policies. Based on the analysis in Table 2.2, the dotted lines show how government policies can explicitly affect various aspects ranging from material selection to market demand. Note that all the involved variables are consistent with the ones in the Grand Product Design Model in Figure 2.1. If a variable is not underlined such as market size (Y) and demand (d), it is a scalar. An underlined variable can be a vector such as a list of product qualities ($\underline{q}$) or labor costs for different workers ($\underline{la}$). It can also represent a composite variable such as a manufacturing plant ($\underline{pd}$) or a waste treatment plant ($\underline{wt}$).

$$\text{Maximize } NPV,\ SI \qquad (2.1)$$

Subject to

$$NPV \leftarrow T_e(pr, d, \underline{c}_m, \underline{c}_{nm}) \qquad \text{(Economics)} \qquad (2.2)$$

$$SI \leftarrow T_s(\underline{x}, \underline{pd}, \underline{la}, \underline{wt}, \underline{mk}, pr, \underline{rd}) \qquad \text{(CSR)} \qquad (2.3)$$

$$\underline{G} \leftarrow [\,\underline{G}_r, \underline{IC}_{PC}, \underline{IC}_{MC}] \qquad \text{(Government policy)} \qquad (2.4)$$

$$[\underline{x}, \underline{pd}] \leftarrow T_{xpd}(\underline{G}_r) \qquad \text{(Materials \& Processes)} \qquad (2.5)$$

$$\underline{q} \leftarrow T_q(\underline{x}, \underline{pd}, \underline{rd}, \underline{IC}_{PC}) \qquad \text{(Quality)} \qquad (2.6)$$

$$pu \leftarrow T_{pu}(\underline{q}, \underline{pr}, \underline{IC}_{MC}) \qquad \text{(Utility)} \qquad (2.7)$$

$$d \leftarrow T_d(pu, \underline{pu}_c, \underline{mk}, Y, \underline{IC}_{MC}) \qquad \text{(Demand)} \qquad (2.8)$$

$$\underline{c}_m \leftarrow T_m(\underline{x}, \underline{pd}, \underline{la}, \underline{wt}, \underline{G}_r, \underline{IC}_{PC}) \qquad \text{(Manufacturing costs)} \qquad (2.9)$$

$$\underline{c}_{nm} \leftarrow T_{nm}(\underline{mk}, \underline{rd}, \underline{IC}_{PC}, \underline{IC}_{MC}) \qquad \text{(Nonmanufacturing costs)} \qquad (2.10)$$

$$\underline{c}^L \leq f\left(\underline{x}, \underline{pd}, \underline{la}, \underline{wt}, \underline{mk}, pr, \underline{rd}\right) \leq \underline{c}^U \qquad \text{(Bounds)} \qquad (2.11)$$

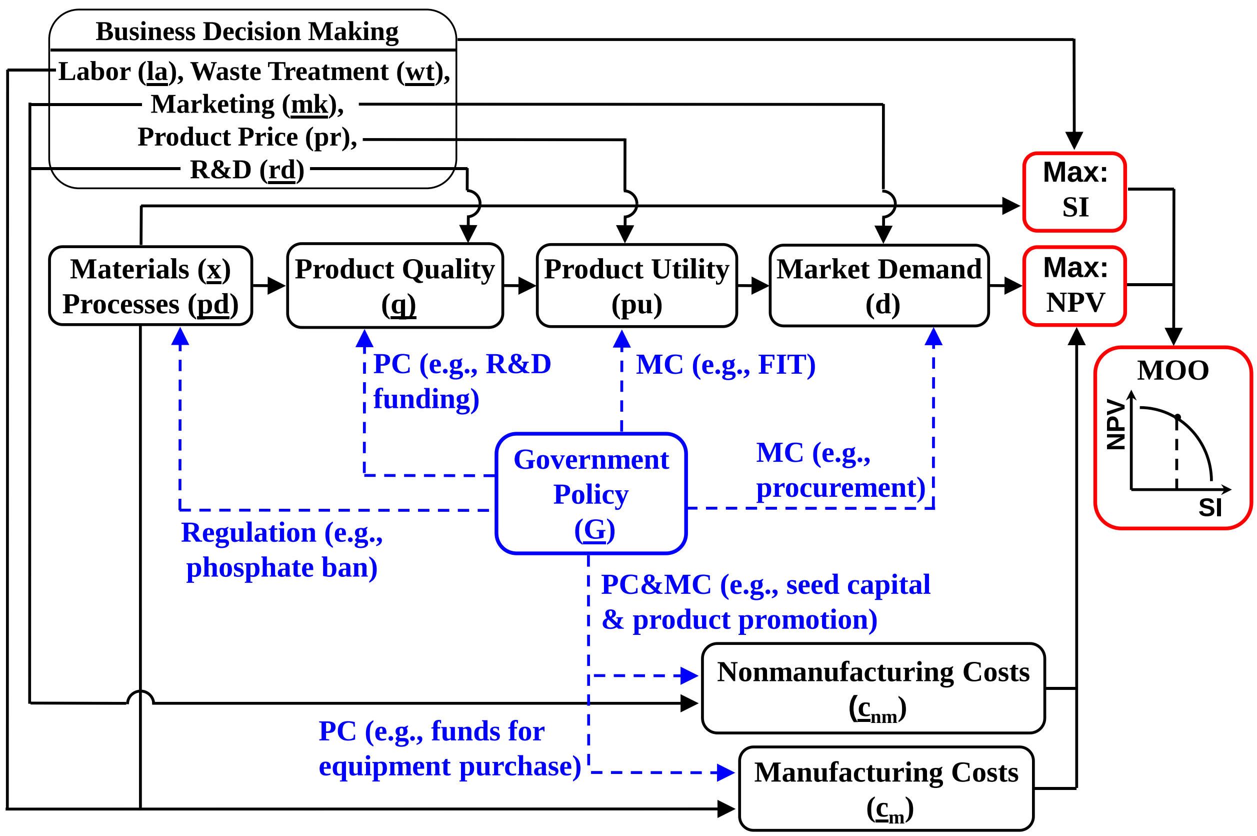


Figure 2.3: Multi-objective optimization framework for business decision making

The supporting models are shown as relationships with an arrow ← instead of an equal sign, which signifies an equation. This emphasizes the fact that the dependent variable (LHS) is determined from the independent variables (RHS) using rule-based methods such as heuristics, model-based methods such as heat and mass transport equations, databases, tools, and experimental results. In this work, heuristics are first used to reduce the relationships to equations, which are then solved using optimization software.

For the new product, material selection and process design are regulated by government regulations in Eq. 2.5 such as the DDT and phosphates examples. In other words, Eq. 2.5 can be interpreted as the constraints on material selection and process design. Additionally, certain product quality as given in Eq. 2.6 should be achieved. Eq. 2.7 shows the dependency of product utility (pu) on consumers' satisfaction of the product. There are two types of utility functions: direct utility function and indirect utility function. The former is a function of the amount of consumed products such as the Cobb-Douglas utility function while the latter is a function of quality and effective price.[47-49] Since indirect utility directly reflects consumer preferences, it is used in this study (Eq. 2.7). Given the market size and competitors' utility ($\underline{pu}_c$), market demand is determined in Eq. 2.8. Furthermore, the manufacturing cost (c_m) is calculated by adding the related costs (e.g., material cost, operational cost, etc.) in Eq. 2.9. The non-manufacturing cost ($\underline{c}_{nm}$) consisting of marketing and R&D expenditures is obtained in Eq. 2.10.

In principle, all the variables in this multi-objective optimization problem can change. For example, market size can vary from time-to-time and is influenced by many factors such as economic conditions, population, social trends, marketing activities, etc.[50] However, to make sure that the model is tractable and to emphasize the importance of government policy and corporate social responsibility, it is assumed that the market size is fixed. These support models are now discussed below:

2.3.1. Quality Model

Eq. 2.6 shows the relationship of product quality to materials, processing, R&D activities, and PC incentives that provide extra resources for R&D to further improve product quality. Often, product quality is described by qualitative attributes such as stability, effectiveness, durability, pleasant to consume or use, aesthetics, and ease of use. These attributes can be transformed into quantitative product specifications, such as physicochemical properties (e.g., viscosity, conductivity, etc.) or specifications regarding the product itself (e.g., product form, product structure, ingredient compositions, etc.). These specifications depend on the materials used in the product and the manufacturing processes. Most of all these technical decisions are made in the R&D phase. Therefore, proper R&D activities should be carried out for obtaining the proper materials and processes to achieve the desired quality.

2.3.2. Utility Model

Eq. 2.7 shows that product utility depends on product quality, price, and some MC incentives which can reduce the effective price the consumer pays.[48] Product utility is decided by the consumer's perception and each consumer has a different perception. Thus, it is necessary to treat the product utility as uncertain. From the researcher's perspective, only a fraction of factors (e.g., price and quality) can be observed to influence consumer purchasing behavior and there exists other unobserved attributes.[51] Therefore, the uncertainty of product utility mainly originates from those unobserved attributes, instead of the observed attributes. Bearing this in mind, the utility of a particular product is decomposed into a representative utility (υ) and a random utility (ε) in the random utility theory (Eq. 2.12a).[52]

$$pu = \upsilon + \varepsilon \tag{2.12a}$$

Here, υ is an average value of product utility taken over all consumers and is a function of product quality, price, and MC incentives. By following the example from Train,[51] Eq. 2.12b expresses a simple linear expression of υ but it can be replaced by any other appropriate relationships.

$$\upsilon = a_\upsilon + \underline{b}_\upsilon \cdot \underline{q} - c_\upsilon \cdot pr + \underline{d}_\upsilon \cdot \underline{IC}_{MC} \tag{2.12b}$$

where a_υ, $\underline{b}_\upsilon$, c_υ, and $\underline{d}_\upsilon$ are utility coefficients that can be determined through fitting of historical sales data from market reports. For a completely new product without historical sales data, consumer preferences have to be obtained through market survey to determine the utility coefficients. This approach has been investigated by Smith and Ierapepritou.[23] ε represents the deviation of a particular consumer's utility from the average value. Considering its random nature, ε is described by a probability density function, $g(\varepsilon)$, such as that given in Eq. 2.12c. This distribution was proposed by McFadden[53] to derive the easily applicable consumer demand model: the logit model. Integration of $g(\varepsilon)$ gives the cumulative distribution function, $G(\varepsilon)$, in Eq. 2.12d.

$$g(\varepsilon) = e^{-\varepsilon} e^{-e^{-\varepsilon}} \tag{2.12c}$$

$$G(\varepsilon) = \int_{-\infty}^{\varepsilon} g(\varepsilon) d\varepsilon = e^{-e^{-\varepsilon}} \tag{2.12d}$$

2.3.3. Demand Model

Eq. 2.8 shows the dependence of product demand on product utility, utilities of competitors' products, marketing activities, market size, and certain MC incentives. Many demand models have been proposed in the literature.[11,51] One of the most used demand model is the logit model which calculates the likelihood that a consumer buys a certain product or not. The model is derived based on the analysis of an individual's purchasing behavior and the statistical data of population behavior. The detailed derivation is shown below. First, the probability P_a that a consumer buys the product *a* instead of competing products such as product *c* is formulated as follows:

$$P_a = P(pu_a > pu_c, \forall c) = P(\varepsilon_c < \varepsilon_a + \upsilon_a - \upsilon_c, \forall c) \tag{2.13}$$

where υ_a and υ_c can be calculated by Eq.2.12b. Assuming that ε follows the distribution expressed in Eq. 2.12c and that each consumer has the same distribution for ε, the probability P_a can be calculated by substituting $(\varepsilon_a + \upsilon_a - \upsilon_c)$ into Eq. 2.12d,

$$P_a(\varepsilon_a) = \prod_c e^{-e^{-(\varepsilon_a + v_a - v_c)}} \tag{2.14a}$$

Since ε_a is a random distribution, P_a is equal to the integral over all values of ε_a (namely Eq. 2.12c).

$$P_a = \int_{-\infty}^{\infty} \left(\prod_c e^{-e^{-(\varepsilon_a + v_a - v_c)}}\right) \cdot g(\varepsilon_a) d\varepsilon_a \tag{2.14b}$$

Finally, the solution for P_a is independent of ε_a as shown below[51]

$$P_a = \frac{e^{v_a}}{e^{v_a} + \sum_c e^{v_c}} \tag{2.15}$$

The market demand for product a is the product of P_a and market size. As stated before, marketing activities and the corresponding market size are considered to be fixed here. In conclusion, as indicated in Eq. 2.12b, the representative utility v_a and v_c depend on quality and price and thus demand is also a function of product quality, price, and market size.

$$d = \frac{e^{v_a}}{e^{v_a} + \sum_c e^{v_c}} \cdot Y \tag{2.16}$$

2.3.4. Cost Model

Manufacturing costs consist of material cost, processing cost, labor cost, and other costs such as rent, and utilities. As shown in Eq. 2.9, government regulations and PC incentives can also affect manufacturing costs. The nonmanufacturing costs which include marketing and R&D expenses are influenced by marketing strategies, such as advertisement media and expenditure, and R&D activities (Eq. 2.10). Many PC and MC incentives can be exploited to reduce nonmanufacturing costs. For instance, an R&D grant from the government can help pay for R&D costs while free promotions contribute to a reduction in marketing cost.

2.3.5. Objective Function

Two objectives are considered in this study. The first is maximization of profit. This is quantified by the NPV calculated in capital budgeting,

$$NPV = \sum_{j=-n}^{m} \frac{PCF_j}{(1+R)^j} \tag{2.17}$$

where R, n, and m represent the discount rate, the number of years for product design and facility construction, and the number of years of factory life, respectively. PCF_j is the project cash flow in the jth year:

$$PCF_j = \begin{cases} -TDC_j - TCI_j & j \leq 0 \\ (pr_j - c_{m,j} - c_{nm,j}) \cdot d_j \cdot (1 - tax) + tax \cdot De_j - \Delta NWC_j & j > 0 \end{cases} \tag{2.18}$$

Before manufacturing starts ($j \leq 0$), PCF_j includes total development cost (TDC_j) and total capital investment (TCI_j). After product sales starts ($j > 0$), PCF_j is obtained by subtracting from the revenue ($pr_j \cdot d_j$), the manufacturing cost ($c_{m,j} \cdot d_j$), nonmanufacturing cost ($c_{nm,j} \cdot d_j$), tax after adjusting for depreciation, and the increase in net working capital (ΔNWC_j). De_j is the capital depreciation at year j.

The second objective is CSR that includes donation to charities, reduction in greenhouse gas emission, potential of damage to ozone, job creation, employee training, and so on. In this study, CSR is quantified as a composite social index (SI), a weighted sum of various normalized indicators of environmental and social performance.[54]

$$SI = \sum_s w_s \cdot I_s^N \tag{2.19}$$

$$I_s^N = \frac{I_s}{I_s^B} \tag{2.20}$$

where w_s is the weighting factor for the sth normalized indicator I_s^N. I_s and I_s^B are the values of the sth indicator and the corresponding benchmark, respectively. Note that as many indicators as necessary can be included in the composite index.

Benchmarks represent the performance of other companies, or government requirements. Indicators may account for positive or negative impacts on SI. For instance, for achieving a large

SI, energy consumption should be reduced while accrued jobs are to be increased. Thus, for these indicators having positive impacts, the corresponding weighting factors are numerically positive while others are negative. Irrespective of the different impacts of indicators, I_s^N takes on a positive value.

The weighting factor representing the importance of an indicator can be obtained from expert opinions, survey, and communication with policymakers while the indicators themselves can be selected from the Global Reporting Initiatives.[55] The indicators that are considered for CSR include materials consumption, energy consumption, total water withdrawal, reduction of greenhouse gas (GHG) emissions, total number of employee hired, average hours of training, benefits provided to full time employees, etc. The selected indicators are in turn quantified by different methods such as life cycle assessment (LCA).[56-58] Normally, the availability of data and the precision requirement determine which method should be selected.

Two caveats should be pointed out regarding the use of a composite index in Eq. 2.19. One is whether or not the use of a composite index is acceptable. The pros and cons of using a composite index has already been discussed in detail.[54] For instance, a poorly constructed composite index may send misleading messages. However, the obvious advantage is that it can succinctly represent complex, multi-dimensional issues with a single metric. Despite their imperfection, complex indices are widely used to support decision-making in many fields such as corporate social responsibility with the Social Index,[59,60] environment with the Environmental Performance Index[61] and the Eco-indicator 99,[62] economy with the Composite Leading Indicators,[63] social science with the Human Development Index,[64] etc. Another point of contention is how the weighting factors should be determined. Clearly, different weighting factors in Eq. 2.19 can lead to different values of the social index and thus different decisions. In general, while it is straightforward to assign a value to each of the weighting factors, it is difficult to fix them with certainty and consensus since each decision maker may have a different view of the relative importance of the various indicators.

2.3.6. Solution Method

For multi-objective optimization, various methods have been employed to generate the Pareto-optimality such as weighted sum method, ε-constraint approach, and genetic algorithm.[65] Due to its ease of use, the ε-constraint approach is used here. The basic idea is to convert one objective function into an inequality constraint and then perform multiple single objective optimization. When NPV is considered as the primary objective, SI is transformed into constraints. The solution procedure is as follows. (1) Maximize NPV without the consideration of SI to determine the lower bound of SI. (2) Maximize SI to get its upper bound. (3) Fix a series of ε to divide the range of lower and upper bounds into several identical intervals (e.g., 20 intervals in this study). (4) Add a series of constraints $SI \geq \varepsilon$ to the model and maximize NPV to get the points for the Pareto front as shown below.

$$\max \quad NPV \tag{2.21}$$

s.t. Eq. (2.2-2.11)

$$SI \geq \varepsilon \tag{2.22}$$

2.4. Case Study – the Solar Photovoltaic Industry

In this section, decision making at a monocrystalline silicon PV module company is discussed to highlight the application of the multi-objective optimization framework. At present, silicon-based PV accounts for over 85% of market share because of its high efficiency and long lifespan. Since PV has been recognized to be one of the key renewable energies, it has received a great deal of support from governments around the world. Table 2.4 lists selected PV incentive programs in different economies. For example, the Chinese government has implemented a national feed-in tariff (FIT) since 2011. Under this scheme, fixed tariffs are offered to households for generating electricity from PV for a long period of time. From the official website, we can find that the tariff rate (S_F) is set by the Chinese government to be 0.15 $/kWh and the timespan T_F is 20 years.[43] Note that if this case study will be expanded to another country such as Germany, similar data for the years 2004-2014 in Germany can be found in reference a3 in Table A2.1.

Table 2.4 PV related incentive programs in different countries

Country	PV Incentive programs
Australia	Feed-in tariff, subsidies for large-scale solar power stations
Canada	Feed-in tariff, subsidies for taxation, and IP protection
China	R&D grants, interest subsidies, feed-in tariff
France	Feed-in tariff, tax exemption, green loans
Germany	Feed-in tariff, tax exemption
Spain	Feed-in tariff
United States	renewable portfolio standard, production tax credit

Consider a firm that plans to invest up to 300 M$ to manufacture silicon-based PV modules. The money should cover capital investment and net working capital. To focus on the variations of business decision making, the manufacturing process is assumed to be sufficiently mature and is fixed. Therefore, PV quality and manufacturing cost are fixed as well. The company decision makers must decide whether the project should proceed and how much money should be invested. If the project moves forward, several business decisions have to be made: PV module price (pr), the percentage of wastewater to be reused (WR), salary ratio (SAR), and whether to take advantage of the government's R&D and promotion incentive schemes. These design variables influence both profit and CSR. All the input parameters as well as their sources are given in Table 2.5.

Table 2.5 Input data in the case study

Parameter	Symbol	Value	Source
PV module efficiency	η	14.8%	66
PV module lifespan	T	25 years	66
Annual solar radiation	SR	1360 kWh/(m^2·year)	67
Performance ratio	λ	0.85	68
Degradation rate	δ	0.005	68
Operational cost of PV	O_t	0 $/Wp	68
Consumer discount rate	R_c	0.07	68
FIT rate in China	S_F	0.15 $/kWh	43
FIT timespan	T_F	20 years	43
Production safety factor	f_{pc}	1.2	assumed
Number of years for factory life	m	5 years	assumed
Number of years for product design and facility construction	n	1 year	assumed
Percentage of capital depreciation	De	0.2	assumed
Price of balance of systems	p_{bos}	0.38 $/Wp	69
Installation cost	p_{it}	0.30 $/Wp	69
Utility parameter	A_{PV}	0 $/kWh	regressed
Utility parameter	A_E	6.9 $/kWh	regressed
Utility parameter	B_{PV}	31	regressed
Utility parameter	B_E	31	regressed
Diffusion demand parameter	γ	0.4	regressed
Electricity grid price	P_e	0.1 $/kWh	assumed
Market size	Y	10 GW_p/year	assumed
Material cost	c_{mat}	0.583 $/Wp	66
Utility cost	c_{ut}	0.073 $/Wp	66
Capital cost of a reference facility	c_{ref}	0.875 $/Wp	70
Production capacity of a reference facility	PC_{ref}	395 MWp	70
PV capital scaling factor	b	-0.18	71
Total volume of wastewater	V_{wt}	0.00233 m^3	72
Cost for recycling 1 m^3 wastewater	f_{wt}	0.6 $/$m^3$	73
Minimum wage in PV industry	WG_{min}	8000 $/year/people	66
Number of employees required	f_e	2.4 people/MWp/year	66
The amount of CO_2 released by CFPP	f_{co_2}	0.877 kgCO_2/kWh	74
Company discount rate	R	0.05	assumed

2.4.1. Quality Model

The quality of a PV module is characterized by its lifespan (T) and efficiency (η). Since the materials and manufacturing processes have been identified, T and η are set at 25 years and 14.8%,[66] respectively. T determines the total amount of electricity generated throughout the entire product life. η determines the annual electricity output per square meter in a given year t (EO_t in kWh/(m^2·year)). EO_t is equal to the solar radiation multiplied by the module efficiency that decreases over time because of energy loss and PV degradation.

$$EO_t = SR \cdot \eta \cdot \lambda \cdot (1 - \delta)^t, \quad t = 1, 2, \dots, T \tag{2.23}$$

where SR, λ, and δ are the annual solar radiation (in kWh/(m^2·year)), performance ratio, and degradation rate, respectively. The performance ratio λ accounts for the energy loss due to temperature variation, contamination, transmission, and so on. Note that although electricity output is expressed on a square meter basis, PV is sold on a peak watt (Wp) basis. Thus, the following equation is used to convert EO_t to E_t (in kWh/(Wp·year)).

$$E_t = \frac{EO_t}{1000 \times \eta} = \frac{SR \cdot \lambda \cdot (1-\delta)^t}{1000} \tag{2.24}$$

where E_t is the annual electricity output per peak watt in a given year t and the denominator $(1000 \times \eta)$ accounts for the number of peak watt for one square meter of PV module.

2.4.2. Utility Model

Instead of the general utility model in Eq. 2.12b, the following relationship for consumer satisfaction υ is assumed,

$$\upsilon = A_{PV} - B_{PV} \cdot LCOE \tag{2.25}$$

Here, A_{PV} and B_{PV} are the utility coefficients. $LCOE$, the levelized cost of electricity, is the ratio of the net cost after subtracting the tariffs received for the electricity produced over the lifetime of the module and accounting for the time value of money.[68] In this case study, the utility coefficients A_{PV} and B_{PV} as well as the parameters used in the following demand model are regressed by using historical *LCOE* and PV installation capacity data from 2010 to 2015 in Mainland China.[67,75-77] The details of the regression processes are described in Appendix B. Moreover, the lower the LCOE is, the more satisfied the consumer is.

$$LCOE = \frac{CI_0 + \sum_{t=0}^{T} \frac{(O_t + M_t)}{(1+R_c)^t} - \sum_{t=0}^{T_F} \frac{E_t \cdot S_F}{(1+R_c)^t}}{\sum_{t=0}^{T} \frac{E_t}{(1+R_c)^t}} \tag{2.26}$$

$$CI_0 = pr + p_{bos} + p_{it} \tag{2.27}$$

$$M_t = 0.005 \times CI_0 \tag{2.28}$$

Here, CI_0 is the consumer's initial investment which is the sum of the PV module price (pr in \$/W$_p$), price for the balance of system (p_{bos} in \$/Wp), and installation cost (p_{it} in \$/Wp). Here, pr is assumed to be bounded between 1 and 2.5 \$/Wp to ensure the optimization problem reasonable. O_t and M_t are the annual operational and maintenance cost, respectively. Since PV uses free sunlight, no fuel cost is considered. The summation of O_t and M_t is calculated as 0.5% of the initial investment. T_F, S_F, and R_c are the FIT duration, FIT rate, and consumer discount rate, respectively.

2.4.3. Demand Model

van Benthem et al.[70] proposed the following equation that is related to the logit model for calculating the market demand for PV.

$$d_j = \frac{e^{\upsilon}}{e^{\upsilon} + e^{\upsilon_E}} \cdot Y + df_j \qquad j = 1, \dots, m \tag{2.29}$$

The first term on the RHS calculates the demand for PV and is the same as that in Eq. 2.16. The utility for PV (υ) and that for electricity from the grid (υ_E) are calculated using Eq. 2.25 and Eq. 2.30, respectively.

$$\upsilon_E = A_E - B_E \cdot P_e \tag{2.30}$$

P_e is the grid electricity price. A_E and B_E are utility coefficients. The second term is the diffusion function that accounts for the adoption of PV due to contacts between existing and potential consumers. The probability of increasing the adoption is proportional to the product of the fraction of existing consumers and fraction of potential consumers as shown below.

$$df_j = \gamma \cdot d_{j-1} \cdot \left(1 - \frac{d_{j-1}}{Y}\right) \qquad j = 1, \dots, m \tag{2.31}$$

The parameter γ indicates the magnitude of diffusion. Note that at year $j = 1$, d_0 is set to 0 Wp. The utility coefficients (A_E and B_E), γ, and Y are regressed in Appendix B.

2.4.4. Cost Model

Goodrich et al.[66] reported the cost structure of silicon PV modules in China. The manufacturing cost (c_m) consists of material cost (c_{mat}), utility cost (c_{ut}), capital cost (c_{cap}), maintenance cost (c_{mt}), cost for wastewater reuse (c_{wt}), and labor cost (c_{la}) as given in Eq. 2.32. Note that all the costs are on a peak watt unit ($/Wp) basis.

$$c_m = c_{mat} + c_{ut} + c_{cap} + c_{mt} + c_{wt} + c_{la} \tag{2.32}$$

$$c_{cap} = c_{ref} \cdot \left(\frac{PC}{PC_{ref}}\right)^b \tag{2.33}$$

$$PC = f_{pc} \frac{\sum_{j=1}^{m} d_j}{m} \tag{2.34}$$

$$c_{mt} = 0.03 \times c_{cap} \tag{2.35}$$

$$c_{wt} = f_{wt} \cdot V_{wt} \cdot WR \tag{2.36}$$

$$c_{la} = WG_{min} \cdot f_e \cdot SAR \tag{2.37}$$

c_{mat} accounts for the costs of silicon feed stock, metal paste, wires, and so forth and is set to be 0.583 $/Wp. The cost of utilities (c_{ut}) is 0.073 $/Wp.[66] Eq. 2.35 shows the typical power law correlation for capital cost. c_{ref} and PC_{ref} are the capital cost and production capacity of a reference facility, respectively. The scaling factor b is set to be that of semi-conductor industry since they have similar production processes.[71] The production capacity, PC, is determined by the estimated market demand as given in Eq. 2.34. The safety factor f_{pc} which is used to ensure sufficient capacity is assumed to be 1.2. c_{mt} is assumed to be 3% of the capital cost. Moreover, the volume of wastewater (V_{wt}) generated by producing 1 Wp PV module is estimated to be $0.00233m^3$. The main pollutants include hydrogen chloride and fluoride-based chemicals. To reuse the wastewater, in addition to chemical (e.g., neutralization and precipitation) and biotreatment, ultrafiltration and reverse osmosis are needed to further purify the water so that certain purity criteria can be met. Note that although other treatment process can be employed, reverse osmosis is the widely used process in the solar photovoltaic industry. Thus, only this process is considered for simplicity. The cost of treating 1 m^3 wastewater in the reverse osmosis process (f_{wt}) is equal to 0.6 \$ and WR is the fraction of wastewater treated by reverse osmosis. The cost of treating the fraction $(1 - WR)$ of wastewater is neglected in comparison with the cost of treatment by reverse osmosis. Finally, the labor cost c_{la} is shown in Eq. 2.37. It equals to the product of the average salary of a full-time employee and the number of employees required for production (f_e). The average salary is equal to the salary ratio (SAR) multiplied by the minimum wage in this group of workers doing similar work (WG_{min}). It is assumed that the maximum wage for these workers is 50% larger than WG_{min}. Thus, SAR is bounded between 1 and 1.5.

2.4.5. Objective Function

Two objective functions are maximized: NPV and SI. NPV is calculated using Eq. 2.17-2.18, with the net working capital assumed to be 10% of the capital investment. For SI, two indicators are selected from the environmental section of the GRI framework and two from the social section. The extent of CO_2 mitigation (I_1) is chosen to be the first indicator. As given in Eq. 2.38, I_1 is the product of the amount of electricity generated by all the PV systems within their lifetime and the amount of CO_2 released by generating 1 kWh electricity from coal fire power plant (CFPP). As given in Eq. 2.39, the second indicator (I_2) is the total volume of wastewater that is reused by the company. An important social factor is the number of accrued jobs (I_3), which is proportional to the production capacity (Eq. 2.40). Lastly, SAR is selected as the fourth indicator (I_4) which represents the benefit that a single employee can receive. The weighting factors and benchmarks for calculating SI are listed in Table 2.6. Note that a composite index with 4 indicators and assumed weighting factors is used to demonstrate how corporate social responsibility can be explicitly quantified. However, a separate and thorough study including interviews with experts is needed to identify a complex index that can truly reflect the consensus of all the stakeholders in the PV industry. This task is beyond the scope of this study.

$$I_1 = f_{co_2} \cdot \sum_{t=0}^{T} E_t \cdot \sum_{j=1}^{m} d_j \tag{2.38}$$

$$I_2 = V_{wt} \cdot WR \cdot \sum_{j=1}^{m} d_j \tag{2.39}$$

$$I_3 = f_e \cdot PC \tag{2.40}$$

$$I_4 = SAR \tag{2.41}$$

Table 2.6 Benchmarks and weighting factors for calculating social index

Selected Indicators	Benchmark	Weighting
Overall extent of CO_2 mitigation (I_1)	1×10^7 ton CO_2	0.35
Total volume of reused water (I_2)	5×10^6 m^3	0.15
Total number of accrued employees (I_3)	500 people	0.25
Ratio of average salary to minimum wage (I_4)	1.25	0.25

Again, the objective function in this case study is the maximization of NPV calculated using Eq. 2.17-2.18 and SI calculated using Eq. 2.19-2.20, 2.22, and 2.39-2.41. The model consists of:

- Eq. 2.23-2.24 for the quality of the PV module
- Eq. 2.25-2.28 for consumer satisfaction

- Eq. 2.29-2.31 for product demand
- Eq. 2.32-2.37 for product cost

The following variables are fixed in these equations: EO_t, E_t, υ_E, η, T, SR, λ, δ, O_t, R_c, S_F, T_F, f_{pc}, m, n, De, p_{bos}, p_{it}, A_{PV}, A_E, B_{PV}, B_E, γ, P_e, Y, c_{mat}, c_{ut}, c_{ref}, PC_{ref}, b, V_{wt}, f_{wt}, WG_{min}, f_e, f_{co_2}, and R. Note that EO_t, E_t, and υ_E are fixed by using Eq. 2.23, Eq. 2.24, and Eq. 2.30, respectively. The values of the fixed variables are listed in Table 2.5. The variables that need to be optimized are: $LCOE$, υ, CI_0, pr, M_t, d_j, df_j, c_m, c_{cap}, c_{mt}, c_{wt}, c_{la}, PC, WR, and SAR.

2.4.6. Results

The optimization problems are solved in GAMS 24.5.5 with the solver CONOPT. NPV is treated as the primary objective function while SI is converted as ε-constraints. In these calculations, 20 equal intervals are used between the lower and upper bounds of SI. Four scenarios are discussed below to understand how business decisions are made.

2.4.6.1.Scenario 1: A 20-year FIT

In Scenario 1, the base case, the government provides FIT at a fixed rate for 20 years. All the input data are given in Table 2.5. The curve on the right in Figure 2.4 shows the Pareto front with FIT set at 0.15 $/kWh and the trade-off between NPV and SI. The solutions under the curve are suboptimal and any solution above the curve is infeasible. As SI increases from 1.12 to 2.71, NPV is reduced from 153 M$ to 18 M$. If FIT is not available (S_F = 0), we get the curve on the bottom left. It can be seen that its objective values (NPV and SI) are much worse than the curve with FIT, signifying the importance of FIT to open up the PV market.

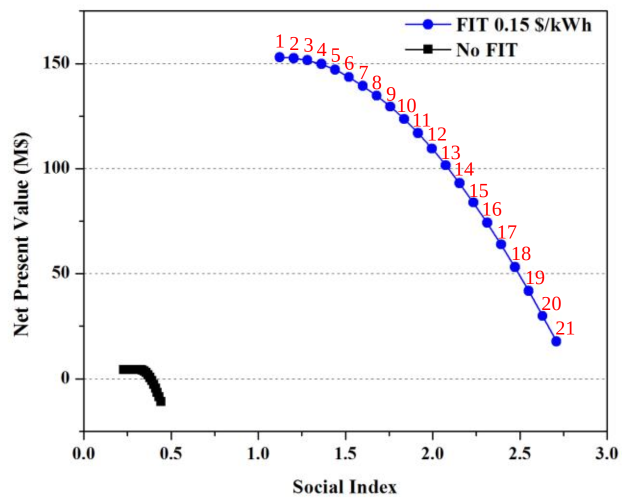


Figure 2.4 Pareto-front obtained by maximizing NPV and SI in Scenario 1

At the Pareto front, each point corresponds to different values of the design variables. Figure 2.5 shows how these values change. From point 1 to 21, the TCI increases from 194 M$ to 405 M$. Note that the total investment at point 9 consisting of 268 M$ TCI and 26.8 M$ net working capital is slightly less than 300 M$. Recall that only 300 M$ is budgeted for this investment. Thus, point 10 and above are not affordable. Additionally, both SAR and WR reach their upper bounds before point 9. This is because labor cost and cost for wastewater reuse only account for small portions of the total manufacturing cost. As price decreases from 1.40 $/Wp to 1 $/Wp, NPV decreases while SI increases.

Since all the points, 1-21, along the Pareto front are equivalently optimal, the decision makers can choose any point from the curve to implement the project. Wang and Rangaiah[78] compared ten mathematical approaches for selecting one solution out of the Pareto-optimality. For instance, based on the LINMAP approach the point with the shortest distance to the positive ideal point; i.e. the point with best objective values, can be selected. In our case, the objective values of the positive ideal point are 153 M$ and 2.71. Then, it is easy to conclude that point 13 that is the closest to the positive ideal point should be selected. However, the required capital investment at point 13 is larger than the company's investment budget of 300 M$. As mentioned, only points 1-9 in Figure 2.5 are affordable. Here, point 9 is selected as the 'base case' for further comparison.

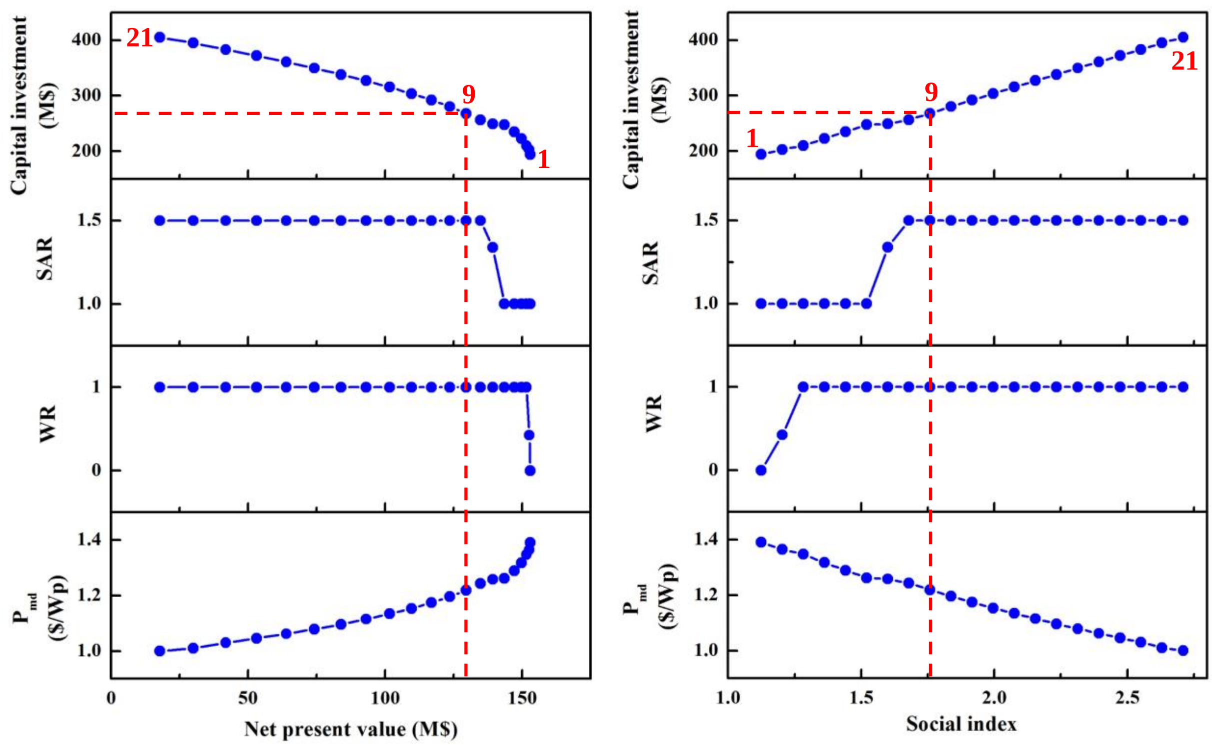


Figure 2.5 Variation of design variables along the Pareto-front in Scenario 1

2.4.6.2.Scenario 2: Regulation on wastewater treatment

In Scenario 2, it is assumed that all wastewater discharged into the environment must be treated by the reverse osmosis plant. With this additional constraint, the new Pareto front (the curve with stars) is shown in Figure 2.6. The two curves ('star' and 'circle') coincide, except for the first two points at the top left. The other points coincide because these points have the same design variables (as shown by point 3-21 in Figure 2.5). Moreover, as SI increases from point 1 to point 21 in Figure 2.5, *WR* reaches the upper bound at point 3. Since the wastewater treatment cost is relatively small compared with other costs (e.g., salary costs, material costs, etc.), it is fine to increase *WR* for achieving a higher SI. In the base case (i.e., point 9 in Figure 2.5), all wastewater is reused (i.e., $WR = 1$). Thus, the company already fulfills the regulation requirement.

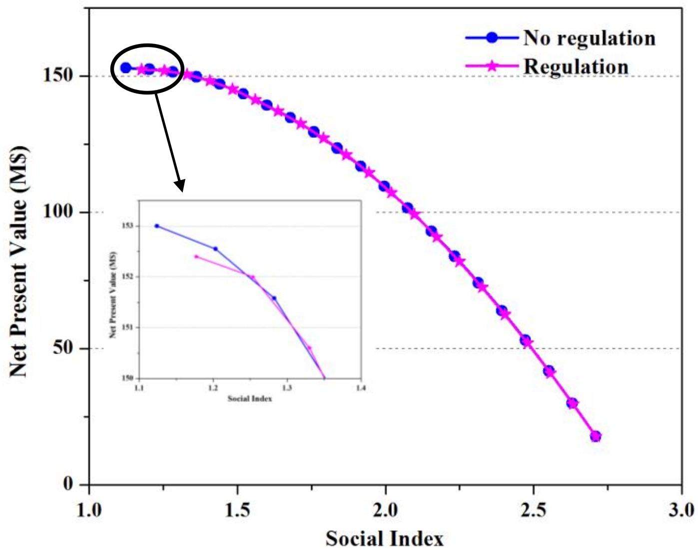


Figure 2.6 Pareto-front obtained with FIT and regulation in Scenario 2

2.4.6.3.Scenario 3: Reduction in tariff after two years

As shown in the reference a3 in Table A2.1, the German government reduced the tariff rate over time. Assume that this situation occurs in China as well. In Scenario 3, it is assumed that S_F is reduced from 0.15 to 0.14 $/kWh after two years to study the influence of FIT variations. Clearly, with the same module price, $LCOE$ will increase suppressing market demand and NPV. Table 2.7 shows the potential impact, which depends on how the company reacts to the reduced tariff. If the company insists on having the same SI (i.e., WR and SAR are kept the same), as shown in the second column labelled as Case B, the company must reduce the module price. NPV decreases by 37% from 130 M$ to 82 M$.

In order to counteract the decrease in FIT, the company can launch R&D projects to reduce product cost within the first two years. The third column labelled Case C in Table 2.7 shows the outcome if the costs can be reduced by 16% after the first two years. Even though the price goes down, NPV is reduced only by 3 M$ while SI remains the same. Figure 2.7 shows the cumulative present value of cash flow in the three cases. The curves of the Base Case and Case C almost overlap. This means that the 16% cost reduction can compensate the negative impact of the reduced FIT. Comparing the Base Case and Case B, the payback time in Case C is around 4 years while it

Table 2.7 The optimization results in Scenario 3

	Base case	Case B#	Case C+
pr ($/Wp)	1.22	1.10*	1.10*
WR	1	1	1
SAR	1.5	1.5	1.5
PC (MWp/year)	291	291	291
Number of employees	698	698	698
NPV (M$)	130	82	127
SI	1.76	1.76	1.76

is 3.5 years in the base case. Therefore, R&D must continue to avoid the decline of project profitability as FIT decreases. Note that since the expenditure for additional R&D activities has not been considered, these are the most optimistic results.

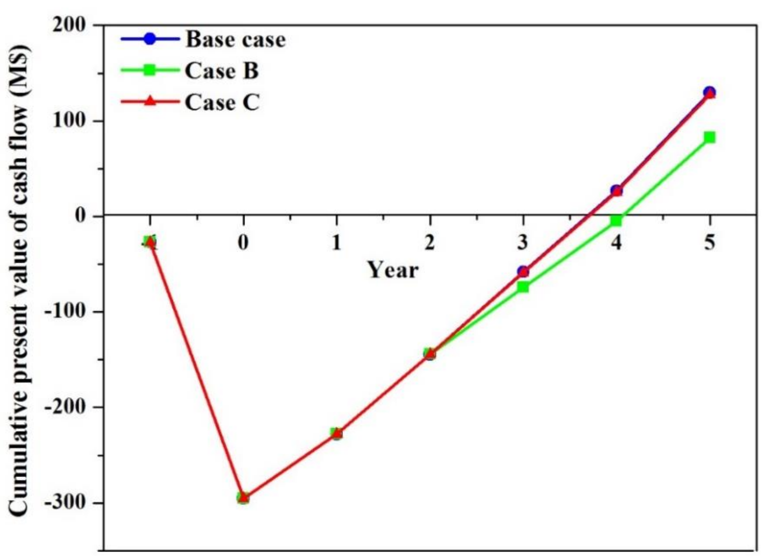


Figure 2.7. Cumulative present value of cash flow of the three cases in Scenario 3

2.4.6.4.Scenario 4: R&D funding and product promotion program

As shown in reference a5 in Table A2.2, the Hong Kong government provides funding to the companies for conducing R&D. In addition, support is offered to promote brand and expand market. Thus, in the last scenario, the local government presumably launches another two incentive programs. The first one offers 10M$ R&D funding for reducing manufacturing cost. The other one provides 5M$ to expand the market. In return, the company must provide an extra 100 jobs to local residents after receiving the benefits for each incentive. Note that, as shown in Figure 2.7, the firm cannot afford R&D and marketing at year 0 due to the limited investment budget of 300 M$.

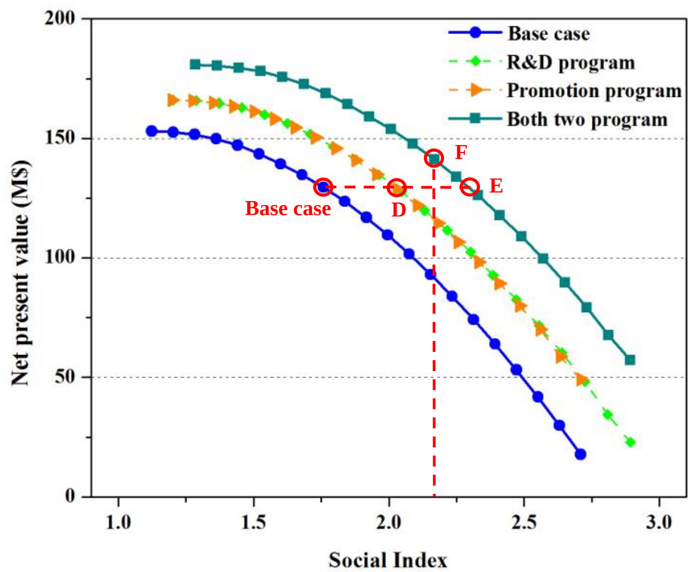


Figure 2.8 The Pareto-fronts obtained in Scenario 4

Let us consider that the firm receives only the R&D funding and that this leads to a 7% cost reduction after the first two years. Figure 2.8 shows the Pareto-front (the curve with diamonds) for this case, which is better than the base case in both NPV and SI. Table 2.8 lists the optimization results of point D. Comparing with the Base Case, an extra 119 jobs can be created for locals which fulfills the government's requirement (100 jobs) and NPV remains the same at 130 M$. In other words, the company becomes more socially responsible without sacrificing NPV. This can be achieved because the product price is reduced to 1.15 $/Wp and the production capacity (and market demand) increases up to 340 MWp/year. Since the number of employees is proportional to the production capacity, extra jobs are created. If the company only executes the promotion program and expands the market size by 10%, we get the Pareto front which basically overlaps with the one with R&D program only (Figure 2.8).

Figure 2.8 also shows the Pareto-front (curve with squares) when the company executes both programs and achieve the same outcomes in cost reduction and market expansion. If NPV remains at 130 M$, we get point E whose results are listed in Table 2.8. The company provides an extra 254 jobs as compared with the Base Case and SI increases up to 2.29. Note that the increase in jobs is more than the minimum requirement of 200 and is more than twice that from only the R&D program (i.e., 119 jobs in point D) because of synergistic effect. If the number of employees is fixed at 898, we get point F, which provides an increased NPV to 140 M$.

Table 2.8 The optimization results in Scenario 4

	Base Case	Point D	Point E	Point F
pr ($/Wp)	1.22	1.15	1.12	1.15
WR	1	1	1	1
SAR	1.5	1.5	1.5	1.5
PC (MWp/year)	290	340	393	375
Number of employees	698	817	952	898
NPV (M$)	130	130	130	140
SI	1.76	2.02	2.29	2.18

2.5.Conclusion

This chapter presents a multi-objective optimization model for decision making in chemical product development taking into account government policies and corporate social responsibility. This is the first attempt in the literature to develop such a systematic approach. Government incentives are classified based on what they try to accomplish for such a product and whether the incentive is a form of cash payment. Government regulations define the rules and bounds on the choice of materials and processes for producing the product. Company reacts to these incentives and regulations, and takes into account consumer preferences to design a product that offers maximum profit while fulfilling social responsibility. The framework is demonstrated by a PV module investment case study. To keep the model manageable, the materials and manufacturing process for the PV case study are fixed and only the business decisions are optimized. Four scenarios are discussed to illustrate how the decisions are made under the impact of different government policies.

Additional work can be done for this chapter. A direct utility model using only quantities of goods as arguments is not suitable for use in this case study where solar panel is the only product. Instead, the models popularized by Lancaster,[49] McFadden,[53] and Hanemann[48] are followed in this chapter. More complex models can be considered for the case study. It is clear that different weighting factors in Eq. 2.19 can lead to different values of the social index and thus different decisions. A more comprehensive and in-depth evaluation of the weighting factors is recommended. Moreover, the government-company-consumer interactions can also be considered from the government point of view. A government should optimally allocate the limited resources to achieve its objectives. This has been recognized as a bi-level optimization problem.

This framework is part of our long-term effort to develop a Grand Product Model that considers most, if not all, of the important factors influencing product design. These include product ingredients, processing, material properties, product structure, product cost, pricing, and so on. Research on further expanding this framework to consider global supply chain and sustainability is underway.

2.6.Appendix A

Table A2.1 Incentive programs in Germany

Abbreviation	Name	Description
ERP[a1]	European Recovery Program	Venture capital funds focusing on German-based high-tech companies to develop new technologies
PG[a2]	Public Guarantees	Acts as guarantor to encourage financial institutions to offer loans to new companies
FIT[a3]	Feed-in Tariff	Offers tariffs to renewable energy producers to accelerate investments in renewable energy technologies
BAFA[a4]	Economic Affairs and Export Control	Provides support to Germany companies to participate in selected fairs and oversea exhibitions

[a1]: http://www.eif.org/what_we_do/resources/erp/
[a2]: https://www.gtai.de/GTAI/Navigation/EN/Invest/Investment-guide/Incentive-programs/public-guarantees.html
[a3]: https://en.wikipedia.org/wiki/Feed-in_tariffs_in_Germany
[a4]:www.bafa.de/EN/Promotion_Economic_Development_SME/promotion_economic_development_sme_node.html

Table A2.2 Incentive programs in Hong Kong

Abbreviation	Name	Description
ITF[a5]	Innovation and Technology Fund	Provides funds to companies for developing new products and technologies in Hong Kong
R&D centers[a6]	/	Provides free information, consultation on product and technology development and networking opportunities
GSP[a7]	General Support Program	For non-R&D projects that contribute to upgrading Hong Kong industries as well as fostering an innovation culture
BDP[a8]	Brand Development and Promotion	Assists Hong Kong enterprises in the establishment, development, and promotion of their brands such as organizing exhibitions and providing free market information

[a5]: http://www.itf.gov.hk/l-eng/about.asp
[a6]: http://www.itc.gov.hk/en/rdcentre/rdcentre.htm
[a7]: http://www.itf.gov.hk/l-eng/GSP.asp
[a8]: http://www.branding.tid.gov.hk/english/support_measures/marketing.html

Table A2.3 Incentive programs in Singapore

Abbreviation	Name	Description
RISC[a9]	Research Incentive Scheme for Companies	Provides government grants to develop R&D capabilities in strategic areas of technology
WSQ[a10]	Workforce Skills Qualifications	Trains, develops, assesses and recognizes individuals for key competencies
DTD[a11]	Double Tax Deduction	200% tax deduction on eligible expenses for supporting market expansion and investment development activities
TXC[a12]	TradeXchange	Trade enhancing infrastructures to offer an integrated electronic system of "work flow, submission and enquiry to the transportation-related agency"

[a9]: https://www.edb.gov.sg/content/edb/en/why-singapore/ready-to-invest/incentives-for-businesses.html
[a10]: http://www.ssg.gov.sg/wsq.html?activeAcc=1
[a11]: https://www.iesingapore.gov.sg/Assistance/Global-Company-Partnership/Market-Access/Double-Tax-Deduction
[a12]: https://www.tradexchange.gov.sg/tradexchange/content/aboutradexchange.html

Table A2.4 Incentive programs in United States

Abbreviation	Name	Description
SBIR[a13]	Small Business Innovation Research	Provides seed funds (early-stage capital) for technology commercialization in the United States
CRADA[a14]	Cooperative Research & Development Agreements	Allows a government agency and a private company or university to work together on research and development
CPG[a15]	Comprehensive Procurement Program	Buys products made with recovered materials to ensure that the materials collected in recycling programs are used again in the manufacture of new products
FEMP[a16]	Federal Energy Management Program	Provides training to foster and maintain a high-performance workforce to conduct and operate in an energy efficient and sustainable manner

[a13]: https://sbir.nih.gov/
[a14]: https://en.wikipedia.org/wiki/Cooperative_research_and_development_agreement
[a15]: https://www.epa.gov/smm/comprehensive-procurement-guideline-cpg-program
[a16]: https://energy.gov/eere/femp/federal-energy-management-program-training

2.7.Appendix B

The parameters, A_{PV}, B_{PV}, A_E, B_E, γ, and Y, in the utility model and demand model are elaborated here. B_{PV} is assumed to be equal to B_E. Additionally, when LCOE is equal to the grid price, only 1 out of 1000 consumers presumably purchases PV. Under this assumption, the probability of purchasing PV can be written as:

$$P = \frac{e^{A_{PV}}}{e^{A_{PV}} + e^{A_E}} = 0.001$$

Thus, if A_{PV} is presumably set to be 0 \$/kWh, A_E is then equal to 6.9 \$/kWh. The parameters B_{PV} (B_E) and γ are regressed from historical LCOE data and annual installed PV capacity from 2010 to 2015 in Mainland China using Eq. 2.25-2.31 (Table B2.1).[67]

Table B2.1 Historical LCOE and installation capacity data from 2010 to 2015 in Mainland China

	2010	2011	2012	2013	2014	2015
LCOE ($/kWh)	0.250	0.042	0.033	0.000	-0.017	-0.033
Installed PV (GWp)	0.5	2.5	5.0	9.5	10.6	15.1
Grid price minus LCOE ($/kWh)	-0.15	0.058	0.067	0.100	0.117	0.133

The regression results with a coefficient of determination R^2 of 0.97 are listed in Table B2.2.

Table B2.2 Regression results

	B_{PV} (B_E)	γ	Y_M (GW_p/year)	R^2
Value	31	0.4	20	0.97

Note that the market size Y_M is countrywide. However, the case study assumes a firm focusing on the market in southern China with a market size of 10 GW_p/year

Chapter 3: Product Design: Incorporating Make-or-buy Analysis and Supplier Selection

3.1.Introduction

The research on the design of chemical products has gradually evolved in breadth and depth. There exist a number of perspective articles offering different viewpoints of product design.[3,5,6,79,80] Many case-studies are available for the design of specific products. These include the design of personal detergent,[81] biofuel blend,[82] refrigerant,[31] disinfectant,[83,84] perfume,[85,86] fuel additive,[30] paint formulation,[87,88] inkjet ink[29] and so on. Systematic approaches and methods include tools, model-based methods, rule-based methods, databases, and experiments have been developed for designing these products. These include chemical product design simulator,[89] inversion model in product design,[16] design based on consumer preference,[23] pricing model,[11,36] model accounting for the interrelationship among various design tasks,[2] government policy and corporate social responsibility.[90] In this chapter, we focus on make-or-buy analysis and supplier selection in product design.

Figure 3.1 shows the relationship between the consumer and the company that makes and markets the new product as well as the relationship between the company and its suppliers. After conceptualizing the product based on consumer preferences, the company sources the ingredients from different suppliers. Some ingredients go directly into the final product while some intermediate ingredients are converted in-house into ingredients that go into the final product. Each ingredient, intermediate or final, can be purchased from suppliers with different production capacity, price, and quality. Therefore, suppliers must be properly selected for achieving reliable supply and low product cost.

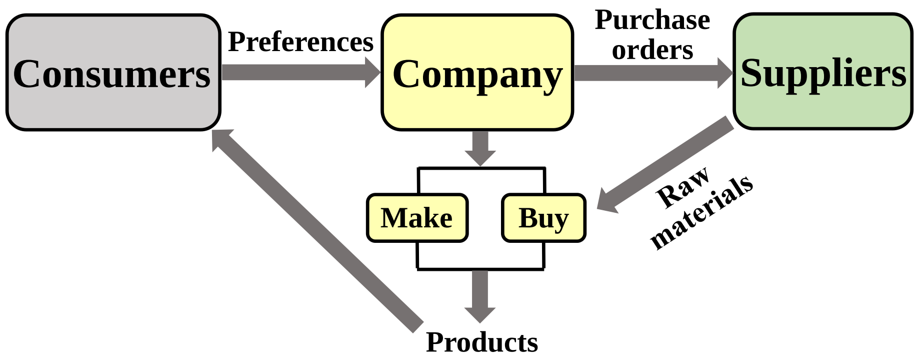


Figure 3.1 Consumers-company & company-suppliers relationships

Generally, make-or-buy decisions are made at the strategic and operational levels.[91] Many approaches have been developed for systematic make-or-buy analysis, such as the transaction cost framework,[92] analytic hierarchy process method,[93] and weighted sum method.[94] Similarly, supplier selection takes many factors into consideration. For instance, Amorim et al.,[95] developed a stochastic mixed-integer programming model for systematic supplier selection in the food processing industry taking into account perishability, model parameter uncertainty, and freshness dependent demand. Ware et al.,[96] reviewed the various issues and methods in supplier selection problems. It is worth noting that the methodologies developed in the supply chain literature were intended for products with fixed formula, quality, price and even market demand. In other words, these two issues were studied only from the supply chain management perspective. In fact, make-or-buy analysis and supplier selection are closely related to product design. However, to the best of our knowledge, few studies consider the two issues from the product design perspective. This motivates us to develop a framework where product design, make-or-buy analysis, and supplier selection are simultaneously considered from the systems engineering perspective. This is particularly important for designing new formulated products and functional products.

The design problem we aim to solve is illustrated in Figure 3.2. The icons on the right (i.e., ingredients, process design, quality, consumer preference, pricing, product cost, nonmanufacturing cost, and economic analysis) are adjusted from the Grand Product Design Model[2] while the supply chain icon (on the left) is newly added. The supply chain icon contains information of the qualified suppliers (e.g., location, price, quality, and production capacity), purity requirements, available manufacturing technologies, and company resources such as initial capital budget. Starting at the middle, a product is conceptualized based on consumer preferences. The total market size, quality, and price of the competitor's product are known. The ingredients and process are identified (top of figure) to provide a product with the desired quality. It is assumed that the company owns a site where the plants for manufacturing the final product and for converting intermediate ingredients to final ingredients, and warehouse are collocated. It allows the simultaneous optimization of the product cost that depends on ingredients and operating costs, and the product formula that satisfies the consumer preferences; that is, the product ingredients are not fixed in advance. However, in order not to handle too many details in this study, it is assumed that product distribution channels are fixed. In other words, the profit is optimized by choosing the ingredients, make-or-buy, suppliers, product price, and market share in the presence of a competing product. Since variables such as market size may vary with time, the year is discretized into multiple periods with a prefixed length (e.g., month or quarter) within which the variable is fixed. Two case studies – light duty liquid detergent and controlled release granular herbicide – are used to demonstrate the application of the proposed framework.

3.2. Procedure for Simultaneous Product Design, Make-or-Buy Analysis, and Supplier Selection

The aforementioned design problem is formulated as a collection of relationship models in Eq. 3.1-3.8. The underlined entities are simply different types of variables. For instance, in Eq. 3.2, $\underline{x}$ accounting for the selected ingredients and their compositions is a vector while $\underline{pd}$ consists of

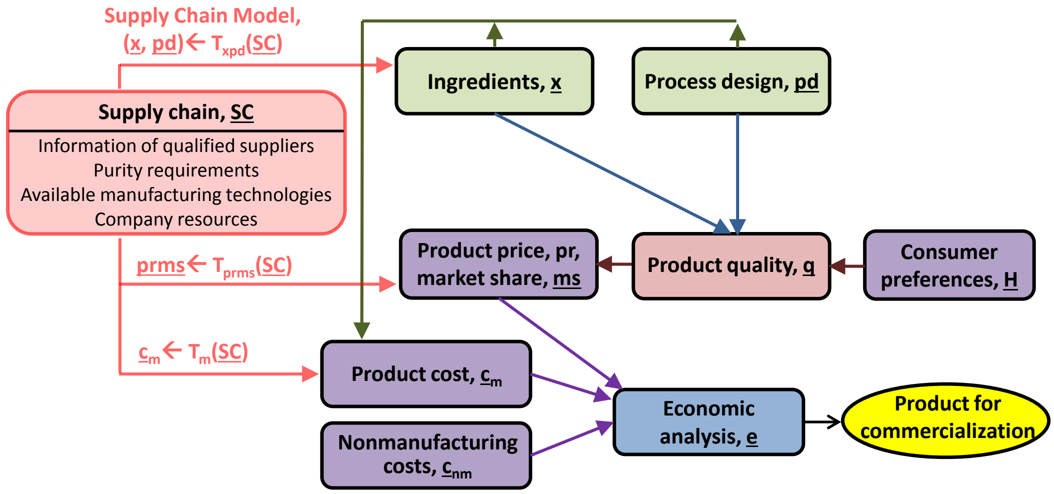


Figure 3.2 Impacts of supply chain on product design activities

process design flowsheet and equipment operating conditions. The arrows ←, instead of equal signs, signify the fact that the LHS variables can be determined from the RHS variables through model-based methods, rule-based methods, databases, tools, and experimental results.

$$max\ \underline{e} \tag{3.1}$$

Subject to

$$\underline{q} \leftarrow T_q(\underline{x}, \underline{pd}) \qquad \text{(Quality)} \tag{3.2}$$

$$\underline{prms} \leftarrow T_{prms}(\underline{q}, \underline{H}, \underline{Y}) \qquad \text{(Pricing)} \tag{3.3}$$

$$\underline{x}, \underline{pd} \leftarrow T_{xpd}(\underline{SC}) \qquad \text{(Supply chain)} \tag{3.4}$$

$$\underline{c}_m \leftarrow T_m(\underline{x}, \underline{pd}, \underline{SC}) \qquad \text{(Product cost)} \tag{3.5}$$

$$\underline{c}_{nm} \leftarrow T_{nm}(\underline{mk}) \qquad \text{(Non-manufacturing cost)} \tag{3.6}$$

$$\underline{e} \leftarrow T_e(\underline{prms}, \underline{c}_m, \underline{c}_{nm}) \qquad \text{(Economics)} \tag{3.7}$$

$$\underline{c}^L \leq f\left(\underline{x}, \underline{pd}, \underline{prms}, \underline{q}, \underline{H}, \underline{Y}, \underline{SC}, \underline{mb}, \underline{su}, \underline{c}_m, \underline{c}_{nm}, \underline{mk}\right) \leq \underline{c}^U \qquad \text{(Bounds)} \tag{3.8}$$

The objective function is the maximization of profit (Eq. 3.1). Product quality ($\underline{q}$) is decided in Eq. 3.2. Here, we consider that product quality includes qualitative product attributes and quantitative technical requirements. Product price ($\underline{pr}$) and market share ($\underline{ms}$) are determined in Eq. 3.3. Note that the price $\underline{pr}$ is considered as a vector because price may vary in different geographical regions and with demographics based on the pricing strategy[36]. $\underline{H}$ captures the consumer preferences and $\underline{Y}$ denotes the given market sizes. Furthermore, $\underline{x}$ and $\underline{pd}$ are influenced by the supply chain $\underline{SC}$ (Eq. 3.4). As the distribution channels are assumed to be fixed in this study, $\underline{SC}$ has two components. Make-or-buy analysis ($\underline{mb}$) decides whether the selected ingredients are made in-house or purchased externally, while supplier selection ($\underline{su}$) determines the selected suppliers and the corresponding order quantities. Eq. 3.5 calculates product cost ($\underline{c}_m$). Nonmanufacturing cost ($\underline{c}_{nm}$) includes administrative and marketing activities ($\underline{mk}$) such as advertising costs (Eq. 3.6). Finally, Eq. 3.7 decides the profit based on price, market share, and costs. Note that the above problem can be expanded by incorporating other objectives such as corporate social responsibility (in Chapter 2), product sustainability, etc. In that case, additional constraints and models are needed.

A five-step design procedure is proposed to solve this design problem (Figure 3.3). It is derived from the Grand Product Design Model in Figure 3.2. At each step, heuristics and rule-based methods (shown on the right of Figure 3.3) are used to make decisions and to convert the relationships into mathematical equations (such as Eq. 3.9-3.37 below) which are then solved by optimizers. The procedure starts with the identification of consumer preferences through which design targets are decided. Then, proper ingredients and process design are generated in Step 2. Step 3 provides a product with the desired qualities. In Step 4, product pricing, make-or-buy analysis, and supplier selection are carried out. Meanwhile, product cost and nonmanufacturing cost are calculated and profit is maximized. Finally, experimental verifications are conducted to ensure a reliable design. The specific models and equations are discussed next.

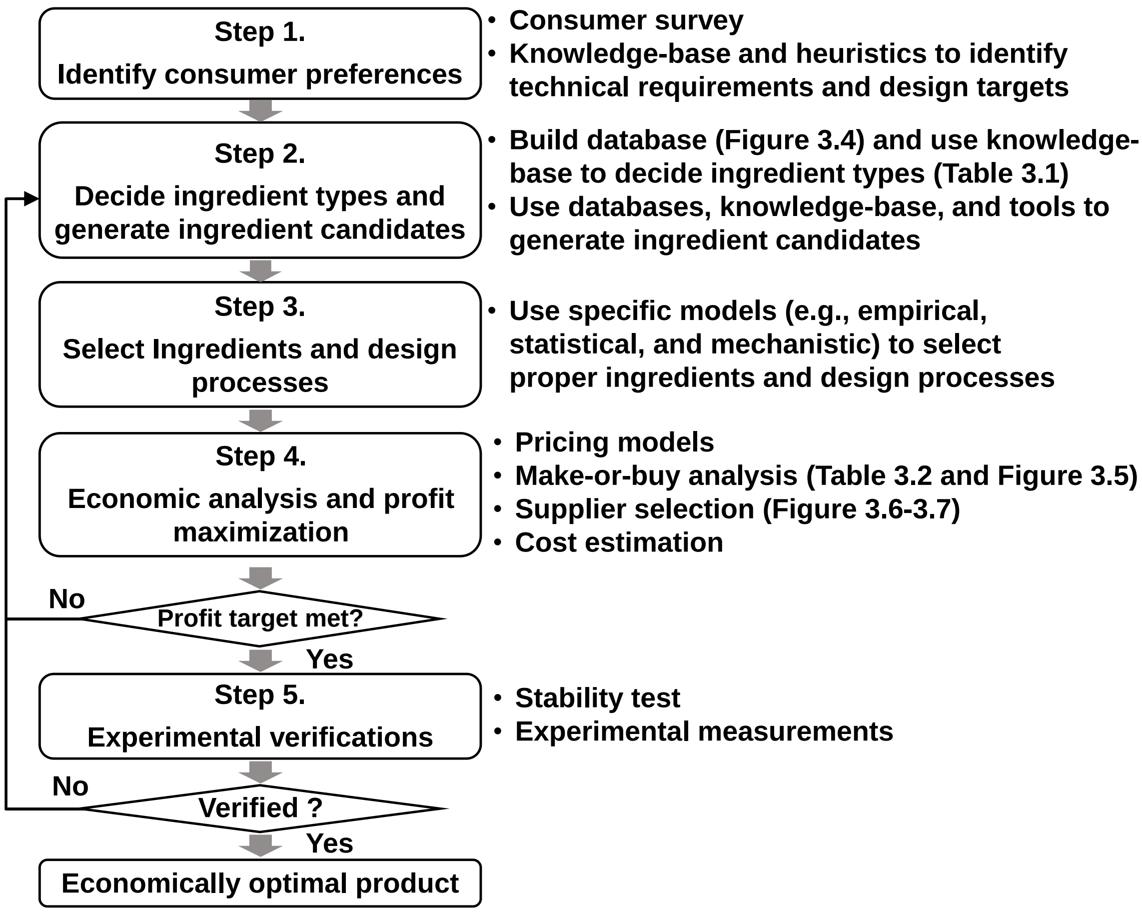


Figure 3.3 Procedure for simultaneous product design, make-or-buy analysis, and supplier selection

3.2.1. Step 1. Identify Consumer Preferences

The consumer preferences $\underline{H}$ in Eq. 3.3 that include various product attributes (e.g., stability, ease of spread, cleanliness) are identified through consumer survey. Generally, how consumers perceive the product can be quantified by the consumer preference function H, which is the weighted sum of the preference scores of the product attributes.

$$H = \sum_n w_n \cdot y_n \tag{3.9}$$

where w_n is the weighting factor ($\sum_n w_n = 1$), which is determined through consumer survey. y_n, in the range of 0-1, is the preference score of the n-th product attribute. Generally, product attributes can be translated into various technical requirements ($\underline{tr}$) through knowledge-base and heuristics in the form of House of Quality[25]. The technical requirements include functional performance (e.g., dissolution time, shelf life), physicochemical properties (e.g., pH, viscosity, solubility), or product characteristics (e.g., particle size, form, smell). Preference scores are calculated by

$$\underline{y} = f(\underline{tr}) \tag{3.10}$$

Meanwhile, rule-based methods can be utilized to determine a set of design targets (lower bound $\underline{tr}^L$ and upper bound $\underline{tr}^U$) on these technical requirements. For instance, the pH of hand lotion must be large than 4 and less than 8 so that the lotion does not harm the skin.

$$\underline{tr}^L \leq \underline{tr} \leq \underline{tr}^U \tag{3.11}$$

3.2.2. Step 2. Determine Ingredient Types and Generate Ingredient Candidates

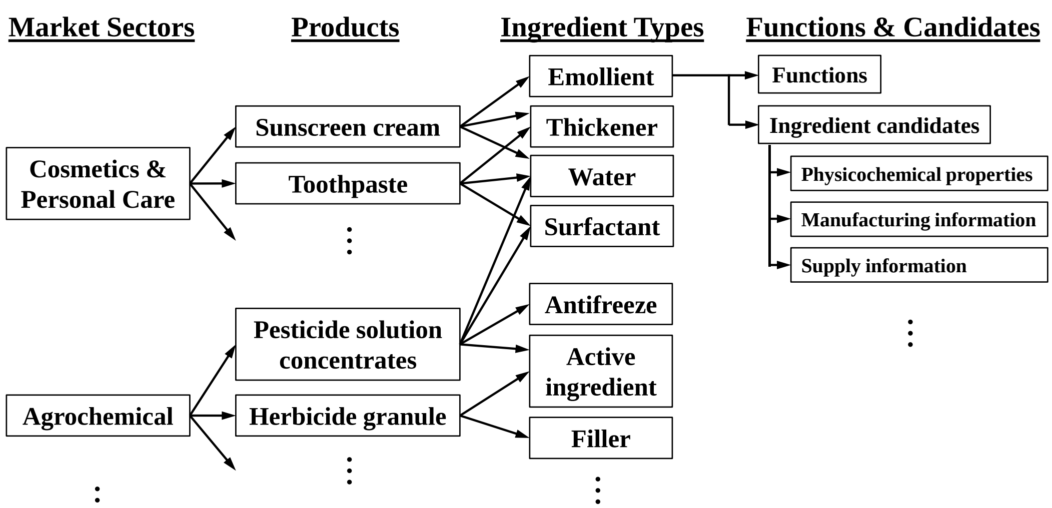


Figure 3.4 Multi-level data structure for chemical product design in different market sectors

Eq. 3.2 shows that product quality depends on the selected ingredients and process design. To do so, data on potential ingredients are needed. Figure 3.4 shows a multi-level database structure for designing products in different market sectors. In each sector, there are many products and each product consists of many ingredients to provide multiple functions. Thus, ingredients can be classified into different types based on their functionalities. The required ingredient types in a product can be identified by knowledge-base and heuristics. For instance, the typical ingredient types used in the agrochemical products[97] and their functions are listed in Table 3.1 (2nd and 3rd columns). In addition, Fung et al.,[98] listed the ingredient types used in the detergents and Cheng et al.,[15] showed the ingredient types in skin-care creams. For products in other sectors (e.g., cosmetics and personal care[99], household and professional care[100,101], paint and coating[102], pharmaceutical[103], adhesive and sealant[104], ink and dye[105,106], and lubricant[107]), the required ingredient types can be similarly identified. For a specific ingredient type, many chemicals can provide the necessary functions. Thus, potential ingredient candidates (e.g., 4th column in Table 3.1) can be generated by using knowledge-base, material databases (e.g., Material Project, NIST chemistry book, NIMS material database) or computer-aided tools[89]. Moreover, for each ingredient candidate, its supply information (e.g., the number of suppliers, purchasing prices, etc.) and manufacturing information (i.e., processing techniques, production capacity, capital cost, etc.) should be collected. Note that if an ingredient candidate cannot be purchased and manufactured in-house, it should not be generated for consideration.

3.2.3. Step 3. Select Ingredients and Design Processes

To meet the design targets, proper ingredients as well as their concentrations should be selected out of the candidates identified in Step 2. Additionally, detailed process design should be determined. Systematic framework has been proposed to synthesize the manufacturing processes for selected formulated and functional products.[8-10] The generic flowsheet usually consists of pre-treatment, mixing, structure formation, post treatment, filling and packaging. Among them,

Table 3.1 Typical ingredients types used in the agrochemical products

Ingredient types	Functions	Candidates	Properties for selection
Absorbent/carrier	Offer solid medium to load liquid ingredients	• Silica • Talc	• Absorptive capacity • Hardness
Active ingredient	Provide product-specific functions (e.g., control pathogen or insect)	• DDT • Captan	• Functional mechanism • Biological property
Antifreeze	Lower freezing point of a liquid	• Ethylene glycol • Propylene glycol	• Efficacy • Solubility
Antifoaming	Prevent formation of foam and break the foam already formed	• Polysiloxanes • Silicone	• Efficacy • Solubility
Binder	Bind solid particles together and to substrates	• PVP solution • Lignosulphonates	• Adhesiveness
Dispersant	Preserve suspension and dispersion of solid particles in liquid to prevent re-aggregation	• Alkylphenol ethoxylates • Aliphatic alcohol ethoxylates	• Molecule weight • Solubility
Disintegrant	Promote break-up of tablets	• Starches • Crosslinked polyvinylpyrrolidone	• Solubility • Diffusivity
Emulsifier	Stabilize emulsion and prevent phase separation	• Alkylphenol • Polyoxyethlene oxo alcohol	• Polar property
Filler	Extend volumes and improve some technical properties (e.g., transparency, conductivity)	• Cellulose • Lignin	• Density • Solubility • Diffusivity
Preservative	Prevent decomposition caused by microbial growth or undesired chemical changes	• Propionic acid • Benzoic acid	• Biological property
Surfactant (wetting agent)	Lower surface tension between two phases (e.g., solid leaf-liquid herbicide) to ease solubility	• Sodium lauryl sulphate • Nonylphenol ethoxylate	• Hydrophilic-hydrophobic property
Solvent	Provide liquid medium to dissolve other ingredients	• Water • xylene	• Ability to dissolve • Toxicity
Thickener	Increase viscosity without greatly changing other properties	• Silica • Clays	• Solubility

structure formation usually involves only a few unit operation alternatives. For instance, homogenization is used for making emulsions, dilute dispersions, etc. Powders and granules are manufactured by bulk solids processing steps such as screening, milling, granulation, etc. Moreover, many specific models (e.g., empirical, mechanistic, and statistical models) can be used for this purpose. Empirical and mechanistic models often depend on the physicochemical properties of the ingredients. The technical requirements can be calculated based on the selected ingredients and process design.

$$\underline{tr} = g(\underline{x}, \underline{pd}) \tag{3.12}$$

3.2.4. Step 4. Economic Analysis and Profit Maximization

Here, product profitability is evaluated using the Net Present Value (NPV).

$$NPV = \sum_{j=-n}^{m} \frac{PCF_j}{(1+R)^j} \tag{3.13}$$

where R, n, and m represent the discount rate, the time for product design and facility construction, and product life, respectively. The subscript j denotes the j-th period of time. PCF_j is the project cash flow in the j-th time period:

$$PCF_j = \begin{cases} -CI - NWC & j \le 0 \\ \left(pr \cdot d_j - c_{m,j} - c_{nm,j}\right) \cdot (1 - tax) + tax \cdot De_j - \Delta NWC_j & j > 0 \end{cases} \tag{3.14}$$

Before manufacturing starts ($j \le 0$), PCF_j includes the capital investment (CI) for production facilities and net working capital (NWC). After sales begin ($j > 0$), PCF_j is calculated by subtracting from the revenue ($pr \cdot d_j$), total product cost ($c_{m,j}$), nonmanufacturing cost ($c_{nm,j}$), tax after adjusting for depreciation (De_j), and increase in net working capital (ΔNWC_j). Upon the end of the project, all the *NWC* is recovered. Product price and market share are calculated using the pricing model and costs are obtained after the make-or-buy analysis and supplier selection. In general, the NPV has to meet a profit target for the project to continue.

3.2.4.1.Pricing

Eq. 3.3 relates product price and market share to product quality, consumer preferences, and market size. Here, market share is represented by market demand ($\underline{d}$). since demand can always be decided with given price and quality, only price is considered as the design variable. Based on microeconomics, specific pricing models have been proposed to account for this relationship in product design[11,36]. Assuming a single competitor, the demand at time j (d_j) is calculated by comparing pr and H with those of the competitor's product (i.e., pr_c and H_c) in Eq. 3.15. In addition, d_j and the competitor's product demand (dc_j) are constrained by the market size (Y_j).

$$\left(\frac{d_j}{dc_j}\right)^{1-\rho} = \alpha^{\rho} \cdot \frac{pr_c}{pr} \cdot \left(\frac{H}{H_c}\right)^{\rho} \tag{3.15}$$

$$pr \cdot d_j + pr_c \cdot dc_j = Y_j \tag{3.16}$$

where the parameter α, in the range of 0-1, is the consumer awareness on the superiority of the new product. ρ is related to elasticity. Chan et al.,[36] developed a three-step framework where α and ρ can be systematically determined for a completely new or improved chemical product. For products with sufficient market data, ρ is regressed from sales data and α is decided by advertising expenditures. For new products without market data, specific pricing strategy (e.g., cost-based, customer-based, and competition-based pricing) is selected based on heuristics and then α and ρ are estimated accordingly.

3.2.4.2.Make-or-Buy Analysis

Figure 3.5 shows the general procedure for the make-or-buy analysis. To begin such an analysis, the external (e.g., regulations and qualified suppliers) and internal information (e.g., purity requirements, manufacturing technologies, and company resources) is collected. Then, the major objectives for make-or-buy analysis should be identified. In general, objectives include cost reduction, quality assurance, risk control, reliable manufacturing, and reduction of time to market.[94] Moreover, many factors such as political issues, company resources, strategic plans, etc. have to be considered since these factors greatly influence the make-or-buy objectives. The heuristics in

Table 3.2 can be used to determine how the objectives can be better achieved. For instance, if the major objective is to reduce costs, the economic factor is the key for make-or-buy analysis. The binary variables (mob^i) indicates the make-or-buy decision for product ingredient i.

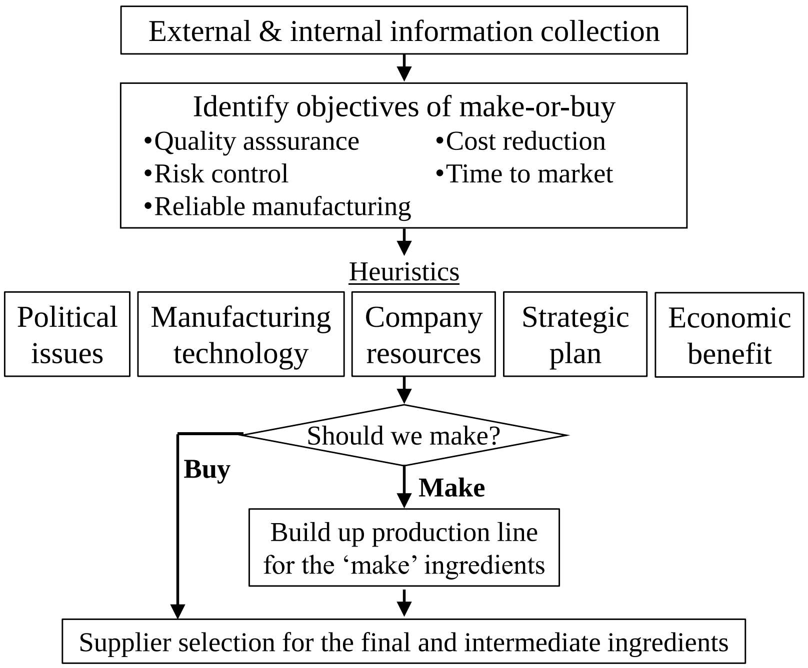


Figure 3.5 General make-or-buy analysis procedures

$$mob^i = \begin{cases} 1 & \text{favoring buy ingredient } i \\ 0 & \text{favoring make ingredient } i \end{cases} \tag{3.17}$$

Note that while mob^i is part of Eq. 3.4, it is an input parameter fixed by using the heuristics in Table 3.2. After this step, the relationship represented by Eq. 3.4 becomes a set of equations as discussed next.

3.2.4.3.Supplier Selection

Three sets of ingredients are defined and used in the following supplier selection model:

$PFI = \{'purchased'\ final\ ingredients\}$ $MFI = \{'make'\ final\ ingredients\}$

$II = \{intermediate\ ingredients\}$.

Table 3.2 Heuristics for make-or-buy decision making

Factors	Favoring 'Make'	Favoring 'Buy'
Political issues	• The company has the license to produce the ingredient of interest	• Company does not have required certification • Manufacturing facilities are hard to fulfill environmental regulations
Strategic plan	• There are risks of non-supply, unreliable supply, etc. • The ingredient is used in many products for various markets • It is required to directly control the ingredient quality • Ingredient provides uniques product quality • The production can leverage or share the existing facilities for in-house production	• The company cannot take the risk of managing a new production line • The ingredient can be easily replaced • The company has close collaboration with suppliers • Suppliers offer a customer-preferred brand regarding quality and reliability • It is necessary to reduce time to market
Manufacturing technology	• The company is in a leading position and has advanced in-house technology • Manufacturing technologies can be purchased in the market • Design secrecy is required to protect proprietary technology • The ingredients can be produced from wastes of other production lines	• Quality requirements cannot be met based on current technology • Manufacturing technology is not available in the market • Suppliers own the patents of the technologies
Resource	• Number of qualified suppliers is limited • The quality of available ingredients does not meet requirements	• The company has limited facilities, space, technical supports, product experiences, and skilled employees for new production lines • The existing production line has insufficient capacity
Economics	• Projected sales are large and building new production capacity can result in economic benefit • Government offers heavy incentives and subsidies to promote the manufacturing	• Limited budget for investment • Suppliers offer a cheaper price • Suppliers own better capability to reduce production costs

Suppliers provide the 'purchased' final ingredients that go into the final product as well as the intermediate ingredients that are used to produce the 'make' final ingredients that go into the final product. Figure 3.6 shows the material flow network. Raw materials are procured from various suppliers. The intermediate ingredients are sent to the intermediate ingredient inventory and then converted to the 'make' final ingredients in the ingredient manufacturing plant. The 'purchased' and 'make' final ingredients are stored in the final ingredient inventory ready for use in manufacturing the new product. Finally, the product is stored in the product inventory for distribution to consumers. The procurement is controlled by the ingredient supplier binary variable $IS^i_{r,j}$.

$$IS^i_{r,j} = \begin{cases} 1 & \text{ingredient } i \text{ is purchased at time } j \text{ from supplier } r \\ 0 & \text{otherwise} \end{cases} \quad i \in PFI \cup II \qquad (3.18)$$

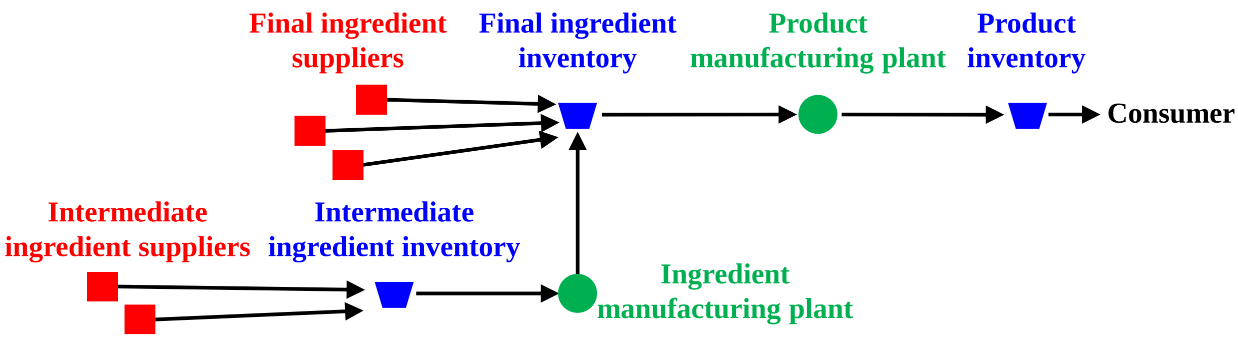


Figure 3.6 General material flow network for procurement and production.

If ingredient i is purchased externally, its suppliers must be selected. Otherwise, no suppliers are needed.

$$\sum_r \sum_j IS^i_{r,j} > 0 \quad if\ mob^i = 1 \qquad i \in PFI \cup II \qquad (3.19a)$$

$$\sum_r \sum_j IS^i_{r,j} = 0 \quad if\ mob^i = 0 \qquad i \in MFI \qquad (3.19b)$$

When the ingredient is purchased ($IS^i_{r,j} = 1$), its purity (PU^i_r) must be larger than the purity requirement (PUR^i) and the order quantity ($OQ^i_{r,j}$) has to be larger than the supplier's minimum order quantity (MOQ^i_r), but less than the maximum production capacity (MPC^i_r). Otherwise, $OQ^i_{r,j}$ is equal to 0.

$$\left. \begin{array}{c} PU^i_r \geq PUR^i \\ MOQ^i_r \leq OQ^i_{r,j} \leq MPC^i_r \end{array} \right\} \quad if\ IS^i_{r,j} = 1 \qquad i \in PFI \cup II \qquad (3.20a)$$

$$OQ^i_{r,j} = 0 \quad if\ IS^i_{r,j} = 0 \qquad\qquad i \in PFI \cup II \qquad (3.20b)$$

Figure 3.7 depicts the ingredient material balances.[108] For the intermediate ingredient inventory, the amount of ingredient i stored at the end of period j (AIS^i_j) is,

$$AIS^i_j = AIS^i_{(j-1)} + \sum_r OQ^i_{r,j} - AIIC^i_j \qquad\qquad i \in II \qquad (3.21)$$

where $AIIC^i_j$ is the amount of intermediate ingredient i consumed during time j, which depends on the amount of 'make' final ingredient manufactured ($AFIM^{ii}_j$) during time j.

$$AIIC^i_j = AFIM^{ii}_j \cdot RII^i \qquad\qquad i \in II,\ ii \in MFI \qquad (3.22a)$$

$$AFIM^{ii}_j \leq pci^{ii} \qquad\qquad ii \in MFI \qquad (3.22b)$$

where RII^i represents the required intermediate ingredient for producing one unit of 'make' final ingredient which is related to the reaction stoichiometry. $AFIM^{ii}_j$ should be less than or equal to

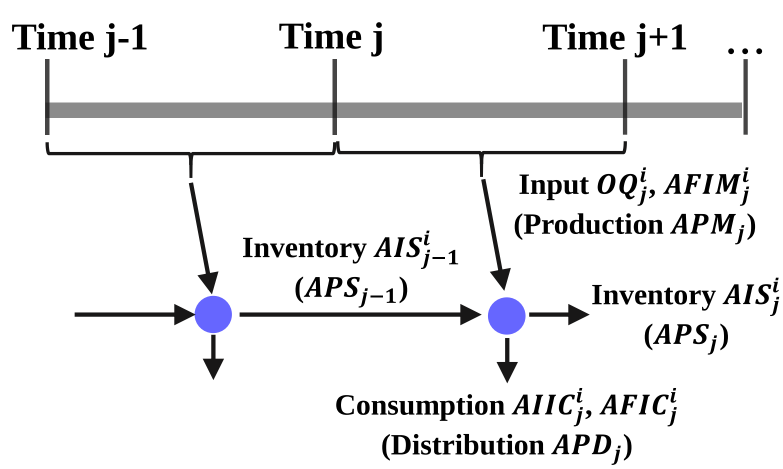


Figure 3.7 Timely-dependent balance of material flows in the inventory

the production capacity of the ingredient manufacturing plant (pci^{ii}). For the final ingredient inventory, the amount of the final ingredient stored at the end of time j is,

$$AIS^i_j = AIS^i_{(j-1)} + \sum_r OQ^i_{r,j} + AFIM^i_j - AFIC^i_j \qquad\qquad i \in PFI \cup MFI \qquad (3.23)$$

where $AFIC_j^i$ is the amount of the final ingredient consumed during time j, which is calculated by

$$AFIC_j^i = APM_j \cdot mf^i \qquad i \in PFI \cup MFI \qquad (3.24a)$$

$$APM_j \leq pcp \qquad (3.24b)$$

where mf^i is the mass fraction of final ingredient i in the product formula. APM_j is the amount of product manufactured during the time j, which is less than or equal to the production capacity of the product manufacturing plant (pcp). Moreover, the total inventory should be less than the maximum storage capacity. $SCII^{max}$ and $SCFI^{max}$ are the maximum storage capacity of intermediate ingredient inventory and final ingredient inventory, respectively.

$$\sum_i AIS_j^i \leq SCII^{max} \qquad i \in II \qquad (3.25a)$$

$$\sum_i AIS_j^i \leq SCFI^{max} \qquad i \in PFI \cup MFI \qquad (3.25b)$$

In addition, the inventory level at time (j-1) should ensure that production can proceed in period j,

$$AIS_{(j-1)}^i \geq \lambda \cdot AIIC_j^i \qquad i \in II \qquad (3.26a)$$

$$AIS_{(j-1)}^i \geq \lambda \cdot AFIC_j^i \qquad i \in PFI \cup MFI \qquad (3.26b)$$

where λ is the safe stock coefficient. The mass balance for the product is given below and depicted in parentheses in Figure 3.7.

$$APS_j = APS_{j-1} + APM_j - APD_j \qquad (3.27a)$$

$$APS_j \leq SCP^{max} \qquad (3.27b)$$

Here, APS_j represents the amount of product stored at the end of time j, which is less than or equal to the maximum storage capacity of product inventory (SCP^{max}). APD_j is the amount of product distributed and sold to consumers during time j. APD_j is equal to the expected market demand which is obtained from the pricing model (Eq. 3.15-3.16).

$$APD_j = d_j \tag{3.28}$$

Similar to the inventory planning of ingredients, the stock must guarantee the product availability for the next period.

$$APS_{j-1} \geq \lambda \cdot APD_j \tag{3.29}$$

3.2.4.4.Cost Estimation

Product cost is determined based on the ingredient selected, process design, and supply chain in Eq. 3.5. Product cost consists of material cost, inventory and distribution cost, operating cost (oc_j), and capital cost. In general, ingredient selection determines the material cost and process design influences the capital cost and operating cost. Make-or-buy decisions and supplier selection dominate material purchasing cost, transportation cost, and inventory cost. The detailed models are given below.

Material cost consists of material purchasing cost (mpc_j) and material transportation cost (mtc_j). Material purchasing cost depends on the order quantity and purchasing unit price ($up_{r,j}^i$).

$$mpc_j = \sum_i \sum_r (OQ_{r,j}^i \cdot up_{r,j}^i) \qquad i \in PFI \cup II \tag{3.30}$$

The unit price is influenced by the order quantity. If the order quantity is less than a threshold value (TV_r^i), the unit price is relatively high (hup_r^i). However, a discount price (lup_r^i) can be obtained when the order quantity exceeds the threshold value.[109]

$$up_{r,j}^i = \begin{cases} hup_r^i & OQ_{r,j}^i < TV_r^i \\ lup_r^i & OQ_{r,j}^i \geq TV_r^i \end{cases} \qquad i \in PFI \cup II \tag{3.31}$$

Material transportation cost is assumed to be linearly proportional to the order quantity and distance.

$$mtc_j = \sum_i \sum_r cti^i \cdot OQ_{r,j}^i \cdot SLD_r^i \qquad i \in PFI \cup II \tag{3.32}$$

where cti^i is the cost of transporting 1 unit of ingredient for 1 unit distance and SLD_r^i is the straight line distance of supplier *r* to company inventory.

Inventory and distribution cost is comprised of ingredient inventory cost (iic_j), product inventory cost (pic_j), and product distribution cost (pdc_j). Inventory costs are assumed to be proportional to the inventory levels.

$$iic_j = \sum_i csi^i \cdot AIS_j^i \qquad i \in PFI \cup MFI \cup II \tag{3.33}$$

$$pic_j = csp \cdot APS_j \tag{3.34}$$

where csi^i and csp are the costs of storing one unit of ingredient *i* and product for one period of time, respectively. Product distribution cost is proportional to the amount of product distributed to consumers.

$$pdc_j = cdp \cdot APD_j \tag{3.35}$$

where cdp is the cost of distributing one unit of product to consumers.

Operating cost at time j is proportional to the amount of product and 'make' final ingredients manufactured during time j.

$$oc_j = APM_j \cdot ocp + \sum_i AFIM_j^i \cdot oci^i \qquad i \in MFI \tag{3.36}$$

where ocp represents the operating cost for manufacturing one unit of product. oci^i is the operating cost for manufacturing 1 unit of 'make' final ingredient. For simplicity, ocp and oci^i are assumed to be constant.

The capital investment is based on the power law correlation.

$$CI = ccp_{ref} \cdot \left(\frac{pcp}{pcp_{ref}}\right)^{\varphi} + \sum_i cci_{ref}^i \left(\frac{pci^i}{pci_{ref}^i}\right)^{\varphi} \qquad i \in MFI \tag{3.37}$$

where ccp_{ref} and pcp_{ref} are the capital cost and production capacity of a reference facility for product manufacturing, respectively. cci_{ref}^{i} and pci_{ref}^{i} are the capital cost and production capacity of a reference facility for producing make final ingredient, respectively. φ is the capital scaling factor.

Non-manufacturing cost includes selling and administrative expenses. In this study, only advertisement cost at time j (adc_j) is considered (Eq. 3.7).

$$c_{nm,j} = adc_j \tag{3.38}$$

In summary, the integrated product design, make-or-buy, and supplier selection problem is explicitly formulated as:

$\max NPV$	(Objective function)
s.t. Eq. 3.9-3.10, Eq. 3.12	(Quality)
Eq. 3.15-3.16	(Pricing)
Eq. 3.17-3.29	(Supply Chain)
Eq. 3.30-3.37	(Product cost)
Eq. 3.38	(Nonmanufacturing cost)
Eq. 3.13-3.14	(Economics)
Eq. 3.11	(Bounds)

The design variables consist of product ingredient ($\underline{x}$), process design ($\underline{pd}$), product price (pr), make-or-buy (mob^i), supplier selection ($IS_{r,j}^{i}$), order quantity ($OQ_{r,j}^{i}$), the amount of product manufactured (APM_j), and the amount of intermediate ingredients manufactured ($AFIM_j^{ii}$).

3.2.5. Step 5. Experimental Verification

If the profit target is met, product prototypes can be fabricated based on the product formulation and process design. In this step, the predicted product quality must be verified with experiments and experimental iterations are performed until the design targets are achieved. This aspect of product design has been discussed elsewhere[15,17,18] and is not included in the following case studies. In case the design targets or profit target cannot be met, we should return to Step 2 and generate new ingredient types and candidates. During the iterations, the information of suppliers, product price, manufacturing technologies, etc. can be considered. This action may improve the design efficiency.

3.3.Light Duty Liquid Detergent in the Household and Professional Care Industry

Light duty liquid detergent (LDLD) is widely used for washing hands, dishes, and fabrics. A company wants to design a new LDLD for handwashing of dishes. A bottle of product contains 1 kg liquid detergent. Table 3.3 lists the input parameters including pricing parameters, information of competitor's product, cost coefficients, tax and discount rate, etc. Some of these input parameters are assumed for solving the optimization problem since they are confidential in the chemical industry. However, every effort has been made so that the assumed numbers are reasonable.

Table 3.3 Input parameters in the LDLD example

Parameter	Symbol	Values
Pricing parameter denoting consumer awareness	α	0.7
Pricing parameter related to elasticity	ρ	0.5
Price of competitor's product	P_c	\$3.5 per bottle
Quality score of competitor's product	H_c	0.9
Safety stock coefficient	λ	0.67
Cost of transporting 1 ton ingredient by 1 km	cti	\$0.25/ton/km
Maximum storage capacity of intermediate ingredient inventory	$SCII^{max}$	600 ton
Maximum storage capacity of final ingredient inventory	$SCFI^{max}$	600 ton
Cost of storing 1 ton ingredient for 1 month	csi	\$30
Operating cost for manufacturing one bottle detergent	ocp	\$0.8
Capital cost of a reference facility for detergent production	ccp_{ref}	\$134000
Production capacity of a reference facility for detergent production	pcp_{ref}	85 ton/month

Operating cost for producing 1 ton LAS	oci	\$1000
Capital cost of a reference facility for LAS production	cci_{ref}	\$8.5M
Production capacity of a reference facility for LAS production	pci_{ref}	300 ton/month
Scaling factor for capital cost	φ	0.6
Maximum storage capacity of product inventory	SCP^{max}	6000 ton
Cost of storing one bottle of detergent for 1 month	csp	\$0.0005
Cost of distributing one bottle of detergent	cdp	\$0.05
Advertisement cost in one month	c_{nm}	\$5M
Time for product design and facility construction	n	4 months
Time of product life	m	36 months
Tax rate	tax	0.4
Discount rate	R	0.07
Percentage of annual capital depreciation	De	33.3%

3.3.1. Step 1: Identify Consumer Preferences

The house of quality (Table 3.4) has six product attributes, five technical requirements, and the weighting factors for the product attributes.[25] Note that only the most dominate technical requirement is identified. Cleanliness is related to the technical requirement, soil removal capability (SRC). For liquid detergent, SRC can be simulated by the soil titration experiment where the amount of soils removed by a certain amount of detergent is measured. The detailed information for performing soil titration experiments is elaborated by Gambogi et al.[110] The foaming ability is quantified by the Ross-Mile Foam Height ($RMFH$).[111] Clearly, large SRC and $RMFH$ are preferred. The attribute of quickly dispersed and dissolved is related to the viscosity. A detergent with low viscosity ($VISC$) is likely to disperse and dissolve in water quickly to achieve detergency. The pH must be close to that of human skin so that the detergent is not irritating. Clear point ($CLPT$) is the temperature at which cloudy liquid turns clear upon warming. Low clear point can maintain the transparency of an aqueous liquid detergent, an important product attribute. The preference scores of the six product attributes are calculated by Eq. 3.39-3.44 based on the five technical requirements. Then, with the weighting factors in Table 3.4, the preference function H for LDLD can be computed. Moreover, design targets are set (i.e., $RMFH \geq 8\ cm$, $SRC \geq 95\ \%$, $250 \leq$

$VISC \leq 400\ cSt$, $CLPT \leq 5$ ℃, and $5.5 \leq pH \leq 7.5$) so that the preference scores are larger than 0.8. This is to ensure that high product quality can be achieved.

Table 3.4 Identified product attributes and technical requirements of LDLD

	Technical requirements					
Attributes	SRC	RMFH	Viscosity	pH	Clear point	Weights
Cleanliness	Eq. 3.38					0.35
Foaming-ability		Eq. 3.39				0.24
Quickly dispersed and dissolved			Eq. 3.40			0.16
Non-irritating to hands				Eq. 3.41		0.15
Transparency					Eq. 3.42	0.06
Stability			Eq. 43			0.04

Eq. 3.39: $y_c = \frac{1}{1+e^{\frac{92.5\%-SRC}{1.75\%}}}$ Eq. 3.40: $y_f = \frac{1}{1+e^{10.3-RMFH}}$ Eq. 3.41: $y_q = \frac{1}{1+e^{\frac{VISC-400}{20}}}$

Eq. 3.42: $y_n = 1 - \left(\frac{pH-6.5}{2}\right)^2$ Eq. 3.43: $y_t = \frac{1}{1+e^{\frac{2.5-CLPT}{1.875}}}$ Eq. 3.44: $y_s = \frac{1}{1+e^{\frac{VISC-250}{20}}}$

3.3.2. Step 2: Determine Ingredient Types and Generate Ingredient Candidates

Table 3.4 shows the required ingredient types for LDLD and their functions.[110] Surfactants are used to remove soils. Foam booster can promote foaming and stabilize the generated foam. Buffers are added to control pH and viscosity. Minor additives provide multiple attributes such as color, smell, anti-microbial, and so on. Specific ingredient candidates for consideration in this case study are also identified for the new LDLD.

3.3.3. Step 3: Select Ingredients and Design Processes

The process flowsheet for LDLD production consists of mixers and a homogenizer (Figure 3.8). Surfactant, stabilizer, solvent, and buffer are added into a mixer for pre-mixing. The pre-mixed mixture is fed into a homogenizer to form a homogeneous product. Then, minor additives are mixed

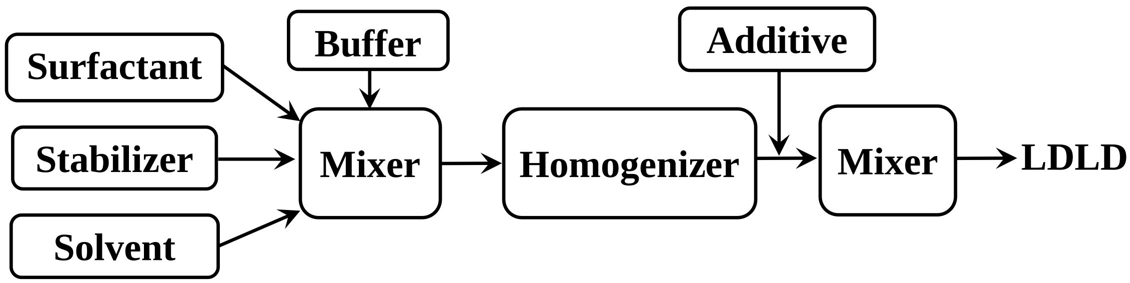


Figure 3.8 General flowsheet structure for LDLD manufacturing

Table 3.5 The required ingredient types for LDLD and CRG herbicide and the generated ingredient candidates

	Ingredient types	Functions	Chemical candidates
LDLD	Surfactant	Lower surface tension between soils and water to facilitate soil removal	LAS, AEO, AEOS
	Buffer	pH and viscosity control	NaOH, NaCl
	Foam booster	Promote foaming and stabilize foam	DEA, TEA, CDEA
	Minor additives	Color, smell, anti-microbial	Formalin, fragrance
	Solvent	Dissolve other ingredients	Water
CRG herbicide	Active ingredient	Kill weeds and retard the regrowth of weeds	24D, MCPA, Metolachlor
	Filler	Offer a solid base to make up granules and control AI release	Starch, lignin, cellulose, PCL
	Binder	Bind all solid particles together	PVP
	Minor additives	Color, flow-ability, etc.	Pigment, gelatin, etc.

LAS: linear alkyl benzene sulfonate; AEO: alcohol ethoxylate; AEOS: alcohol ethoxysulphate;
DEA: diethanolamine; TEA: triethanolamine; CDEA: coconut diethanolamine;
24D: 2,4-dichlorophenoxyacetic acid; MCPA: 2-methyl-4-chlorophenoxyacetic acid;
PCL: polycaprolactone; PVP: Polyvinylpyrrolidone

in to generate the LDLD. For minor additives, only formalin is considered for antimicrobial purpose and its mass fraction is fixed as 0.2%. Product quality is decided by the selection and composition of surfactant, stabilizer, and buffer. For proper ingredient selection, correlation models for predicting the five technical requirements are constructed here. Using the ingredient candidates generated in Table 3.5, Chan and Kavanagh[111] prepared 20 different LDLD formulas and measured the five technical requirements. For each formula, the mass fraction (mf) of selected ingredients and the measured technical requirements are listed in Table S3.1 in Supporting Information. For simplicity, the Supporting Information is provided in https://github.com/zx2012flying/Thesis-Supporting-Information/blob/master/Supporting%20Information%20in%20Chapter%203.docx. Based on these experimental data, linear equations are regressed to calculate the five technical requirements (Eq. 3.45-3.49). The mean absolute percentage errors, as a measure of statistical accuracy, are less than 10% (Table S3.2 in Supporting Information). Note that if a candidate is selected, its mass fraction is larger than zero. Otherwise, the mass fraction is equal to 0.

$$RMFH = 4.14 + (0.86mf^{LAS} + 0.06mf^{AEO} + 0.28mf^{AEOS}) + (0.6mf^{DEA} - 0.17mf^{TEA} + 0.4mf^{CDEA}) \tag{3.45}$$

$$SRC = -17.25 + (12.46mf^{LAS} + 9.56mf^{AEO} + 4.99mf^{AEOS}) - (1.06mf^{DEA} + 1.27mf^{TEA} - 16.59mf^{CDEA}) \tag{3.46}$$

$$VISC = -31.68 - (3.31mf^{LAS} - 1.78mf^{AEO} + 0.15mf^{AEOS}) + (19.34mf^{DEA} + 15.59mf^{TEA} + 5.79mf^{CDEA}) + (43.02mf^{NaOH} + 13.62mf^{NaCl}) \tag{3.47}$$

$$CLPT = -55.43 + (41.73mf^{LAS} + 4.72mf^{AEO} + 0.57mf^{AEOS}) - (99.27mf^{DEA} + 83.03mf^{TEA} + 1.49mf^{CDEA}) - (251.77mf^{NaOH} - 36.54mf^{NaCl}) \tag{3.48}$$

$$pH = 6.56 - 4.42mf^{LAS} + (12.46mf^{DEA} + 9.38mf^{TEA} + 0.70mf^{CDEA} + 31.17mf^{NaOH} \tag{3.49}$$

where the superscripts *LAS, AEO, AEOS, DEA, TEA,* and *CDEA* represent the ingredient candidates listed in Table 3.5.

3.3.4. Step 4: Economic Analysis and Profit Maximization

3.3.4.1.Pricing

The pricing model in Eq. 3.15-3.16 is employed. The information of the main competitor's product is listed in Table 3.3. Its price is assumed to be \$3.5/bottle (1 kg) and the preference score is 0.9. The pricing model parameters are fixed. One month is considered as one period in the planning horizon. The market size of LDLD in the summer is assumed as \$42M per month from May to August, but \$28M per month from November to February. The remaining months are \$35M per month.

3.3.4.2.Make-or-Buy Analysis

The objective of the make-or-buy analysis is cost reduction. Therefore, the heuristics relating to economics in Table 3.2 are considered. All the ingredient purities are required to be larger than 95%. It is assumed that the company owns the technologies to produce the LAS in-house by sulphonation of linear alkylbenezenes (LAB) with oleum and then neutralized with NaOH. As shown in Table 3.6, the maximum purity and production capacity can be up to 99% and 1000 ton/month, respectively. When the company decides to make LAS in-house, LAS becomes the only element in the MFI set.

3.3.4.3.Supplier Selection

The supplier selection model in Eq. 3.18-3.29 are applied here. Table 3.6 lists the detailed information of qualified suppliers for LAS such as purity, plant location, price, etc. The location of the production site is at the origin (0, 0) and the suppliers' locations are given in X-Y coordinates. The estimated cost for manufacturing 1 ton LAS in-house is \$3400. The supplier information for other final and intermediate ingredients is provided in Table S3.3 in Supporting Information.

Table 3.6 Supplier information for LAS in the LDLD example

	LAS						
Supplier	1	2	3	4	5	6	In-house
Purity	95%	96%	97%	98%	95%	95%	up to 99%
Plant location	(-115, 972)	(-1160, 187)	(100, 1163)	(400, 150)	(-200, 694)	(181, 1190)	(0, 0)
MPC* (ton/m)	400	800	400	160	350	1500	up to 1000
MOQ* (ton)	5	20	1	1	20	20	/
Price ($/ton)	< 50 t, 3750 ≥ 50 t, 3250	< 100 t, 3250 ≥ 100 t, 3000	< 20 t, 3900 ≥ 20 t, 3400	< 20 t, 3750 ≥ 20 t, 3500	< 100 t, 3000 ≥ 100 t, 2630	< 100 t, 3000 ≥ 100 t, 2750	3400**

*MPC: maximum production capacity MOQ: minimum order quantity. ** Estimated cost for producing LAS in-house

3.3.4.4.Cost estimation

The product costs are calculated using Eq. 3.30-3.37. The cost coefficients are listed in Table 3.3. Before manufacturing starts, net working capital is assumed to be 10% of capital investment.

3.3.5. Results

Four scenarios for this case study are discussed to demonstrate the application of the proposed framework. In Scenario 1, the traditional method, the purchasing department acquires the ingredients selected by the R&D team. In Scenario 2, the integrated approach which is proposed in Eq. 3.1-3.8 is employed. The new method represents an integrated design and supply chain team that conducts product design and materials purchasing concurrently. The solutions are then compared to show how the integrated approach improves profit. In Scenario 3, ingredient purity is required to be larger than 98%, instead of 95% in Scenario 1 and 2. Scenario 4 considers the impact of make-or-buy decision on product formulation.

The optimization problem was coded in GAMS 24.7.4 and solved by using the MINLP solver DICOPT. Note that due to the inherent non-convexity, global optimum cannot be guaranteed. To improve the quality of the solutions, different initial values were used and the best results are reported.

3.3.5.1.Scenario 1: Traditional Method

Again, the ingredients are selected by product designers to hit the design targets. Then, the ingredient suppliers are selected using the fixed formula by the supply chain department. The results are presented in the first column of Table 3.7. LAS is selected as the surfactant because of its strong foaming ability and soil removing capability. Both TEA and CDEA are used as stabilizer and NaOH is used to control the pH as LAS is acidic. Moreover, Table 3.6 shows that the purity of all the LAS provided by the suppliers meet the minimum requirement (≥ 95%) and suppliers' products are cheaper. It is assumed that the company does not own the manufacturing technologies for other ingredients. Therefore, all ingredients are purchased externally. In this case, the NPV of the base case formula is equal to $72.5 M.

Table 3.7 Computational results for the LDLD example

		Scenario 1	Scenario 2	Scenario 3	Scenario 4
Product formula (mass fraction)	LAS	9.12%	7.41%	5.07%	6.75%
	AEO	/	/	/	/
	AEOS	/	/	2.71%	/
	DEA	/	1.43%	1.60%	1.78%
	TEA	0.72%	/	/	/
	CDEA	1.46%	2.18%	3.62%	2.45%
	NaOH	1.01%	0.44%	/	0.20%
	NaCl	/	/	/	/
	Additives	0.20%	0.20%	0.20%	0.20%
	Water	87.49%	88.34%	86.80%	88.62%
Technical requirements	RMFH(cm)	12.4	12.3	11.7	12.0
	VISC (cSt)	303.6	304.1	307.2	306.3
	CLPT(°C)	-2.3	-2.2	-6.7	-3.4
	SRC (%)	119.3	109.7	117.7	105.7
	pH	6.8	6.8	6.6	6.7
Quality score		0.96	0.96	0.95	0.96
Product cost ($/bot)		1.29	1.25	1.36	1.23
Price ($/bottle)		3.4	3.3	4.1	3.5
Demand (M bottle/year)		54.3	55.2	38.9	51.2
Market share		43.7%	43.8%	38.4%	42.6%
Capital investment (M$)		1.6	1.6	1.3	9.6
NPV (M$)		72.5	75.2	63.8	67.3

3.3.5.2.Scenario 2: Integrated Approach

The results for integrated product design and supplier selection are shown in the second column of Table 3.7. All the ingredients are again purchased externally. Comparing with the base case, less LAS is used and thus less NaOH is needed to maintain the pH. DEA and CDEA are selected as stabilizers, instead of TEA and CDEA. Although the new formula uses a smaller amount of the key ingredients (i.e., surfactant, stabilizer, and buffer), the quality score is still maintained at 0.96. The product cost is lower than that of the base case formula and the NPV is raised to $75.2M.

Figure 3.9 shows the order quantities during the first 12 months. LAS, DEA, and CDEA are procured every month to lower inventory costs since their monthly demands are large. Nonetheless, since the monthly demands of NaOH and formalin are small, they are purchased in large quantities periodically at discount prices and then used for the subsequent several months.

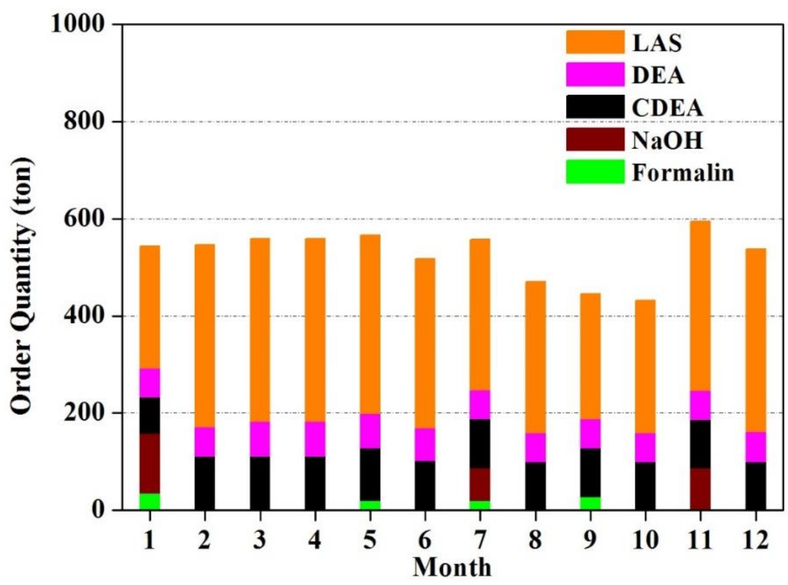


Figure 3.9 Ingredient order quantity in the first 12 months in Scenario 2 for LDLD example

3.3.5.3.Scenario 3: Higher Purity Constraint and Buy Option

In this scenario, all the ingredient purities are required to be larger than 98% for quality assurance. Table 3.6 shows that only the supplier 4 fulfills this requirement, but the supply capacity

(160 ton/month) is not sufficient to meet the demand. In this situation, if we adjust the product formula to the amount of LAS that is available on the market, the optimization results are listed in the third column of Table 3.7. The mass fraction of LAS is reduced to 5.07% and another surfactant AEOS is added. Furthermore, product price is increased to $4.1 per bottle and annual demand is decreased to 38.9 million bottles. The NPV is decreased to $63.8 M.

3.3.5.4.Scenario 4: Higher Purity Constraint and Make Option

It is now assumed that the company makes 98% LAS in-house to meet the demand when the quality of available ingredients does not meet requirement. The input data (e.g., operating cost, capital cost, etc.) for the make option are listed in Table 3.3. The results are shown in the fourth column of Table 3.7. Comparing with Scenario 3, only LAS is used, the product cost is reduced, and the quality score increases. Furthermore, due to a lower product price, a larger market share is achieved. Although the capital investment is increased to $9.8M due to the construction of LAS manufacturing facility, the NPV is increased to $67.3M.

3.4.Controlled Release Granule Herbicide in the Agrochemical Industry

Herbicides have been used to kill undesired broadleaf weeds while leaving the crops to grow unmolested. Traditional herbicide is easily lost due to rainwater washing, leaching, and volatilization. To reduce herbicide loss, it can be produced in the form of controlled release granule (CRG) where active ingredient (AI) is uniformly dispersed within a polymeric matrix. An agrochemical company wants to develop a new CRG herbicide formula. The input parameters including granulation model parameters, pricing model parameters, information of competitors' product, cost coefficients, etc. are listed in Table S3.4 in Supporting Information.

3.4.1. Step 1. Identify Consumer Preferences

Table 3.8. Identified product attributes and technical requirements in CRG herbicide example

Attributes	Technical requirements: Coverage area	Time for 50% AI release	Time for 85% AI release	Tensile strength	Mean diameter	Weights
Large coverage area	Eq. 3.50					0.32
Efficiently kill weed		Eq. 3.51				0.32
Duration to retard weed regrowth			Eq. 3.52			0.16
Hardness				Eq. 3.53		0.1
Ease of use					Eq. 3.54	0.1

Eq. 3.49: $y_c = \frac{1}{1+e^{\frac{0.0777-A_{cr}}{0.0222}}}$ Eq. 3.50: $y_k = 1 - \left(\frac{T_{50}-7}{5}\right)^2$ Eq. 3.51: $y_r = 1 - \left(\frac{T_{85}-21}{4}\right)^2$

Eq. 3.52: $y_h = \frac{1}{1+e^{\frac{100-\sigma_{ts}}{20}}}$ Eq. 3.53: $y_e = 1 - \left(\frac{d_m-800}{350}\right)^2$

The identified product attributes and technical requirements are shown in Table 3.8. Large coverage area is desired by farmers. The AI should be released at a fast rate at the beginning to quickly kill weeds, followed by a lower rate to retard the regrowth of weeds. The AI release profile is represented by two variables: the time for 50% and 85% AI release (T_{50} and T_{85}). The former corresponds to the efficiency of killing weeds and the latter stands for the duration of retarding weed regrowth. Moreover, tensile strength (σ_{ts}) must be sufficiently large so that the granules are not easily deformed. For ease of use, the mean diameter (d_m) should be neither too large nor too small to avoid uneven and inconvenient spreading. Eq. 3.50-3.54 are used to calculate the preference scores of the five attributes. Moreover, design targets are fixed (i.e., $\sigma_{TS} \geq 115\ Pa$, $600 \leq d_m \leq 1000\ \mu m$, $A_{cr} \geq 0.045$ hectare, $4.5 \leq T_{50} \leq 9.5$ days, and $9.5 \leq T_{85} \leq 23.5$ days) so that all the preference scores are larger than 0.7.

3.4.2. Step 2. Determine Ingredient Types and Generate Ingredient Candidates

Table 3.5 shows the typical ingredient types in the CRG herbicide and their functions. In addition to the AI, polymeric filler, and binder, minor additives are added to provide color and enhance particle flowability. Moreover, for each ingredient type, several typical ingredient candidates are given in Table 3.5.[112] . For instance, the commonly used filler includes starch, lignin, cellulose, and polycaprolactone.

3.4.3. Step 3. Select Ingredients and Design Processes

In this example, for simplicity, only one candidate of AI, filler, and binder is selected and the minor additives are not considered. The process flowsheet consists of a blender pre-mixing the AI, filler, and additive particles. Then, the mixed ingredients are fed into the granulator where binder liquid is sprayed on the solid particles to form granules (Figure 3.10). Mechanistic granulation models have been developed to calculate the technical requirements (e.g., mean diameter, tensile strength) of the granules [113]. The technical requirements are determined by ingredient properties (e.g., density, contact angle, diffusion coefficient) and operating conditions of the granulator. The detailed models are given in Appendix (Eq. A3.1-A3.19).

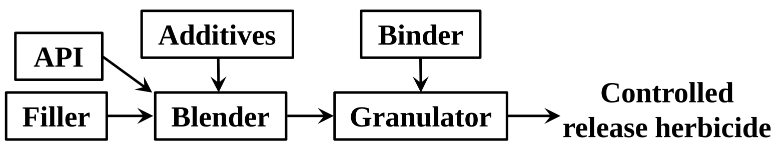


Figure 3.10 General flowsheet structure for CRG herbicide manufacturing

3.4.4. Step 4. Economic Analysis and Profit Maximization

3.4.4.1.Pricing

The market demand is calculated using the pricing model with the input parameters in Table S3.4 in Supporting Information. One period of time is one quarter of the year. Usually, farmers use herbicide in the spring and autumn to kill weeds before seeding. Thus, it is assumed that the market sizes in these two seasons are \$50 M per season. The market sizes in summer and winter are negligible compared with those of spring and autumn.

3.4.4.2.Make-or-buy Analysis

It is assumed that the company has an initial capital budget of \$5M. 2,4-dichlorophenoxyacetic acid (24D) and 2-methyl-4-chlorophenoxyacetic acid (MCPA) are widely used. The company does not own the technology to manufacture 24D nor MCPA. The metolachlor is a relatively new herbicide, which was commercialized in 1996. It is assumed that the company has developed a low-cost technology to synthesize metolachlor from two intermediate ingredients (CAC and MEA). The production capacity can be up to 300 ton/quarter. Therefore, if metolachlor is selected as AI, it can be either purchased externally or made in-house. Moreover, the candidates for filler and binder are commonly-used chemicals and many qualified suppliers can be found in the market. The objective of make-or-buy analysis is simply to reduce cost.

3.4.4.3.Supplier Selection

The aforementioned supplier selection model in Eq. 3.18-3.29 is applied. Table S3.5 in Supporting Information provides the required supplier information for the candidates of AIs, fillers, and binder and the intermediate ingredients (i.e., CAC and MEA) for making metolachlor.

3.4.4.4.Cost Estimation

Product cost is calculated based on Eq. 3.30-3.37 using the cost coefficients listed in Table S3.4 in Supporting Information. The net working capital is assumed to be 10% of capital investment.

3.4.5. Results

Three scenarios are discussed. In Scenario 1, the design problem is solved using the integrated approach. In Scenario 2 and 3, it is assumed that management decides to go for the newer AI metolachlor. Given different capital budgets, the impacts of making or buying metolachlor on the product formula and product profit are considered.

Table 3.9 Computational results for the CRG herbicide example

		Scenario 1		Scenario 2		Scenario 3	
Product formula (mass fraction)	AI	24D:	3.1%	Metolachlor:	2.0%	Metolachlor:	2.6%
	Filler	Lignin:	63.0%	Lignin:	70.0%	Lignin:	84.7%
	Binder	PVP:	33.9%	PVP:	28.0%	PVP:	12.7%
Average shear rate (s^{-1})		2104		2041		2096	
Technical requirements	TS (N/m^2)	469		345		132	
	d_{50} (μm)	727		751		726	
	T_{50} (days)	5		5		5	
	T_{85} (days)	22		23		22	
	A_{ca} (hectare)	0.13		0.1		0.13	
Preference score		0.89		0.81		0.87	
Product cost ($/bag)		15.9		14.7		12.9	
Price ($/bag)		33.9		31.0		36.5	
Demand (k bag/year)		473		518		394	
Market share		16%		16%		14%	
Capital investment (M$)		3.6		3.7		9.8	
NPV (M$)		15.6		13.9		11.5	

3.4.5.1.Scenario 1: Integrated Approach

The product design problem is solved using the integrated approach. The results are listed in the first column of Table 3.9. 24D is used as AI since it already can meet the design targets and the cost is less than the other two AIs. Lignin is used as filler. Since the company does not possess the technologies for manufacturing 24D and lignin, they are purchased externally. The NPV is $15.6M.

3.4.5.2.Scenario 2: Buy Metolachlor

In this scenario, the newer metolachlor is selected as AI. Since the initial capital budget is limited to $5M, the company cannot afford the extra expenses for the construction of a new metolachlor production facility. Hence, it is decided to purchase metolachlor externally. A new product formula is generated in the second column of Table 3.9. The new product formula has a lower preference score. In order to compete in the market, product price is decreased to $31/bag. Compared with the results of Scenario 1, the profit margin is lower. The NPV is reduced to $13.9M.

3.4.5.3.Scenario 3: Make Metolachlor In-house

The company plans to increase the capital budget up to $10 M and make metolachlor in-house by using the low-cost technology. The results are listed in the third column of Table 3.9. The product cost is reduced to $12.9 per bag. Compared with the results in Scenario 2, the preference score and product price are higher, resulting in a larger profit margin. However, due to the extra expenses on metolachlor manufacturing facilities, the capital investment is increased to $9.8M. Finally, the NPV drops to $11.5M. Therefore, making metolachlor in-house is not recommended.

3.5.Conclusion

This chapter presents a new product design framework with the simultaneous consideration of make-or-buy analysis and supplier selection. This framework can tell the product designers when and how the two issues should be incorporated to generate a more profitable product. To the best of our knowledge, this is the first attempt in the literature to develop such a systematic approach in the process systems engineering community. Chemical ingredients are classified into various types based on the functionalities. For each type, many ingredient candidates can be generated from databases and computer-aided tools. Then, proper ingredients are selected out of the candidates to form a product. This is followed by economics analysis consisting of pricing, make-or-buy analysis, supplier selection, and cost estimation are performed to maximize the profit. The framework is demonstrated using two examples: light duty liquid detergent and controlled release granular herbicide. In each example, various scenarios are discussed to illustrate how make-or-buy analysis and supplier selection can affect the ingredient selection, product quality, and cost which finally determine product profitability.

This study is an extension and elaboration of the proposed Grand Product Model, which integrates most of the important issues related to product design, such as ingredient selection, process design, microstructure design, product cost, government policy, etc. The continuous progress towards a complete product design model is inevitable for the success of product design. The extension to product sustainability is in progress.

3.6.Appendix: Mechanistic Models for Calculating CRG Technical Specifications

The tensile strength σ_{TS} can be calculated as [113]

$$\sigma_{ts} = C \cdot S \cdot \frac{1-\varepsilon}{\varepsilon} \cdot \frac{\gamma \cdot cos\theta}{d_m} \tag{A3.1}$$

Here, the material constant C is equal to 6 by assuming that solid particles are spheres. ε is the porosity of the granules. γ and θ are the binder surface tension and contact angle, respectively. S is the liquid saturation of a wet granule as calculated by

$$S = MC \cdot \frac{\rho_s}{\rho_l} \cdot \frac{1-\varepsilon}{\varepsilon} \tag{A3.2}$$

where ρ_s and ρ_l are the true density of solids (i.e., AI and filler) and liquids (i.e., binder) in the CRG, respectively. MC is the moisture content which is the ratio of liquid mass to dry solid mass.

$$MC = \frac{mf^B}{mf^{AI} + mf^F} \tag{A3.3}$$

where mf^{AI}, mf^F and mf^B are the mass fraction of AI, filler, and binder, respectively.

The formation of granule is modelled by considering two key mechanisms: coalescence and breakage [113]. Large granule forms as a result of successful coalescence of smaller particles and then they can also break into pieces when they are so large that the collisions between granules deform themselves. Thus, d_m is calculated based on two critical sizes: the critical size for coalescence (d_{coal}^{cr}) and for deformation (d_{def}^{cr}). The granule size is finally decided by the relative values of these two sizes. Assuming $d_{coal}^{cr} < d_{def}^{cr}$, the mean diameter will stabilize at a size between d_{coal}^{cr} and d_{def}^{cr} as shown

$$d_m = (1 - f_1) \cdot d_{coal}^{cr} + f_1 \cdot d_{def}^{cr} \quad \text{(A3.4)}$$

Here, f_1 implies the importance of layering on the granule growth which is assumed to be 0.6. The values of two critical sizes depend on either capillary or viscous effect that holds the granule together. Generally, for most industrial granulation processes that have high shear rates, viscous effect dominates. Thus, the two sizes are calculated as

$$d_{coal}^{cr} = 2(\frac{9\mu\cdot\left(1+\frac{1}{e}\right)\ln(\frac{h}{h_a})}{8\rho_p\cdot\dot{\omega}}) \quad \text{(A3.5)}$$

$$d_{def}^{cr} = 2\left(\frac{2\tau_y\cdot St_{def}^*}{\rho_p\cdot\dot{\omega}^2}\right)^{0.5} \quad \text{(A3.6)}$$

Here, μ and e are the binder dynamic viscosity (0.001-0.03 Pa·s, depending on the concentration of PVP solutions) and coefficient of restitution (0.5). h/h_a represent the ratio of asperities over liquid layer which is assumed to be 5. $\dot{\omega}$ is the average shear rate inside the granulator which is the process design variable. τ_y and St_{def}^* are yield stress (3000 Pa) and critical Stokes' number for deformation (assumed as 0.5). ρ_p is the particle density which is calculated by considering the porosity within the granule.

$$\rho_p = \rho_{gt}(1 - \varepsilon) \quad \text{(A3.7)}$$

where ρ_{gt} is the granule true density as expressed by

$$\rho_{gt} = \frac{M_{gt}}{V_{gt}} = \frac{M_{gt}}{\frac{M_{gt}\cdot mf^{AI}}{\rho^{AI}}+\frac{M_{gt}\cdot mf^{F}}{\rho^{F}}+\frac{M_{gt}\cdot mf^{B}}{\rho^{B}}} \Rightarrow \left(\frac{mf^{AI}}{\rho^{AI}} + \frac{mf^{F}}{\rho^{F}} + \frac{mf^{B}}{\rho^{B}}\right)\rho_{gt} = 1 \quad \text{(A3.8)}$$

In the granulator, granules gradually consolidate to a lower porosity. Since the viscous effect dominates, a model featuring inter-particle gap distance can be used as a measure of porosity. The reduction in inter-particle gap distance increases with increasing Stokes' number for viscous effect. By replacing gap distance in the equation by Ennis et al., [114] with $2(h_0 - h)$, the following equation can be obtained.

$$\frac{d\varepsilon}{dh} = \frac{3(1-\varepsilon)}{0.5d_m+h} \quad \text{(A3.9)}$$

where h is the thickness of binder liquid layer which is calculated by.

$$h = \frac{h_0}{2}(1 + e^{-St_v}) \quad \text{(A3.10)}$$

where h_0 is the liquid layer thickness before consolidation (assumed to be 100 μm). The Stokes' number St_v is written as

$$St_v = \frac{2\rho_p \cdot \dot{\omega} \cdot d_m^2}{9\mu} \quad \text{(A3.11)}$$

Assuming h is equal to 0 and the spheres are random close packing, the theoretical maximum porosity is 0.36. Based on this initial condition, Eq. A3.12 is obtained by integrating Eq. A3.9.

$$\frac{1-\varepsilon}{1-0.36} = \left(\frac{0.5d_m}{0.5d_m+h}\right)^3 \quad \text{(A3.12)}$$

The coverage area is proportional to the mass fraction of AI in the granule.

$$A_{cr} = \frac{m_{CRG} \cdot mf^{AI}}{F^{AI}} \quad \text{(A13)}$$

Here, m_{CRG} represents the mass of one bag herbicide product (5 kg) and F^{AI} denotes the mass of AI needed for treating 1 hectare land.

AI release is controlled by two mechanisms: the dissolution of granule and AI diffusion within the granule. When either starch or lignin is used as filler, the release is controlled by the AI diffusion from the interior of a granule into the soil. Diffusion within a granule can be modeled using Fick's second law and the percentage $p^{df}(t)$ of the released AI at time *t* is calculated by

$$p^{df}(t) = 1 - \frac{6 \times \sum_{m=1}^{\infty}\left(\frac{1}{m^2} \cdot e^{-\frac{4m^2 \cdot \pi^2 \cdot D^F \cdot t}{d_m^2}}\right)}{\pi^2} \quad \text{(A3.14)}$$

Here, D^F is the filler's diffusion coefficient. Thus, if $p^{df}(t)$ is set equal to 50%, the corresponding T_{50}^{df} is expressed as

$$\sum_{m=1}^{\infty}\left(\frac{1}{m^2}\cdot e^{-\frac{4m^2\cdot\pi^2\cdot D^F\cdot T_{50}^{df}}{d_m^2}}\right) = (1-0.5)\times\frac{\pi^2}{6} \quad \text{(A3.15)}$$

In the same manner, the time for 85% AI release (T_{85}^{df}) is calculated as

$$\sum_{m=1}^{\infty}\left(\frac{1}{m^2}\cdot e^{-\frac{4m^2\cdot\pi^2\cdot D^F\cdot T_{85}^{df}}{d_m^2}}\right) = (1-0.85)\times\frac{\pi^2}{6} \quad \text{(A3.16)}$$

If either cellulose or PCL is applied as filler, the release of AI depends on their dissolution rates. In this case, the percentage $p^{ds}(t)$ of the released AI at time *t* is calculated as

$$p^{dS} = 1 - \left(1 - \frac{2k^F\cdot t}{\rho_p\cdot mf^F\cdot d_m}\right)^3 \quad \text{(A3.17)}$$

Here, k^F is the dissolution rate constant of the filler. Therefore, the T_{50}^{ds} and T_{85}^{ds} are equal to

$$T_{50}^{ds} = \frac{(1-\sqrt[3]{0.5})\cdot\rho_p\cdot mf^F\cdot d_m}{2k^F} \quad \text{(A3.18)}$$

$$T_{85}^{ds} = \frac{(1-\sqrt[3]{0.2})\cdot\rho_p\cdot mf^F\cdot d_m}{2k^F} \quad \text{(A3.19)}$$

Note that the detailed derivation of Eq. A3.14 and A3.17 was written in the Chapter 5 of Seider, et al.[25]

Chapter 4: Sustainable Product Design: A Life-Cycle Approach

4.1.Introduction

Product design plays an increasingly important role in the chemical industry[3] and much progress has been made in the past two decades. In teaching, several books have been published.[25,115-117] In research, different approaches such as model-based methods, rule-based methods, databases, and experiments have been used to design perfume,[86] paint,[87] inkjet ink,[29] smart window,[118] etc. Moreover, the Grand Product Design model has been proposed to capture the conceptual relationships among various product design tasks (e.g., ingredient selection, process design, costing, etc.).[2] Recently, it has been expanded by incorporating the influence of business and management issues such as pricing,[36] government policy and corporate social responsibility.[90] With the depletion of natural resources and awareness of the damage to the environment, the quest for sustainability has been recognized. Many perspective papers identified the needs and opportunities to move towards sustainability.[119-122] In this chapter, we focus on the design of sustainable chemical products.

Sustainability consists of economic, environmental, and social (EES) pillars. Sustainable product can be considered as a product that has minimal EES impact over its life cycle.[123] Figure 4.1 shows the generic product life cycle including raw material production, product manufacturing, and product use. At end of use, some can be recycled by recovering certain ingredients for manufacturing the same product or other products. Otherwise, the product is disposed by landfill or incineration. The arrows denote the transportation of materials and products. To assess product sustainability, the state-of-the-art life cycle sustainability assessment (LCSA) framework was proposed.[124,125] In this framework, life cycle costing (LCC) which aggregates all costs related to a product over its life cycle is used to assess the economic impact. In addition, life cycle assessment

(LCA) and social life cycle assessment (SLCA) are used to evaluate the environmental and social impact, respectively. Accordingly, LCSA = LCC + LCA + SLCA.[124] While LCSA provides in principle quantitative results, its applicability relies on the availability of accurate life cycle inventory (LCI) data which accounts for the input and output of processes involved in a product life cycle.[126] In practice, collecting LCI data is time-consuming and there are limited LCI data for most processes. Alternatively, rule-based methods can be applied to qualitatively assess sustainability for decision-making. The one often used is the sustainability checklist consisting of various questions related to the major EES impact at each life cycle stage.[126-128] Although rule-based methods cannot generate quantitative and holistic results, it is useful to screen design alternatives in the early phase of sustainable product design.

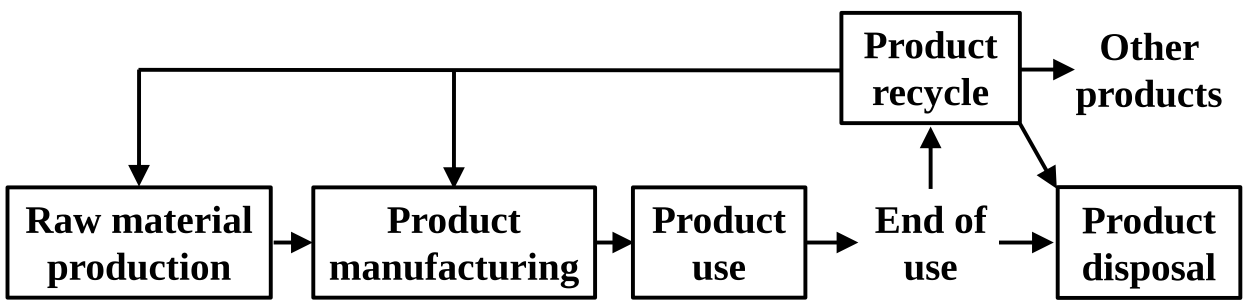


Figure 4.1. Generic product life cycle

As the EES impact at each life cycle stage can vary for different products, different solutions are needed to improve product sustainability. At present, many general principles, guidelines, and tools can be used to reduce the EES impact of a product at different life cycle stages.[129-133] For instance, Go et al.[131] listed the guidelines to design products that can be easily recycled. Heintz et al.[133] developed a computer-aided molecular design tool to design bio-based products. However, re-designing a product with improvement at one single life cycle stage cannot ensure a sustainability improvement in the entire life cycle. General sustainable product design solutions cannot be used alone and must be applied in conjunction with life-cycle-based sustainability assessment tools. Thus, a framework integrating general sustainable product design solutions and life-cycle-based assessment tools is highly desired.

So far, many sustainable product design frameworks have been proposed. For instance, Badurdeen et al.[134] proposed a multi-objective optimization framework for ingredient selection to minimize life-cycle-based economic and environmental impact of a product. Ahmad et al.[132] found that most of the existing product design frameworks only focused on economic and environmental aspects of product sustainability. To fill this gap, LCSA and sustainability checklist can be used to assess all three dimensions of sustainability. However, these approaches have only been used to evaluate given products. No one considered how these methods can be integrated into a systematic framework for designing sustainable chemical products.

In this chapter, a generic framework is developed where LCSA, rule-based methods, and general sustainable product design principles and knowledge are properly integrated. If the needed LCI data are available, the most sustainable product is obtained through optimization. Otherwise, the sustainable design alternative is identified using sustainability checklist. This framework that can be utilized in different phases of sustainable product design has two major novelties. First, the generic and coherent framework incorporates rule-based and model-based methods for sustainable chemical product design. Second, LCSA is incorporated into optimization to provide a comprehensive and quantitative view of the EES aspects of sustainability. The chapter is organized as follows. First, the sustainable product design problem is described. Then, the proposed framework is elaborated to solve the sustainable product design problem. Finally, two case studies–composite bumper beam and lithium ion battery–are provided to illustrate the applicability of the framework.

4.2.Problem Statement

Figure 4.2 shows how sustainability can be achieved in product design. All icons except sustainability (i.e., ingredient, process design, product cost, consumer preferences, product quality, supply chain, and government policies) are extracted from the Grand Product Design Model.[2] Starting at the middle, a base-case product can be generated based on consumer preferences. The ingredients and manufacturing process of the base-case product are identified to ensure that its quality meets consumer needs. Then, a more sustainable product will be designed through analyzing and improving the base-case product. The new product must fulfill the consumers' requirements. The sustainability icon (at the top) contains the information on the way in which the product is disposed and recycled, including the available recycle processes and possible collection rate. Conceptually, sustainability is related to ingredient selection,[135] process design,[136-138] supply chain,[139,140] consumer preference,[141] and government policy[142] as captured in Figure 4.2. Clearly, the design space is very broad and it is not practical to use rigorous models for considering the variations of all these variables. In this study, to ensure that the problem is tractable and solvable, only the selection of ingredient, process, and end-of-use strategy are varied. The consumer preferences are fixed. The variations of government policy and supply chain are not considered. Also, only a limited number of product design alternatives will be generated based on which the sustainable product is obtained. Accordingly, the problem to be formally addressed is as follows. First, the new product must meet a set of consumer needs and technical requirements. Second, a base-case product with known ingredients and manufacturing process is available. The objective is to design a more sustainable product than the base-case one based on a number of design alternatives identified. Design considerations include the selection of ingredients, manufacturing process, and end-of-use process (i.e., landfill, incineration, or any available recycle process). To keep the research focused, process details (e.g., operating conditions and equipment) are not considered.

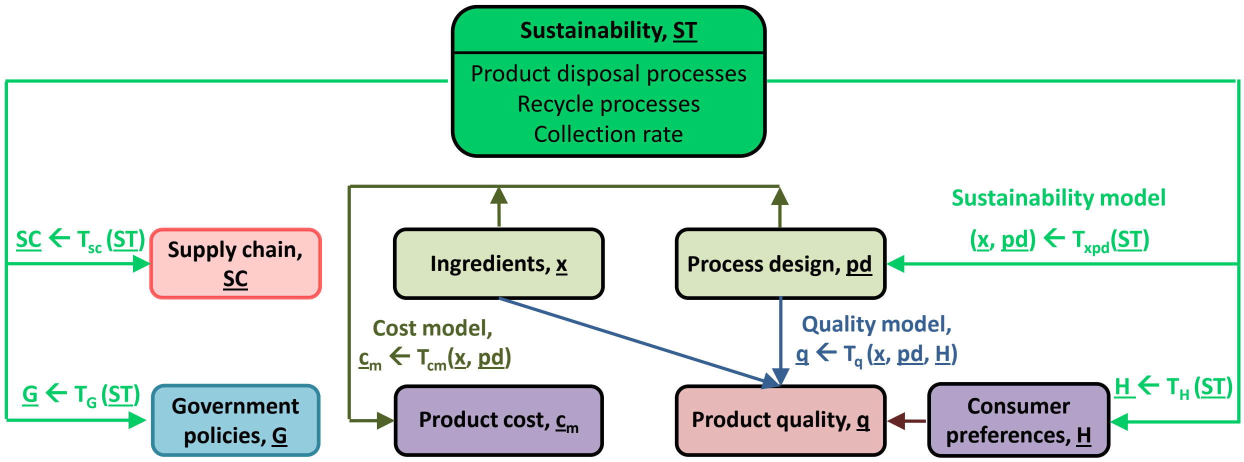


Figure 4.2. Conceptual product design models by incorporating sustainability

The sustainable product design problem is formulated as the relationship models in Eq. 4.1-4.5. The objective function (Eq. 4.1) is the maximization of product sustainability ($\underline{ST}$). This objective considers the benefits to the entire society and might conflict with the conventional profitability measures. In other words, it may not result in a profitable product to the manufacturer. $\underline{ST}$ accounts for the EES impact in raw material production ($\underline{EES}_{RMP}$), product manufacturing ($\underline{EES}_{PM}$), product use ($\underline{EES}_{PU}$), and end of use ($\underline{EES}_{EOU}$) stages in Eq. 4.2a. Based on Figure 4.2, these impact depend on many variables (Eq. 4.2b-e). For instance, $\underline{EES}_{PM}$ is decided by ingredient selection ($\underline{x}$), manufacturing process selection ($\underline{pd}$), supply chain ($\underline{SC}$), and government policies ($\underline{G}$). $\underline{EES}_{EOU}$ depends on $\underline{x}$, $\underline{SC}$, $\underline{G}$, collection rate ($\underline{cr}$), and the selection of recycle process ($\underline{rpd}$) and product disposal ($\underline{pdis}$). As an example of government policies, regulation can be imposed on certain environmental or social indicators (e.g., CO_2 emissions, water consumption, minimum wage, etc.). In this case, the regulation should be considered as constraints in the optimization problem.As stated above, only $\underline{x}$, $\underline{pd}$, $\underline{rpd}$, and $\underline{pdis}$ are regarded as design variables. The consumer preferences

($\underline{H}$), $\underline{SC}$, $\underline{G}$, and $\underline{cr}$ are fixed parameters. Moreover, product cost ($\underline{c_m}$) depends on $\underline{x}$ and $\underline{pd}$ in Eq. 4.3. Product quality ($\underline{q}$) is decided in Eq. 4.4a and design constraints in Eq. 4.4b must be fulfilled. Eq. 4.5 accounts for the lower and upper bounds ($\underline{c}^L$ and $\underline{c}^U$) of the variables. The underlined entities are different types of variables. For instance, $\underline{x}$ consisting of ingredient selections and their compositions is a vector while $\underline{pd}$ includes process flowsheet, operating conditions, etc. The arrows ←, instead of equal signs, signify that the LHS variables can be decided from the RHS variables through different approaches such as mathematical models, rule-based methods, databases, etc. For instance, with the needed LCI data, Eq. 4.2a-e can be represented using LCSA model. Otherwise, rule-based methods are utilized. Note that for ease of reading, a list of symbols for the variables and parameters is given in the Nomenclature in Supporting Information.

$$\max_{\underline{x},\underline{pd},\underline{rpd},\underline{pdis}} \quad \underline{ST} \tag{4.1}$$

$$\text{s.t. } \underline{ST} \leftarrow [\underline{EES}_{RMP}, \underline{EES}_{PM}, \underline{EES}_{PU}, \underline{EES}_{EOU}] \tag{4.2a}$$

$$\underline{EES}_{RMP} \leftarrow T_{rmp}(\underline{x}, \underline{SC}, \underline{G}) \tag{4.2b}$$

$$\underline{EES}_{PM} \leftarrow T_{pm}(\underline{x}, \underline{pd}, \underline{SC}, \underline{G}) \tag{4.2c}$$

$$\underline{EES}_{PU} \leftarrow T_{pu}(\underline{x}, \underline{H}, \underline{SC}, \underline{G}) \tag{4.2d}$$

$$\underline{EES}_{EOU} \leftarrow T_{EOF}(\underline{x}, \underline{SC}, \underline{G}, \underline{rpd}, \underline{cr}, \underline{pdis}) \tag{4.2e}$$

$$\underline{c_m} \leftarrow T_{cm}(\underline{x}, \underline{pd}) \tag{4.3}$$

$$\underline{q} \leftarrow T_q(\underline{x}, \underline{pd}, \underline{H}) \tag{4.4a}$$

$$\underline{q}^L \leq \underline{q} \leq \underline{q}^U \tag{4.4b}$$

$$\underline{c}^L \leq f\left(\underline{x}, \underline{pd}, \underline{rpd}, \underline{pdis}, \underline{c_m}\right) \leq \underline{c}^U \tag{4.5}$$

4.3.Sustainable Product Design Framework

The systematic framework is proposed in Figure 4.3 to solve the sustainable product design problem. It consists of five steps. At each step, the models and rules (shown in parentheses) are used for decision-making. In Step 1, product technical requirements are identified as design constraints. In Step 2, a base-case product is generated and available recycle processes are collected. In Step 3, LCSA or a rule-based method is used to decide the life cycle of base-case product. Meanwhile, the hotspots (i.e., life cycle stages with major impact) are identified. To improve the hotspots, a few design targets and design alternatives are generated in Step 4. Finally, LCSA or a rule-based method is used to determine the sustainable product design. Note that many heuristics are applied in the design framework to provide general guidance for facilitating decision making, instead of detailed solutions to specific problems.

Step 1: Identify Product Technical Requirements

Step 2: Identify Base-case Product and Available Recycle Processes

- Generate a base-case product
- Search for available recycle processes (Table 4.1)

Step 3: Decide Base-case Product Life Cycle and Hotspots

- Using LCSA (Figure 4.4 and Eq. 4.7-4.16)

or

- Using rule-based methods (Table 4.2-4.3)

Step 4: Generate Design Targets and Alternatives for Enhancing Sustainability

- Propose product design targets to improve the hotspots (Table 4.4)
- Generate potential product design alternatives

Step 5: Product Design towards Sustainability

- Using LCSA to optimize the most sustainable product (Eq. 4.17-4.20)

or

- Using rule-based method to screen promising design alternatives (Table 4.5)

Figure 4.3. Sustainable product design framework

4.3.1. Step 1: Identify Product Technical Requirements

The consumer preferences $\underline{H}$ includes various qualitative product attributes (e.g., cleanliness for detergent, stability for lotion, crashworthiness for bumper beam, etc.), which can be identified through consumer survey. Then, $\underline{H}$ is translated into a set of technical requirements ($\underline{tr}$) by using a knowledge-base and heuristics. The technical requirements can be physicochemical and

Table 4.1. Available recycle processes in the current market

Processes	Description	Ingredient recovery rate[a]
Mechanical/Physical Recycle Processes		
Milling and screening	Break solid materials into smaller pieces and recover materials within pre-specified sizes by screening	70-90%
Dissolution and re-precipitation	Recover materials based on their solubility differences in selected solvents (e.g., PE and PP in xylene)	up to 98%
Re-melting and remolding	Recover some metals (e.g., aluminum), alloys, and thermoplastic polymers (e.g., polyurethane)	60~90%
Magnetic separation	Recover ferromagnetic materials (e.g., iron, cobalt, nickel, etc.) from non-magnetic materials	85-95%
Gravity separation	Recover materials based on different material density (e.g., metal and plastics, rubber and plastics, etc.)	40-90%
Electrostatic separation	Recover materials based on the different charge carrying properties (e.g., solid conductors and plastics, PE/PVC)	40-90%
Chemical/Thermal Recycle Processes		
Processes	Description	Ingredient recovery rate
Decomposition	Decompose polymers to recover other valuable materials by using solvolysis, hydrolysis, pyrolysis, gasification, etc.	up to 99%
Pyro-metallurgical process	Use smelting process to separate valuable metals from complex structured product and recover metals by using dissolution, crystallization, etc.	50~90%
Hydrometallurgical process	Dissolve valuable metals from complex structured products and recover metals by leaching, precipitation, etc.	40~95%

[a] recovery rate = amount of recovered ingredients / total amount of input ingredients to be recycled

mechanical properties (e.g., pH, viscosity, mechanical modulus), functional performance (e.g., dissolution time, shelf life), or product characteristics (e.g., color, smell). To ensure high product quality, the design constraints for the technical requirements (i.e., $\underline{tr}^L$ and $\underline{tr}^U$) should be specified.

$$\underline{tr}^L \leq \underline{tr} \leq \underline{tr}^U \tag{4.6}$$

4.3.2. Step 2: Identify Base-Case Product and Available Recycle Processes

4.3.2.1. Generate a base-case product

Serving as a reference, a base-case product that fulfills the design constraints is generated. In general, the base-case product can be an existing product which has already been manufactured or a completely new product prototype conceptualized in the laboratory. For an existing product, the information of product ingredients as well as manufacturing process can be identified from the literature, patents, company websites, etc. For a totally new prototype, it can be generated based on the brainstorming, technical know-how, heuristics, and marketing experience.[25]

4.3.2.2. Search for available recycle processes

For recycle processes, certain ingredients are separated and recovered while the others are disposed. Regarding the base-case product, the information of product recycling (i.e., available recycle processes and possible collection rate) must be identified. These will be used for decision-making in Step 3. Currently, the development of many product recycle processes are in their infancy. Available recycle techniques are limited and most of them are developed to recycle waste electronical and electronic equipment, polymers, papers, and metals. Table 4.1 shows two types of product recycle techniques and the typical ingredient recovery rates. For the mechanical processes, ingredients are separated based on their different physical properties (e.g., solubility, density, magnetism, etc.) without changing chemical structures. Magnetic separation and gravity separation are examples.[143,144] For chemical/thermal processes, the ingredients undergo a series of reactions to recover the desired materials. For instance, the pyro-metallurgical process is widely used to recover metals from waste electronics.[144]

4.3.3. Step 3: Decide Base-case Product Life Cycle and Hotspots

In Step 3, the first task is to decide the life cycle of base-case product. In particular, we must decide whether and which available recycle process should be applied. The second task is to identify the hotspots. These tasks can be achieved by using LCSA or rule-based methods. When LCI data is available, using LCSA is preferred as it offers quantitative and holistic results. Otherwise, rule-based methods can be applied for decision-making, especially in the early phase of sustainable product design.

4.3.3.1.Using LCSA

LCSA is carried out in four phases: 1) goal and scope; 2) life cycle inventory analysis; 3) impact assessment; 4) intepretation.[125]

In the first phase, the functional unit, system boundary, and allocation method should be identified. The functional unit is a measure of the functionalities that the product needs to provide such as fuels with 1 GJ energy, detergents for cleaning 1000 dishes, etc. This ensures that the comparison of different products in LCSA is on an equal basis. The system boundary defines which life cycle stages are included for consideration in the assessment. In general, the five life cycle stages (in boxes) in Figure 4.1 should be included. Since a production system may produce many products, an allocation method must be specified to fairly allocate the total impact to each product. So far, many methods have been developed such as system expansion, partitioning, substitution, etc. The ISO 14044-2006-2 manual recommends using system expansion and partitioning although they still have many limitations.[145] Currently, there is no consensus on the selection of allocation method in the LCSA field. It depends on the research topic and objectives. For instance, as used in the case study in this chapter, the substitution method is often applied when the production system involves recycle process.[145] In this method, the credit of using recycled materials is not allocated to recycle process, but to the raw material production. This is because the production of raw materials is avoided in the future.

The second phase is to collect the LCI data of processes for sustainability assessment. Figure 4.4 shows the inventory data for a unit process consisting of facilities (e.g., land and equipment), energy (e.g., natural gas and electricity), materials (e.g., steam and chemicals), social information (e.g., accrued jobs and wage levels), products, by-products, and emissions (e.g., waste water and VOC).[146,147] Clearly, the LCI data is influenced by the selection of ingredient and process. As an example, Table S4.1-S4.8 in Supporting Information list the LCI data of the processes involved in the life cycle of composite bumper beam. The Supporting Information is provided in https://github.com/zx2012flying/Thesis-Supporting-Information/blob/master/Supporting%20Information%20in%20Chapter%204.docx. In general, LCI data can be retrieved from the literature and databases (e.g., Ecoinvent, social hotspot, PSILCA). Ecoinvent contains the data of facilities, energy, materials, and output emissions for many processes. The social hotspot and PSILCA databases offer the social information of thousands of processes.

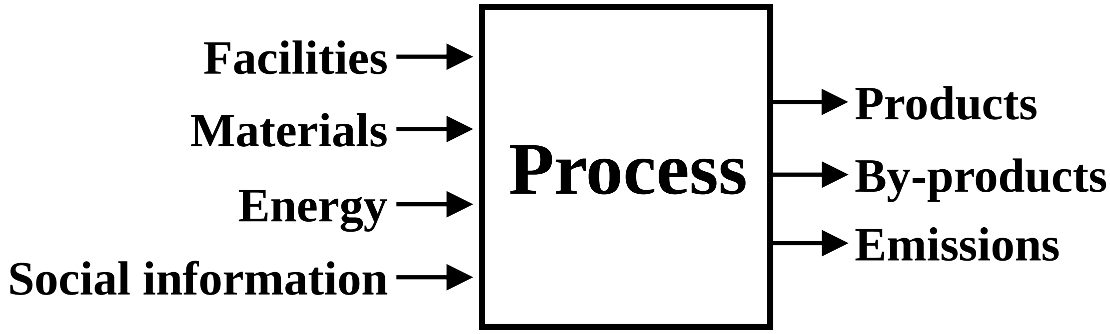


Figure 4.4. Input-output inventory for process units

In the third phase, LCI data is translated into EES impact by using the specific impact assessment models of LCC, LCA, and SLCA. In LCC, the inputs are monetized and these costs are aggregated by cost categories.[125] These calculations may involve many assumptions and approximations. For instance, if the amount of an input is very small, its costs can be neglected. In addition, market prices can be used to monetize the input materials when the data of life cycle cost coefficients of materials are not available. Bearing these in mind, the cost (c_i) at stage i is calculated as follows

$$c_i = cfa_i + cma_i + cen_i + cla_i \tag{4.7}$$

Four categories are considered here, consisting of facilities cost (cfa_i), material cost (cma_i), energy cost (cen_i), and labor cost (cla_i). Other costs are presumably negligible. cfa_i depends on the amount of the f-th input facility at stage i ($IF_{i,f}$ in piece of plant). $CIF_{i,f}$ is the capital cost of the f-th input facility (in $/plant).

$$cfa_i = \sum_f IF_{i,f} \cdot CIF_{i,f} \tag{4.8}$$

cma_i is linearly proportional to the amount of m-th input material at stage i ($IM_{i,m}$ in kg). $CIM_{i,m}$ is the unit cost of the m-th input material (in $/kg).

$$cma_i = \sum_m IM_{i,m} \cdot CIM_{i,m} \tag{4.9}$$

cen_i depends on the amount of e-th input energy at stage i ($IE_{i,e}$ in MJ). $CIE_{i,e}$ is the unit cost of the e-th input energy (in $/MJ).

$$cen_i = \sum_e IE_{i,e} \cdot CIE_{i,e} \tag{4.10}$$

cla_i is the number of input labor headcount at stage i (IL_i in full-time equivalent for a year) multiplied by the average wage level (WL_i in $/headcount/year).

$$cla_i = IL_i \cdot WL_i \tag{4.11}$$

Thus, the life cycle economic impact (EcI) of a product is obtained as follows

$$EcI = \sum_i c_i \tag{4.12}$$

In LCA, the inventory data (i.e., facilities, materials, energy, and emissions) are first translated into 18 midpoint factors (e.g., real damages such as ozone concentration, algae growth, etc.) that cause damage to three endpoint factors (i.e., human, ecosystem, and resource). Then, the three endpoint factors are further aggregated into an environmental index. After selecting the region boundary (e.g., European region or world region), the corresponding normalization parameter set for midpoints and endpoints is used. These procedures are elaborated in detail by Huijbregts et al.[148] and can be performed using commercial software such as Simapro and Gabi. Thus, the environmental impact (e_i) at stage i is equal to the aggregated impact of facilities (efa_i), materials (ema_i), energy (een_i), and emissions (eem_i):

$$e_i = efa_i + ema_i + een_i + eem_i \tag{4.13}$$

Accordingly, the life cycle environmental impact (EnI) is calculated as:

$$EnI = \sum_i e_i \tag{4.14}$$

In SLCA, the social information is converted into various indicators such as unemployment, minimum wage, etc.[147] Again, various normalization parameters can be used for this conversion. Then, they are aggregated into one index (s_i) that denotes the product's social impact at stage i. Similarly, the life cycle social impact (SoI) is calculated as follows

$$SoI = \sum_i s_i \tag{4.15}$$

The fourth phase is to analyze the results for generating conclusions and recommendations. For base-case product, a proper end-of-use strategy should be selected. Using landfill as the reference, the optimal end-of-use strategy can be decided by solving the following minimization problem.

$$\min_J \frac{EcI_J^b}{EcI_{Landfill}^b} + \frac{EnI_J^b}{EnI_{Landfill}^b} + \frac{SoI_J^b}{SoI_{Landfill}^b}$$

$$\text{s.t.} \quad J \in \{\text{landfill, incineration, recycle process } 1, \dots, \text{j}\} \tag{4.16}$$

The superscript b stands for the base-case product. J denotes landfill, incineration, or recycle processes. After this, the hotspots of base-case product should be identified.[149] By analyzing the EES impact at each life cycle stage, the stages associated with major impact can be identified and should be improved. Note that due to the limitations of current sciences and technologies, it is always difficult to improve the stage with the highest impact. Clearly, reducing the impact at any stage can contribute to product sustainability. Thus, we can consider the stages with the second highest or third highest impact as hotspots although the potential improvement on sustainability may be smaller. The stage with the highest impact can be identified to indicate the direction for future technology innovation and development.

4.3.3.2.Using heuristics

If the needed LCI data is not available, heuristics are used. Three tasks are conducted: analyze product recyclability, select recycle process (if necessary), and identify hotspots.

Product recyclability is analyzed to decide if the product is worth recycling. Economic, environmental, and social factors affect this decision-making. The heuristics in Table 4.2 can be used to help make a decision. For instance, if a product (i.e., battery and electronics) consists of rare metals, it should be recycled to preserve the mineral reserves. In contrast, some liquid products such as liquid detergent and hand lotion are directly consumed and cannot be re-collected for recycling.

Given multiple techniques are available to recycle the product, a proper recycle process should be selected. To do so, we need to decide which product ingredients should be recovered. Clearly, the expensive and rare materials are preferred to recycle. Three rules can be used to select a relatively safe, economic, and environment-friendly recycle process.

Table 4.2. Factors and heuristics for recycle-or-not decisions

Factors	Situations favoring 'recycle'	Situations favor 'not recycle'
Economic	• The product can be easily re-collected and sorted (concentrated). The re-collection channels and facilities are available. • Government subsidy is provided to stimulate product recycling. • Certain product ingredients are very valuable in the market.	• The product cannot be recycled as it is directly consumed or hard to separate from other wastes. • Recycling technologies are not available in the market or still under development. • The product consists of cheap and abundant commodities or renewable materials. • The recovered materials are hard to reuse, due to non-removable impurities or structural changes.
Environmental	• The product consists of scarce materials with limited reserve (e.g., rare metals). • The product consists of toxic and erosive materials that harms the environment or human. • Certain ingredients are produced by using energy-intensive or polluting processes	• Debris or toxic wastes would be produced during the re-collection or recycling stages. • The recycle processes use hazardous chemicals or release harmful pollutants. • The product is degraded in nature in a short period of time.
Social	• Government regulates that the product or certain product ingredients must be recovered. • Many jobs can be created by establishing the recycle facilities.	• The products should not be recycled for infection control, such as surgical masks and gloves, etc. • Recycle processes lead to fatal accidents (e.g., explosion, worker injury, etc.)

- Rule 1. Select the widely-used and easily accessible process
- Rule 2. Select the process through which the desired materials are recovered with less loss
- Rule 3. Select the process using less processing, energy, and chemicals/solvents

The last task is to decide the hotspots. As listed in Table 4.3, chemical products can be classified into two types: consumable and durable.[150] The consumable products are directly used up such as perfume, food, shampoo, etc. The typical hotspots of consumable products are raw material production and product disposal. On the other hand, the durable products are not consumed directly such as battery, refrigerant, light bulb, etc. The typical hotspots of durable products are product use and product recycle.[150]

Table 4.3. Typical hotspots for two types of chemical products[150]

	Characteristics	Examples	Typical hotspots
Consumable product	Products are directly consumed throughout their use.	Pesticide, shampoo, food, paint, perfume, inkjet ink, etc.	Raw material production and product disposal
Durable product	Products are not consumed directly, and last for a long time in the same product form.	Battery, air purifier, bumper beam, light bulb, etc.	Product use and product recycle

4.3.4. Step 4: Generate Design Targets and Alternatives for Enhancing Sustainability

4.3.4.1.Propose product design targets to improve the hotspots

Various product design targets can be proposed to improve the identified hotspots. Currently, the design targets cannot be automatically generated by using any methods or tools. Therefore, heuristics and knowledge-base are applied. As stated before, many general principles and guidelines have been proposed to promote product sustainability.[129-132] Based on these solutions, Table 4.4 lists some widely-used design targets. For instance, using materials produced from renewable feedstocks can be an effective approach to reduce the environmental impact at the raw material production stage. Note that for a specific product, the domain knowledge is essential for generating proper design targets for sustainability.

4.3.4.2.Generate potential product design alternatives

To achieve the proposed design targets, promising product design alternatives (i.e., ingredient alternatives or processing technologies) should be generated. Product ingredients can be classified into different types based on their functionalities. Many ingredient candidates offering the same functions can be generated by knowledge-base, material databases or computer-aided tools.[151] For instance, Cheng et al.[15] listed the typical ingredient types and candidates for skin-care creams. The generated ingredient candidates can be regarded as new design alternatives. As listed in the third column of Table 4.4, specific examples are provided to show how new ingredients were used to

Table 4.4. Typical design targets for enhancing product sustainability

Life cycle stage	Design targets	Examples of using new ingredients to achieve design targets
Raw material production	• Reduce the use of rare and heavy metals • Reduce the use of complex polymers and derivatives • Use materials produced from renewable feedstocks	• Use blend of biodiesel and petro-diesel to reduce the consumption of limited crude oil.
Product manufacturing	• Reduce the use of organic solvents • Reduce the number of product ingredients and production steps • Reduce the drop in production yield	• Naturally colored cotton is used to produce clothes so that dying process can be avoided.
Product use	• Reduce the use of toxic and carcinogenic materials • Reduce the use of heavy and non-durable materials • Develop better quality and long lifespan products	• Use light fiber-matrix composite materials to replace heavy steel for manufacturing vehicle body panel
Product recycle	• Reduce the use of non-recyclable materials that release pollutants during product recycling • Use the non-recyclable materials that can be easily separated or removed in the recycle processes • Use the recyclable materials	• Use recyclable PET to manufacture bottles for drinkable water, beverages, etc.
Disposal	• Reduce the use of polycyclic aromatic hydrocarbons • Reduce the use of materials releasing the oxides of sulfur and nitrogen upon exposure • Use biodegradable materials	• Use bio-degradable polymers to manufacture plastic bags, potting cups, etc.

achieve various design targets. For instance, biodegradable polymer can be used for manufacturing plastic bags to reduce the environmental impact at the product disposal stage.[152] Moreover, various methods on synthesizing sustainable processes have been developed such as indicator-based approach,[153] process intensification,[154] techno-ecological synergy,[155] etc. Similarly, process alternatives can be generated and then selected for enhancing sustainability.

4.3.5. Step 5: Product Design towards Sustainability

The generated design alternatives should be assessed by using LCSA or rule-based method (i.e., a sustainability checklist). When LCI data is available, LCSA is used for model-based optimization to determine the most sustainable product. Otherwise, the sustainability checklist is used to qualitatively screen the sustainable design alternatives.

4.3.5.1.Using LCSA to optimize the most sustainable product

As LCSA is applied, Eq. 4.1-4.5 can be re-formulated as a multi-objective optimization problem (Eq. 4.17-4.20) for sustainable product design.

$$\min_{d,K} EcI_K^d, EnI_K^d, SoI_K^d \tag{4.17}$$

$$\text{s.t. } [EcI_K^d, EnI_K^d, SoI_K^d] = LCSA(d, K) \quad \text{(Sustainability assessments)} \tag{4.18}$$

$$\underline{tr}^d = F(d) \quad \text{(Technical requirements)} \tag{4.19}$$

$$\underline{tr}^L \leq \underline{tr}^d \leq \underline{tr}^U \quad \text{(Design constraints)} \tag{4.20}$$

The objective function is formulated in Eq. 4.17. EcI_K^d, EnI_K^d, and SoI_K^d are the EES impacts of *d*-th product design alternative with *K*-th end-of-use process. In Eq. 4.18, the EES impacts are calculated by using LCSA model (i.e., Eq. 4.7-4.15 in Step 3). Furthermore, design constraints must be fulfilled (Eq. 4.19-4.20). $\underline{tr}^d$ denotes the technical requirements of d-th product design alternative. Generally, the multi-objective optimization problem can be solved by various methods to generate the Pareto front such as ε-constraint approach, genetic algorithm, etc.[65] The Pareto front provides a better understanding on the tradeoffs in sustainability. Moreover, in principle, a new product can be treated as more sustainable if it improves at least one of the EES aspects without compromising the others. However, this is always hard to achieve in practice due to the trade-offs of the EES aspects and the limited design space. From the designer's perspective, certain optimal solution can be identified for further consideration. For instance, when equal weights for EES impacts are assumed, Eq. 4.21 can be solved directly.

$$\min_{d,K} \frac{EcI_K^d}{EcI_J^b} + \frac{EnI_K^d}{EnI_J^b} + \frac{SoI_K^d}{SoI_J^b} \tag{4.21}$$

where EcI_J^b, EnI_J^b, and SoI_J^b are the EES impacts of base-case product decided by Eq. 4.16 in Step 3. Note that there is no universal consensus on how to balance the EES performance. If their relative importance can be accurately quantified in the future, this equal-weight assumption can be relaxed.

4.3.5.2.Using rule-based method to screen promising design alternatives

As stated above, sustainability checklist is often used as a rule-based method to qualitatively assess sustainability performance. Table 4.5 shows a sustainability checklist that can be used to screen the promising design alternatives. At each life cycle stage, three questions related to the critical EES issues are considered. For instance, for product manufacturing, the number of processing steps and operating conditions greatly influence the costs and environmental burdens. Safety is one of the major issues in the social aspect of sustainability. Thus, the exposure to toxic or erosive chemicals affecting worker safety is an important consideration. The required information for answering the questions is listed in the third column of Table 4.5. Taking the

Table 4.5. Qualitative sustainability checklist[127,128]

Life cycle stage	Questions	Required information
Raw material production	• Do the purchasing costs of raw materials increase? • Do the raw materials have limited supply in the market? • Do the number of accidents associated with raw material production increase?	• Material purchasing costs • Suppliers' production capacity • Suppliers' production report
Product manufacturing	• Does the number of production steps increase? • Do the operating conditions get demanding? • Are the workers exposed to toxic or erosive chemicals?	• Manufacturing process design • Material properties
Product use	• Does the product quality get worse? • Does the efficiency decrease if the product uses water or energy? • Is the product dangerous or harmful to use?	• Product attributes • Product use conditions • Material toxicity data
Product recycling	• Will the valuable ingredients be lost during recycling? • Are extra waste treatments needed in the recycling facility? • Will the workers be exposed to new hazardous emissions?	• General structure of recycle processes
Disposal	• Can the product be safely incinerated to recover energy? • Is the product harder to be degraded naturally? • Does the product release toxic pollutants upon exposure?	• Material properties (e.g., heating value, bio-degradability, etc.)

product manufacturing stage as an example, the first two questions can be answered based on the manufacturing process design and the last one on the materials' toxicity data. Note that if the answer to a question is 'No', it means that the new design alternative is as good as the existing one on this specific aspect. In general, if a design alternative improves the hotspot without making other stages worse, it can be kept as a potential solution for improving product sustainability. As the project proceeds, it should be further verified by model-based methods (e.g., LCSA).

4.4. Case Study 1: Composite Bumper Beam for Automotive Vehicle

Bumper beam is used in automobiles to protect passengers and the vehicle itself. The European Commission regulates that from 2015, at least 95% (by weight) of the vehicle must be recycled to foster sustainable development. Thus, a more sustainable bumper beam is highly desired. The proposed framework is applied for this design problem.

4.4.1. Step 1. Identify Product Technical Requirements

Crashworthiness is the most important product attribute for a bumper beam.[156] It should bear the force and absorb the energy generated in a crash. In general, crash accidents occur in the *X*-*X*, *Y*-*Y*, and *X*-*Y* (or *Y*-*X*) directions. *X* indicates the direction in which the vehicle heads and Y stands for its transverse direction. For protection purpose, the bumper beam must have high values of mechanical strength in these directions.[157] Thus, three technical requirements have to be considered, namely the Young's modulus in *X*-*X* and *Y*-*Y* directions and the shear modulus in *X*-*Y* direction. Young's modulus is the ratio of the stress to the strain along an axis. Shear modulus is the ratio of the shear stress to the shear strain. The larger the modulus is, the larger force the bumper beam can bear.

Table 4.6. Candidates of reinforcing fiber and polymeric matrix for use in composite bumper beam and their properties

		Young's modulus E (GPa)	Shear modulus G (GPa)	Poisson's ratio η	Density ρ (kg/m^3)	Heating value HV (MJ/kg)
Reinforcing fiber	Carbon fiber	220	17	0.26	1900	32.8
	Glass fiber	75	33	0.21	2490	0
	Kenaf fiber	40	16	0.20	1450	15.8
	Jute fiber	20	7	0.38	1300	17.7
Polymeric matrix	Polyester resin (PR)	3.5	1.4	0.42	1300	34
	Epoxy resin (ER)	3.5	1.4	0.42	1200	34
	Polypropylene (PP)	0.9	0.4	0.42	946	39.8
	Polyethylene (PE)	0.7	0.3	0.42	950	43.5
	Polyethylene terephthalate (PET)	3.9	1.4	0.39	1320	21.9

For a commercial bumper beam, the Young's modulus in the *X-X* and *Y-Y* directions (E_{XX} and E_{YY}) must exceed 20 and 5 GPa, respectively. The shear modulus in the *X-Y* direction (G_{XY}) must be larger than 2.5 GPa.[157]

4.4.2. Step 2. Identify Base-Case Product and Available Recycle Processes

4.4.2.1.Generate a base-case product

The bumper beam can be made of aluminum, alloy, or composite material due to their high strength. Among them, the lightweight composite material is preferred for higher fuel efficiency. Composite material is made by embedding reinforcing fibers into polymeric matrix. Kim et al.[157] reported that glass fiber and polypropylene (PP) have been used by a Korea automotive company to manufacture bumper beams. Here, this existing product is generated as the base-case. In addition, it is assumed that the base-case product can be manufactured using injection molding. Again, process details (e.g., operating conditions and equipment) are not considered. Meanwhile, he volume fractions of fiber (VF_f) and matrix (VF_m) as well as the fiber's spatial orientation ($\underline{SO}$) are decided by solving the following minimization problem: Given the volume of bumper beam, minimize its weight subject to the strength constraints.[156]

Table 4.7. Computational results for the composite bumper beam example

		Base-case product	Sustainable product
Fiber	Candidate (F_s)	Glass fiber	Carbon fiber
	Weight (kg)	2.49	0.63
Matrix	Candidate (M_k)	PP	PP
	Weight (kg)	1.89	2.53
Fiber spatial orientation ($\underline{SO}$)		[-1, 0, 0], [0.64, 0.77, 0]	[-0.987, 0.161, 0], [-0.635, -0.773, 0]
Total weight (kg)		4.38	3.15
Product cost c_m ($)		4.9	6.9
Young's modulus E_{XX} (GPa)		20	20
Young's modulus E_{YY} (GPa)		5	5
Shear modulus G_{XY} (GPa)		2.5	2.5
End-of-life strategy EOU_J		Incineration with energy recovery	Pyrolysis
Economic impact EcI (M$)*		283	229
Environmental impact EnI (MPt) *		140	124
Social impact SoI (jobs)*		485	370

* Based on the functional unit of 10 million pieces of bumper beam

$$\min M_{cbb} = (\rho_{glass} \cdot VF_f + \rho_{PP} \cdot VF_m) \cdot V_{cbb} \tag{4.22}$$

$$\text{s.t. } E_{XX} \geq 20\ GPa, \quad E_{YY} \geq 5\ GPa, \quad G_{XY} \geq 2.5\ GPa \qquad \text{(Design constraints)} \tag{4.23}$$

$$[E_{XX}, E_{YY}, G_{XY}] = rFGM(VF_f, VF_m, \underline{SO}) \qquad (rFGM \text{ model})$$

$$VF_f, VF_m, \underline{SO} \in R \qquad \text{(Design variables)}$$

where M_{cbb} and V_{cbb} are the mass and volume of composite bumper beam, respectively. V_{cbb} is set equal to 0.003 m^3. ρ_{glass} and ρ_{PP} are the density of glass fiber and PP, respectively. Design constraints are expressed in Eq. 4.23. In addition, the revised Fabric Geometry Model (*rFGM*) is used to predict the Young's modulus and shear modulus.[158] They are calculated based on the properties of glass fiber and PP, VF_f, VF_m, and $\underline{SO}$. The properties are listed in Table 4.6 and the detailed *rFGM* is elaborated in Eq. S4.1-S4.36 in Supporting Information.

This problem is solved using the global solver BARON in GAMS 24.7.4. The solutions are listed in the first column of Table 4.7. The base-case product is made of 2.49 kg glass fiber and 1.89 kg PP. All three design constraints are met. In addition, the product cost (i.e., cost of glass fiber and PP and manufacturing cost) is equal to \$4.9 per bumper beam.

4.4.2.2.Search for available recycle processes

Two recycle processes are available: pyrolysis process and mechanical process. In the pyrolysis process, composites are cut into fragments and fed into a heated furnace. The matrix is decomposed into lower molecular weight organic substances that are burnt to generate electricity. The fiber is recovered and the recovery rate can reach 95%. It can be assumed that the properties of recovered fibers do not change while the average length of recovered fibers is shorter. Regarding fiber re-manufacturability, it can only be recycled once after pyrolysis.[159] In the mechanical process, composites are cut and ground for size reduction. The small pieces are sieved into two fractions. The fine fraction (fiber rich) can be used as filler. The coarse fraction (matrix rich) is incinerated for electricity generation.[160]

4.4.3. Step 3: Decide Base-case Product Life Cycle and Hotspots

LCSA is applied here. The EES impacts with four end-of-use processes (i.e., landfill, incineration, pyrolysis, and mechanical recycle) are determined to identify the proper one. In addition, the EES impacts at each life cycle stage are calculated to identify the hotspots.

4.4.3.1.Using LCSA

The LCSA is applied in this example. In the first phase, the functional unit is defined as 10 million pieces of the bumper beam providing the desired strengths (Eq. 4.23). Note that this number is around half of the vehicle production capacity in China in 2015. The system boundary consists of all the life cycle stages as shown in Figure 4.1. Note that how the recovered materials are exactly used in other products is not included. The substitution method is employed. The credits of the materials and electricity recovered from recycle processes are allocated to the raw material production stage.

In the second phase, LCI data is modelled and collected in the form of Figure 4.4. Tables S4.1-S4.8 report the LCI data at each life cycle stage. Various assumptions have been made. For instance, the transportation distance between any two life cycle stages is set equal to 300 km. It is assumed that the amount of input energy of the injection molding process only depends on the selection of polymeric matrix. The consumption of diesel is affected by the weight of the bumper beam and is used to quantify the impact of product use. Moreover, the social hotspot and PSILCA databases for SLCA are not available in our group. Thus, for simplicity, the number of accrued jobs is used to represent the social impact.

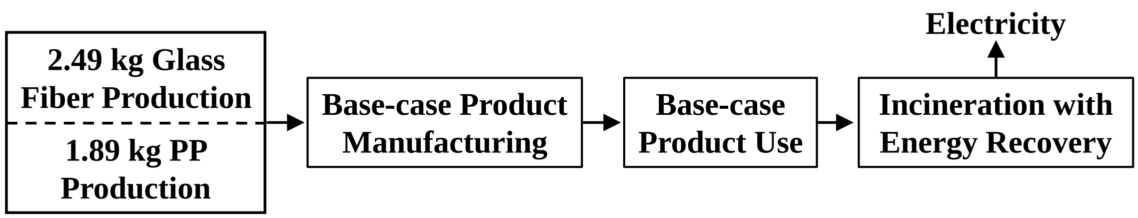
In the third phase, the life cycle cost of the base-case product is calculated by using Eq. 4.7-4.12. Table S4.9 lists the cost coefficients of input materials and energy (i.e., CIM and CIE). Note that if the mass of certain input material is less than 0.001 kg, its cost is neglected. Table S10 lists the cost coefficients of input facilities (i.e., CIF). These cost coefficients are market prices because there is no available database for life cycle cost coefficients. The translation of LCI data into environmental impact was performed in Simapro. The world region boundary is specified and the

Table 4.8. LCSA results of the base-case product with different end-of-use scenarios for the composite bumper beam example

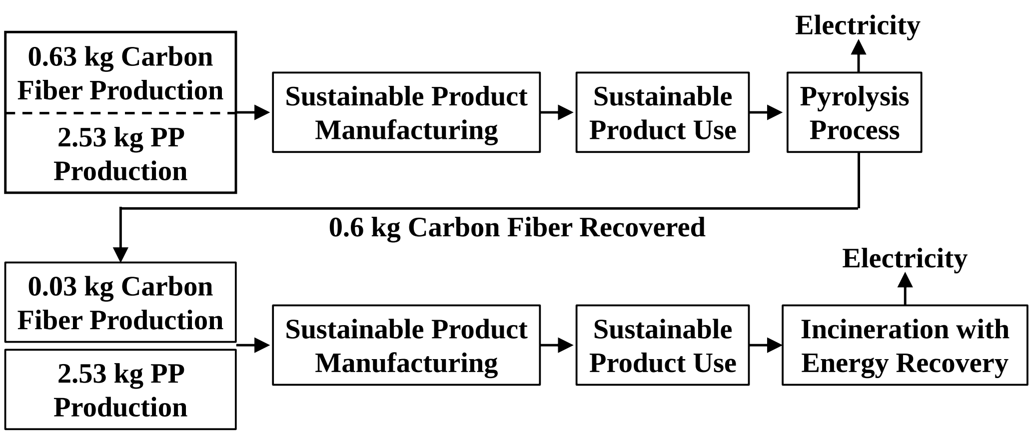
	Pyrolysis process	Mechanical process	Incineration with energy recovery	Landfill
Economic impact EcI^b (M$)*	292	301	283	286
Environmental impact EnI^b (MPt)*	155	159	140	141
Social impact SoI^b (jobs)*	497	570	485	461

* Based on the functional unit of 10 million pieces of bumper beam

set of World Recipe H/A normalization parameters was applied. For assessing social impact, the number of locally accrued jobs is directly retrieved from Tables S4.1-S4.8.



(a)



(b)

Figure 4.5. (a). Life cycle of base-case product; (b). Life cycle of sustainable product for composite bumper beam case study

In the fourth phase, Table 4.8 lists the LCSA results with different end-of-use strategies for the base-case product. The number of jobs created by using incineration is larger than that of using landfill. Using incineration also leads to the minimum life cycle cost and environmental impact. Using landfill as the reference, incineration with energy recovery should be applied for the base-case product. The life cycle of the base-case product is shown in Figure 4.5(a). In addition, Figure 4.6 shows the EES impact of the base-case product at each life cycle stage (black bar). Clearly, product use stage accounts for most of the economic and environmental impact. The number of accrued jobs at the product recycle stage is small. Based on these data, the product use and product recycle stages are considered as the hotspots for further improvement.

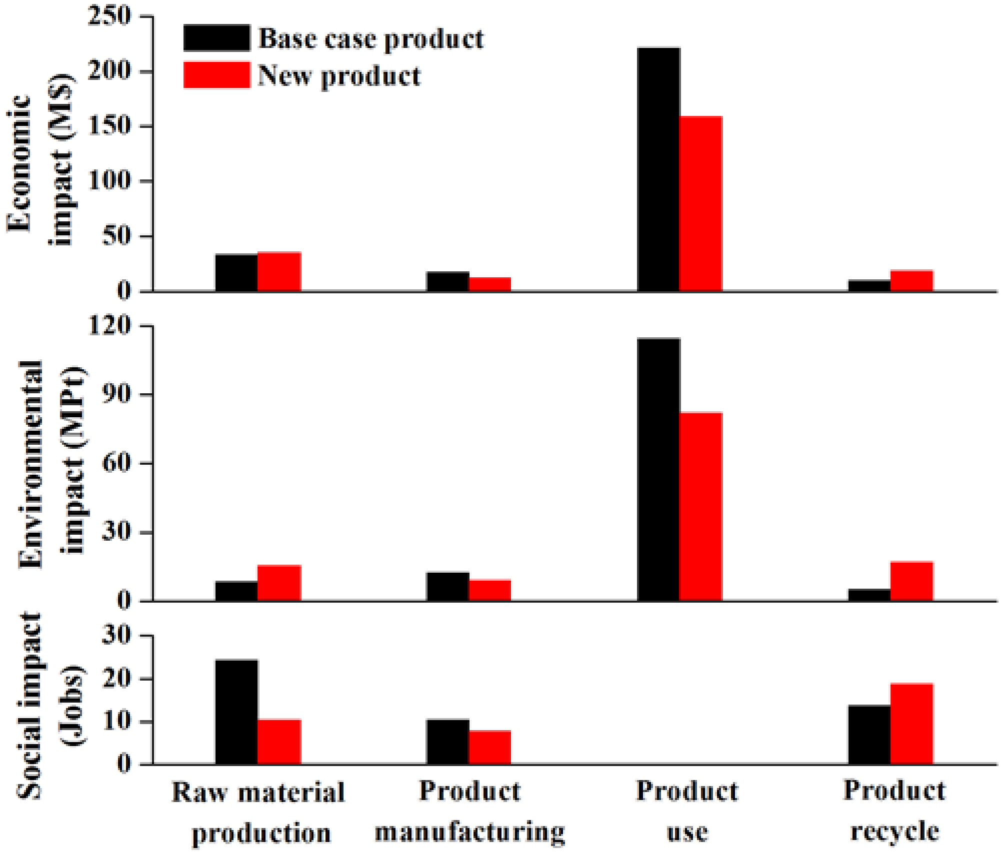


Figure 4.6. Economic, environmental, and social impact of base-case product and sustainable product at each life cycle stage for composite bumper beam example

4.4.4. Step 4: Generate Design Targets and Alternatives for Enhancing Sustainability

4.4.4.1.Propose product design targets to improve the hotspots

Based on heuristics in Table 4.4, the following design targets are proposed to improve hotspots:

1. Use another fiber or matrix for designing more lightweight composites to reduce the impact at product use stage
2. Use another fiber or matrix to match another recycle process so that more materials can be recovered and more jobs are created

3. Develop cheaper lightweight high-strength materials to replace composite materials
4. Develop new recycle techniques so that the recovered materials can be reused in multiple generations

Here, the first two design targets are considered to show how ingredients and end-of-use strategy should be selected for promoting sustainability.

4.4.4.2.Generate potential product design alternatives

Table 4.6 lists new fiber and matrix alternatives generated from Mallick[161] such as carbon fiber, jute fiber, PE, PET, etc. All these ingredient alternatives are considered to design a more sustainable bumper beam. The four end-of-use strategies consisting of landfill, incineration with energy recovery, pyrolysis, and mechanical process are considered as well.

4.4.5. Step 5: Sustainability Assessment for Design Alternatives

4.4.5.1.Using LCSA to optimize the most sustainable product

The sustainable composite bumper beam can be generated by solving the multi-objective optimization problem in Eq. 4.24. The economic and environmental impacts should be minimized while the number of accrued job should be maximized. The EES impact of sustainable product is denoted by $EcI, EnI,$ and SoI and calculated by using LCSA method. The LCI data, cost coefficients and the number of accrued jobs are listed in Supporting Information. The impact depends on the selection of fiber (F_s) and matrix (M_k), their volume fractions (VF_f and VF_m), and the selection of end-of-use process (EOU_J). In addition, design constraints must be met and the modulus are calculated by the $rFGM$ (Eq. S1-36). Design variables consists of the binary variables F_s, M_k, and EOU_J as well as continuous variables VF_f, VF_m, and $\underline{SO}$.

$$\min \frac{EcI}{EcI^b} + \frac{EnI}{EcI^b} - \frac{SoI}{SoI^b} \qquad (4.24)$$

s.t. $[EcI, EnI, SoI] = LCSA(F_s, M_k, VF_f, VF_m, EOU_J)$ ($LCSA$ model)

$E_{XX} \geq 20\ GPa, \quad E_{YY} \geq 5\ GPa, \quad G_{XY} \geq 2.5\ GPa$ (Design constraints)

$[E_{XX}, E_{YY}, G_{XY}] = rFGM(F_s, M_k, VF_f, VF_m, \underline{SO})$ ($rFGM$ model)

Design variable: $F_s, M_k, EOU_J \in \{0,1\} \qquad VF_f, VF_m, \underline{SO} \in R$

$s \in \{carbon\ fiber, glass\ fiber, kenaf\ fiber, and\ jute\ fiber\}$

$k \in \{PR, ER, PP, PE, PET\}$

$J \in \{landfill, incineration, pyrolysis, mechanical\}$

This multi-objective optimization problem was solved using the ε-constraint approach due to its ease of use. The detailed solution procedure can be found in Rangaiah.[65] Here, EcI is considered as the primary objective while EnI and SoI are converted into inequality constraints. In addition, a series of ε are fixed to divide the range of EnI and SoI into 10 equal intervals. In doing so, multiple ε-constrained single-objective optimization problems were solved using BARON. Figure 4.7 shows the Pareto front representing the trade-offs among the EES aspects. The minimum economic and environmental impacts are 229M$ and 129MPt, respectively. The maximum number of accrued jobs is 738 jobs.

By using base-case product as the reference and assuming equal weights of EES impacts, the minimum of $\frac{EcI}{EcI^b} + \frac{EnI}{EcI^b} - \frac{SoI}{SoI^b}$ is solved to generate an optimal product design for comparison. EcI^b, EnI^b, and SoI^b are the EES impact of the base-case product decided in Step 3 (third column in Table 4.8). The result which happens to be one of the Pareto optimal solutions in Figure 4.7 is listed in the second column of Table 4.7. The new product is made up of carbon fiber and PP. Product cost for one piece of bumper beam increases up to $6.9 while the weight decreases to 3.15 kg. In addition, the number of accrued jobs decreases by 24% to 371 jobs. Compared with the base-case product, there are 114 fewer jobs for the new product. However, the life cycle cost is reduced to M$229 and life cycle environmental impact is decreased to 129 MPt. In this case, the overall sustainability performance improves if equal weight is given to the EES impacts.

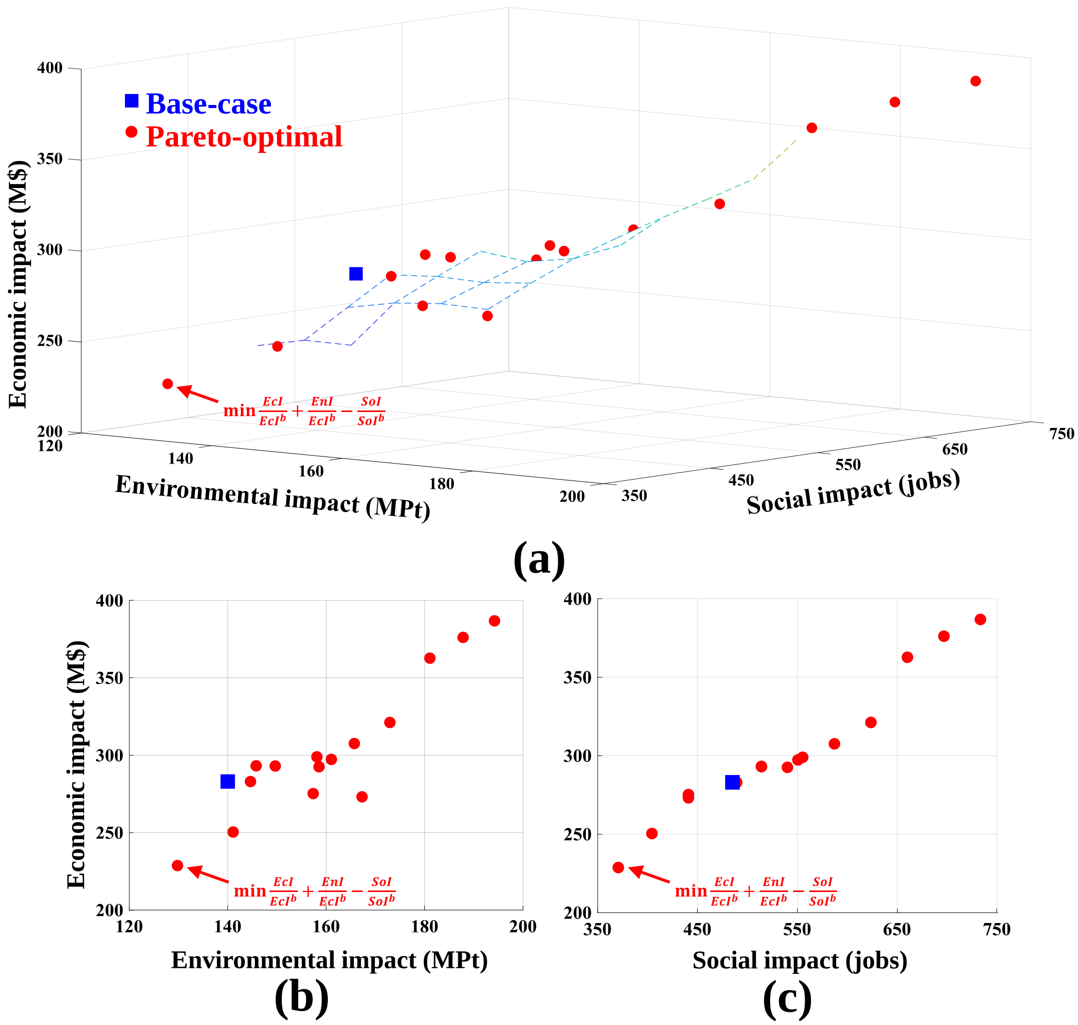


Figure 4.7. (a) Pareto Front for Bumper Beam Example; (b) Projection of Pareto Front to Economic-Environmental Coordinate; (c) Projection of Pareto Front to Economic-Social Coordinate

Figure 4.5(b) shows the life cycle of one piece of the new product. 0.63 kg carbon fiber and 2.53 kg PP are used to manufacture the bumper beam. After product use, pyrolysis process is applied to generate electricity and 0.6 kg of carbon fiber. These fibers are used with additional raw materials in the second generation of product.

Figure 4.6 shows the EES impact of the new product at each life cycle stage. At product use stage, the associated cost and environmental impact are greatly reduced since the sustainable bumper beam is lighter. Therefore, the first design target is achieved. Moreover, at raw material production stage, the cost and environmental impact increase. This is because the production of carbon fiber is expensive and energy intensive. In this case, pyrolysis process is applied so that the expensive carbon fiber can be recovered and reused in another generation. In addition, using pyrolysis increases the number of accrued jobs at the product recycle stage.

The other two design targets are not considered at present. However, with the future development of technologies, they may be achieved so that more sustainable bumper beam can be designed accordingly.

4.5.Case Study 2: Lithium ion Battery for Electric Vehicle

Lithium ion batteries (LIBs) have been used to power the propulsion of electric vehicles (EVs). Widely used LIBs include lithium iron phosphate (LFP), lithium nickel manganese cobalt oxide (NMC), etc. Note that LIBs are named after the cathode material in use. With the rapid expansion of the EV market, more sustainable LIBs are highly desired. In this example, we will not perform calculations as in the bumper beam example. This is because most relevant LCI data are not available for LIBs. The absence of data does not mean that nothing can be done. Instead, the aim of this example is to show how the framework can be used to efficiently identify the information needed for designing a sustainable product, rather than getting a detailed design solution.

4.5.1. Step 1. Identify Product Technical Requirements

Figure 4.8 lists the five product attributes for LIBs, including large full charge capacity, long life span, quick charging, cheap and safe. These attributes are translated into five technical requirements by heuristics, which includes energy density, cycle number, charge rate, costs, and cell materials. Only the most dominant attributes and technical requirements are identified here. The specifications of a commercial LIB battery are regarded as design constraints.[162]

- Energy density ≥ 120 Wh/kg
- Cycle number ≥ 2000
- Charge rate ≥ 4C
- Cost per kWh ≤ 0.4 $/kWh
- Safe cells

Product attributes \ Technical requirements	Energy density	Cycle number	Charge rate	Costs	Cell materials
Large full charge capacity	**9**				**9**
Long life span		**9**			**3**
Charge quickly			**9**		**3**
Cheap				**9**	**3**
Safe					**9**

Figure 4.8. House of quality for lithium ion battery in electric vehicle

4.5.2. Step 2. Identify Base-Case Product and Available Recycle Processes

4.5.2.1. Generate a base-case product

Due to its good thermal stability and enhanced safety, LFP has been widely applied in EVs. In this example, the existing LFP battery is considered as the base-case product, which can meet the pre-specified design targets. Referring to the *BatPac* database,[162] Table 4.9 lists the components and ingredients in the LFP battery cell. It consists of anode, cathode, separator, electrolyte, and current collectors. The organic solvent n-methyl-2-pyrrolidone (NMP) is used to dissolve the binder polyvinylidene fluoride (PVDF) which binds the active material particles as well as the current collector together. Moreover, the detailed battery assembly processes have been illustrated by Nelson et al.[163] The electrodes are first manufactured through a series of steps (e.g., coating, solvent evaporation, and slitting) and then packed into a battery cell in a dry room. Afterwards, the battery cell is sent for formation cycling following be sealing, testing, module assembly, etc.

Table 4.9. LFP battery cell formula

Components	Ingredients
Anode	Graphite
Cathode	LFP salt, carbon
Current collector	Copper (for anode), aluminum (for cathode)
Electrolyte	$LiPF_6$, ethylene glycol, dimethyl ether
Separator	PP, PE
Binder	Polyvinylidene fluoride (PVDF)
Solvent (evaporated)	N-methyl-2-pyrrolidone (NMP)

4.5.2.2.Search for available recycle processes

Two major recycle processes have been developed for recycling metals from spent LIBs: pyro-metallurgical process and hydro-metallurgical process. In the pyro-metallurgical process, LIBs are directly fed to a high temperature furnace where carbon, graphite, electrolyte solvents, and polymers are burnt off. The produced gases go through a post-combustion chamber for post-treatment. The copper and iron form an alloy and then can be further separated for reuse. The aluminum and lithium form a slag for use in other applications (e.g., cement industry).[164] For the hydro-metallurgical process, the spent LFP batteries first go through a series of pretreatments (e.g., dismantled, crushing, and screening) to separate different components. After recovering the current collectors (i.e., copper and aluminum), the cathode powders go through a series of processes (e.g., dissolution, precipitation, etc.) to recover lithium metal for reuse.[165]

4.5.3. Step 3: Decide Base-Case Product Life Cycle and Hotspots

4.5.3.1.Using rule-based methods

Since most LCI data for LFP battery is not available, using rule-based methods is necessary. According to Figure 4.3, decision has to be made on whether to apply the available recycle processes identified in Step 2. Based on the heuristics in Table 4.2, The LFP battery must be recycled due to the following reasons. First, many countries have regulated that LIB makers or EV manufacturers must collect and recycle the used LIBs. Second, because of a huge demand for lithium metal and its limited reserve, the lithium used in the cathode should be recycled for reuse. Lastly, the electrolyte $LiPF_6$ should be properly treated since its exposure in nature damages the environment.

Based on the second rule for recycle process selection, the hydro-metallurgical process is selected for LFP recycling because it allows the recovery of lithium to re-manufacture new batteries. As stated above, the binder, separator, electrolyte, graphite, and carbon cannot be recovered in the two recycle processes. After selecting the recycle process for LFP battery, its product use and product recycle stages are considered as the hotspots (see heuristics in Table 4.3), since the LFP battery is a durable product.

4.5.4. Step 4: Generate Design Targets and Alternatives for Enhancing Sustainability

4.5.4.1.Propose product design targets to improve the hotspots

Three potential design targets are proposed to improve the identified hotspots.

- Design a new cathode with higher energy density and cycle number to reduce the impact at product use stage
- Develop a new green binder that does not emit toxic gases upon combustion for easy recycling
- Develop new recycle processes to recover $LiPF_6$ and PVDF

4.5.4.2.Generate potential product design alternatives

Table 4.10. The application of sustainability checklist on LFP battery

Life cycle stages	Answers	Needed information
Raw material production	• The cost of PAA (~$1.5/kg) is lower than that of PVDF (~$20/kg) • The supply of PAA is abundant with more than 10 suppliers. • PAA can be produced by well-developed polymerization processes.	• Market price of PAA • Number of PAA suppliers • PAA production process
Product manufacturing	• Solvent recovery process is not needed, as PAA is water-soluble. • Since battery assembly requires dry environment, using water as solvent may lead to more demanding operating conditions. • PAA is not a toxic material (LD_{50}>2.5 g/kg).	• Process design of battery assembly • PAA properties (e.g., toxicity, solubility)
Product use	• It has been reported that using PAA in LFP battery can lead to a higher cycle number,[166] a higher energy density, a smaller resistance of solid electrolyte interphase and charge exchange.[167]	• Quality specifications of new battery
Product recycle	• Using PAA will not affect the recovery of lithium and other metals. • The combustion of PAA only releases CO_2 and H_2O • No additional hazardous emissions will be generated.	• Hydro-metallurgical process design • PAA combustion reaction

For simplicity, only the second design target (i.e, developing a new binder) is discussed. It is found that the aqueous binders such as polyacrylic acid (PAA), carboxymethyl cellulose, and polyethylene glycol have been investigated to replace the PVDF.[168] Here, these three ingredient candidates are considered as new design alternatives.

4.5.5. Step 5: Sustainability Assessment for Design Alternatives

4.5.5.1.Using rule-based method to screen promising design alternatives

Since PAA is the cheapest among the three aqueous binders, the sustainable checklist (see Table 4.5) is applied to qualitatively assess the sustainability of new LFP battery using PAA. The answers to the questions are listed in the second column of Table 4.10. The information needed for designing such a sustainable product is shown in the third column. For instance, at the raw material production stage, the abundant PAA (around $1.5/kg) is much cheaper than PVDF (around $20/kg). At the product use stage, it has been reported that using PAA can increase product quality such as cycle number, energy density. Moreover, the combustion of PAA only release CO_2 and H_2O in the hydro-metallurgical process, instead of toxic gases. In this case, additional waste treatment is not needed.

4.6.Conclusion

This chapter presents a systematic framework for sustainable product design where LCSA, sustainability checklist, heuristics, and knowledge-bases are properly integrated and applied. This is the first attempt to develop such an approach in the process systems engineering community. Product technical requirements are first identified. Then, a base-case product is generated and available recycle techniques are collected. Afterwards, the life cycle of base-case product as well as the hotspots are decided by using LCSA or rule-based methods. To reduce the impact of hotspots, a few design targets and product design alternatives are generated based on knowledge-base and heuristics. Finally, LCSA or sustainability checklist is used to determine the most sustainable product design. This framework is demonstrated by two examples: composite bumper beam and lithium ion battery. Although many assumptions have been made in solving the complex sustainable product design problems, the framework is useful for generating promising sustainable product design from a large design space. As the design proceeds, the obtained solutions can be further verified using rigorous models or experiments. This improves the efficiency and shortens the development time.

Although the framework can be used to generate a more sustainable product, much work is still needed before sustainability can be truly claimed. For instance, uncertainties are involved in the problem formulation and solutions due to the imprecise data, model assumptions, etc. In the literature, many approaches have been proposed to facilitate decision making under uncertainties such as probability simulation, interval numbers, and rigorous modeling.[169,170] However, it is still not clear how those approaches can be employed to handle uncertainties in sustainable product design. Thus, a proper integration should be studied for enhancing design reliability. Furthermore, LCSA framework can be used to assess the EES dimensions of sustainability. However, this framework still have many limitations. For instance, the impact of human behavior is not included. Recently, Bakshi[171] proposed six necessary but not sufficient requirements that sustainability assessment methods should satisfy. For instance, one of the requirements is that the issues of intergenerational equity must be concerned for sustainability. How the requirements can be specifically used to improve the current assessment methods should be pursued. Moreover, Eq. 4.21 assumed that the economic, environmental, and social aspects are equally important. In fact, the relative importance among the three metrics and their inter-connections still need to be studied in the future. For instance, the economy is nested inside society. Both the economic and society are nested in the environment.

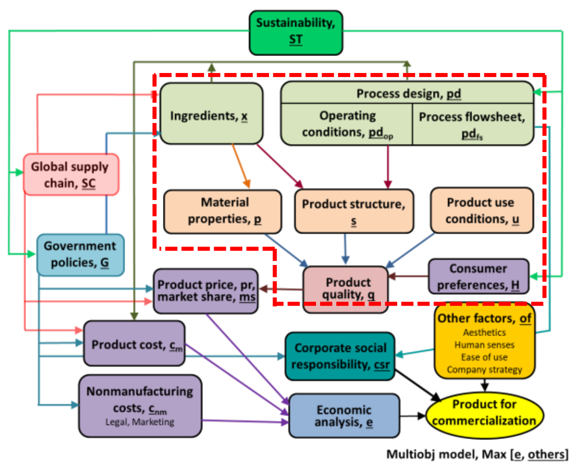
Chapter 5: Food Product Design: A Hybrid Machine Learning and Mechanistic Modeling Approach

5.1.Introduction

The food industry is very competitive, with a few multinational companies and many small enterprises competing in any given market.[172] Food products are complex and have short product life. To prosper in such an environment, the rapid development of new food products that consumers like is obviously a suitable strategy.[173] However, food products are often designed based on experience, which is expensive and time-consuming. Thus, an efficient and effective approach for expediting new food product design is highly desired.

During the past two decades, much work has been accomplished in the Process Systems Engineering community on product design such as integrated product and process design,[33,87] hybrid modeling,[30] statistical-based,[83,84] and heuristic-based[174] methods for product formulation. Only limited amount of work is focused on food products. For example, Meeuse[175] proposed a process synthesis procedure for structured food products. Dubbelboer et al.[176] applied neural network, population balance model, emulsion rheology model, etc. to design mayonnaise.

In this study, the Grand Product Design Model (Figure 5.1a) will be expanded for the design of new food products. This comprehensive model accounts for sustainability, government policies, global supply chain, selection of ingredients, process design, product pricing, and so on. It captures the conceptual relationships among various design tasks and can be readily applied to any type of product.[2,90,177,178] Figure 1b shows how it is adapted to design food products with desired quality. Starting at the top left corner, manufactured food products such as mayonnaise tends to consist of many ingredients (e.g., egg, milk, and flour) in certain compositions. The task is to select the suitable ingredients and their compositions. Each food ingredient has its own properties (e.g., taste, smell, color, and nutritional value). Various unit operations (e.g., mixing, freezing, drying, and baking) are used to process the ingredients to manufacture the food product. Some food products such as ice cream would have an internal structure that depends on the ingredients used and the manufacturing process. In general, food products can be consumed directly or after certain preparation steps (e.g., cooking instant noodles and frozen dumplings in boiling water). Food quality at the bottom of Figure 5.1b has two components. One is sensorial attributes (i.e., sight, touch, hearing, taste, and smell) perceived by the five senses of human.[179] These sensorial



(a)

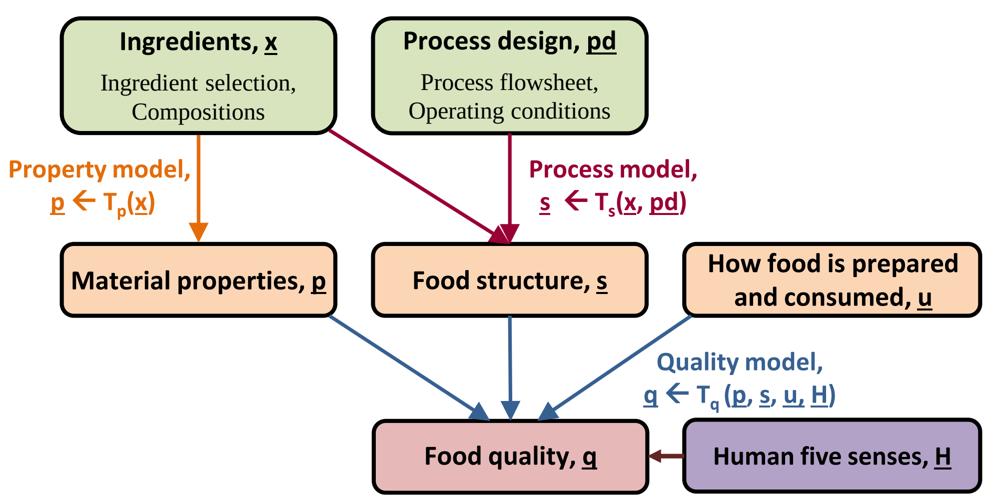


Figure 5.1. (a) The Grand Product Design model; (b) Application of Grand Product Design model for food product design

attributes are related to food characteristics such as color, viscosity, and crispness as listed in Table 5.1. Another food quality is nutritional value but, because of the intended scope of this chapter, it will not be considered in this work.

At present, nutritional values aside, new food products are designed to match identified targets by trial-and-error for certain food characteristics and thus satisfy the consumers' preferences in sensorial attributes. Then, food quality in terms of sensorial attributes is evaluated by a group of panelists. The average of the panelists' sensorial ratings is used to represent food quality.[179,180] Clearly, it is highly desirable to develop methods which can accelerate food product design.

Fortunately, considerable efforts have been made to develop mechanistic models relating food characteristics to processing conditions.[176,181] For example, the color of cookies can be related to

Table 5.1. Sensorial attributes and related food characteristics

Sensorial attributes	Related food characteristics
Sight	Shape, size, surface, color, color intensity, color depth, clarity, shininess
Touch	Cohesiveness, elasticity, viscosity, adhesiveness, hardness, crumbliness, chewiness, crispness
Hearing	Cooking sound, chewing sound, sound volume
Taste	Acidity, sweetness, spiciness, bitterness, saltiness, fattiness, aftertaste, taste intensity
Smell	Spices, bakery, edible, fruit, stinky, sour, odor intensity

the ingredient, baking time and temperature.[181] However it is still difficult to predict consumer satisfaction on food products because sensorial perception is elusive and subjective. In addition to food characteristics, it can be affected by consumer status and environment.[182] Additionally, each consumer can have significantly different preferences. Statistical methods such as response surface methodology (RSM) have been applied to analyze sensorial ratings.[183,184] Based on rating data, simple functions are regressed to correlate input and output variables. Their applicability is limited to a small number of input variables. Machine learning is an ideal option to overcome this limitation. With advanced algorithms, machine learning can deal with many input variables and there is a lot of data on consumer satisfaction on food products. However, machine learning cannot replace mechanistic models because there is only a limited amount of data relating process operating conditions to food characteristics.

In this work, a generic hybrid mechanistic modeling and machine learning approach is developed to design new food products. Mechanistic models derived from the underlying mechanisms offer reasonable estimates of food characteristics while the machine learning model predicts sensorial satisfaction. The chapter is organized as follows. First, a hybrid modeling framework where machine learning, mechanistic models, knowledge-base, and databases are employed is formulated for food product design. Then, genetic algorithm (GA) is applied to solve this grey-box optimization problem. Finally, a chocolate chip cookie case study is discussed to illustrate the applicability of this hybrid modeling approach.

5.2.Food Product Design by the Hybrid Modeling Approach

5.2.1. Hybrid Modeling Framework

Food product design problem is formulated in Eq. 5.1-5.5. The objective function is to maximize food product quality quantified by sensorial ratings ($\underline{q}$). Design variables consist of the selection and composition of food ingredients ($\underline{x}$) and the key operating conditions($\underline{pd}$) in food processing. Food characteristics $\underline{Z}$ are calculated using mechanistic models. Design constraints ($\underline{Z}^L$ and $\underline{Z}^U$) on food characteristics are defined in Eq. 5.3. Although food quality is influenced by food characteristics (see Figure 5.1), this relationship is hard to model based on physicochemical principles. Hence, food quality is correlated to the ingredients and operating conditions by using a machine learning model in Eq. 5.4. Collection of training data for sensorial rating, ingredients, and operating conditions is relatively easy. Eq. 5.5 denotes the lower and upper bounds ($\underline{c}^L$ and $\underline{c}^U$) of design variables.

$$\max_{\underline{x},\underline{pd}} \ \underline{q} \qquad \text{(Objective function)} \qquad (5.1)$$

$$\text{s.t.} \quad \underline{Z} = G(\underline{x}, \underline{pd}) \qquad \text{(Mechanistic models)} \qquad (5.2)$$

$$\underline{Z}^L \leq \underline{Z} \leq \underline{Z}^U \qquad \text{(Design constraints)} \qquad (5.3)$$

$$\underline{q} = F(\underline{x}, \underline{pd}) \qquad \text{(Machine learning model)} \qquad (5.4)$$

$$\underline{c}^L \leq \underline{x}, \underline{pd} \leq \underline{c}^U \qquad \text{(Bounds)} \qquad (5.5)$$

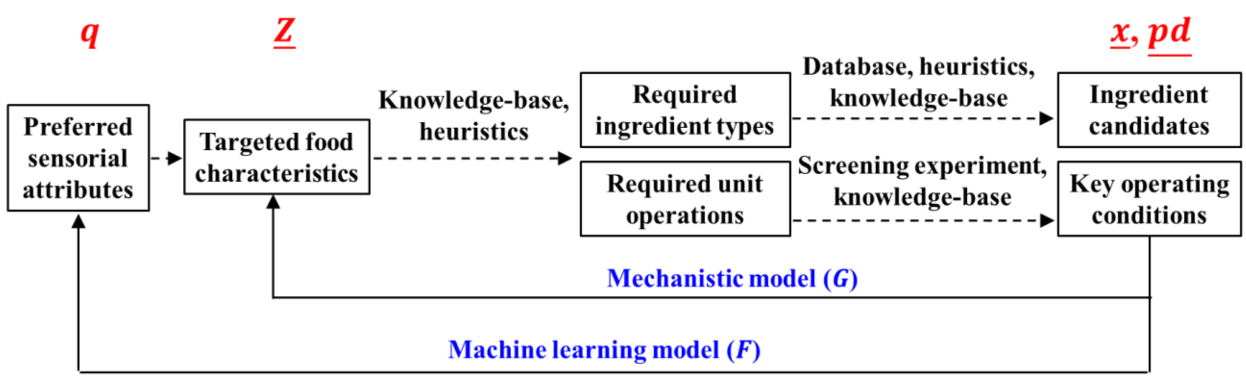


Figure 5.2. Hybrid modeling framework for food product design

A systematic hybrid modeling framework is proposed in Figure 5.2 to specify the above design formulation. Starting from the left, the preferred sensorial attributes and related food characteristics should be identified and design targets are defined. Then, a set of ingredient candidates are generated for selection. Meanwhile, the key operating conditions of required unit operations are identified as design variables. Machine learning model is built to predict sensorial ratings. Mechanistic models are used to calculate food characteristics.

5.3.1.1.Identify Preferred Sensorial Attributes and Targeted Food

As stated above, food quality depends on the sensorial attributes preferred by consumers. Although other factors such as labeling, packaging, and nutritional values may affect consumer's perception on food products, these factors are not considered in this work. To design a high-quality food, the preferred sensorial attributes for the particular food product should be first identified. Then, the importance of each sensorial attribute are assessed through heuristics or consumer survey. For instance, crisp texture is important for designing potato chips and being brown in color is essential for chocolate chip cookies.

Moreover, sensorial attributes are related to food characteristics (Table 5.1). For instance, the sight can be affected by the shape, color, clarity, etc. Food taste is related to sweetness, spiciness, aftertaste, taste intensity, etc.[179,180] In general, the variations in food characteristics can lead to different sensations and the desired food characteristics are specified to obtain the new food products. These target food characteristics are equivalent to technical requirements for non-food products and are considered as design constraints in Eq. 5.3.

5.3.1.2.Identify Ingredient Candidates and Key Operating Conditions

To make the food, the required ingredient types can be identified using heuristics and knowledge-base. Food ingredients can be classified based on their functionalities.[185] For instance, a food-grade emulsifier is used for phase stability in emulsion-based foods (e.g., mayonnaise and margarine). An essential oil can be used to obtain the desired aroma. In general, various ingredient types are needed to provide multiple desired food characteristics. For instance, the first column in Table 5.2 lists the ingredient types required for making chocolate chip cookie such as sugar, flour, and condiment.[186] For each ingredient type, numerous ingredient candidates can be selected. The consideration of all the possible ingredient candidates is not practical. Thus, a preliminary screening should be carried out to identify the high potential ingredients. Food ingredients are often generated from databases, knowledge-base, and heuristics. For instance, the composition of raw food ingredients and branded food products is available in websites by FooDB (http://foodb.ca/) and USDA (https://ndb.nal.usda.gov/ndb/). A set of ingredient candidates can be identified based on availability and properties. Table 5.2 lists 43 commonly-used ingredient candidates for chocolate chip cookie such as all-purpose flour, baking soda, egg, butter, and so on.

Table 5.2. Typical ingredient types and ingredients candidates for chocolate chip cookie

Ingredient types	Typical ingredient candidates	
Sugar and syrup	1. brown sugar	2. corn syrup
	3. white sugar	
Fat and oil	4. butter	5. peanut butter
	6. melted semisweet chocolate	7. shortening
	8. vegetable oil	
Dairy product	9. cream cheese	10. egg
	11. milk	
Flour	12. all-purpose flour	13. rice cereal
	14. whole wheat flour	15. oats
	16. cake mix	
Leavening agent	17. baking powder	18. baking soda
Chocolate additive	19. semisweet chocolate chip	20. white chocolate chip
	21. milk chocolate chip	22. cocoa powder
Coating	23. melted milk chocolate candy	24. confectioners' sugar
	25. melted semisweet chocolate	
Condiment	26. almond extract	27. cinnamon
	28. instant vanilla pudding mix	29. instant coffee granule
	30. nutmeg	31. orange zest
	32. salt	33. vanilla extract
Flavor/texture additive	34. water	35. dry cherry
	36. pumpkin puree	37. raisin
	38. almond chip	39. flaked coconut
	40. macadamia nut	41. peanut
	42. peanut butter chip	43. walnut

The unit operations that are required to process the ingredients (e.g., blending, frying, freezing, and baking) should be identified. The function and usage of major food manufacturing processes are elaborated in the book by Berk[187]. For each unit operation, many operating conditions should be decided as well. By using knowledge-base or screening experiments (e.g., single factor experiment, Plackett-Burman design),[183] the key operating conditions can be identified as design variables.

5.3.1.3.Build Machine Learning and Mechanistic Models

Figure 5.3 shows the general workflow of applying machine learning for regression and prediction. The vector $\underline{X}$ and $\underline{Y}$ are input and output variables, respectively. The training dataset $[\underline{X}, \underline{Y}]$ is imported into the learning algorithm to build a black-box model. Given an unknown input $[\underline{XU}]$, the model predicts the output $[\underline{YU}]$. Learning algorithms include random forest, support vector machine, neural network, etc. For each algorithm, there are two types of parameters: hyper- and model-parameters. The hyper-parameters defining model structure must be specified manually while the model-parameters are generated automatically. The selection of algorithm and hyper-parameters depends on the experience of users.[188] Table A5.1 in Appendix provides heuristics for selecting training algorithm and hyper-parameters. May be useful for beginners. For instance, the scaling of input data is required to apply support vector machine. After choosing the algorithm and hyper-parameters, model accuracy for new or unknown data must be assessed using cross-validation such as *K*-fold cross validation and leave-p-out cross validation. The most popular one is *K*-fold cross-validation that is elaborated in Figure A5.1 in Appendix. When using machine learning to predict sensorial ratings, the historical data of sensorial evaluations can be used as training data. For each data sample, the input variables should include the chosen ingredients and the operating conditions. The output variables are the sensorial ratings. Considering the one in ten rule, the number of data samples is preferably ten times more than the number of input variables.

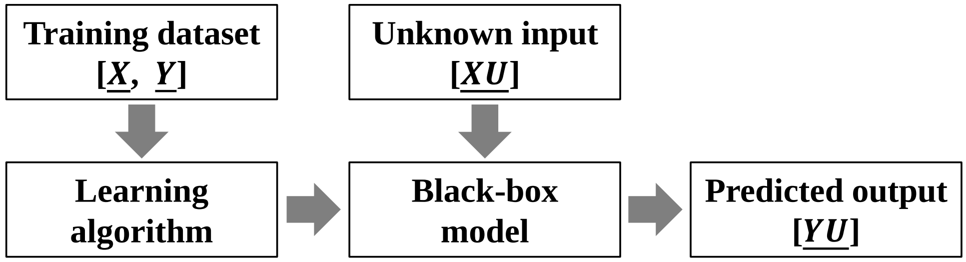


Figure 5.3 General workflow of applying machine learning for regression and prediction

Food characteristics are determined using mechanistic models. Most food characteristics are directly related to food properties. For instance, sweetness depends on sugar content. Wine acidity is decided by its pH.[12] Some food characteristics (e.g., chewiness and hardness) are related to the food structure as well. Many mechanistic models for food processing operations have already been developed based on transport phenomena, balance equations, kinetics, and so on.[189-192]

Table 5.3 shows how the hybrid modeling framework in Figure 5.2 is applied to three different food products: bread, mayonnaise, and dehydrated fruit. For instance, to make mayonnaise, egg yolk, salt, sugar, and water are used. The ingredients should be well-mixed in a homogenizer. The rotational speed, gap size, and flow rate are the key operating conditions. The sight, taste, and

Table 5.3. Application of hybrid modeling framework for the bread, mayonnaise, and dehydrated fruits examples

	Bread[181]	Mayonnaise[176]	Dehydrated fruit[193,194]
Ingredient candidates	Baking soda, water, flour, sugar, etc.	Egg yolk, salt, sugar, water, etc.	Fresh fruit
Key operating conditions	Baking temperature, baking time	Rotation speed of homogenizer, flow rate, gap size	Drying time, air flow rate, air temperature, air humidity
Machine learning model for sensorial attributes	Sight, taste, smell, touch	Sight, taste, touch	Sight, taste, touch
Mechanistic model for food characteristics	Color, crumbliness, surface crispness, softness	Color, flavor, taste intensity, viscosity	Color, chewiness, nutrient retention, rehydration properties

touch are the key sensorial attributes for mayonnaise. If the required training data is available, the ratings of various attributes can be predicted using machine learning models. The relevant food characteristics such as color and viscosity can be determined using mechanistic models.[176]

5.2.2. Solution Strategy

Eq. 5.1-5.5 is a grey-box optimization problem where both mechanistic (i.e., white-box) model and machine learning (i.e., black-box) model are used. It cannot be directly solved by derivative-based solvers (e.g., conopt and ipopt) since the derivative information of black-box models is generally not available.[195] Currently, two approaches are used to solve grey-box problems. The first one is to use a surrogate mathematical model to approximate the black-box model. The surrogate model should allow for the use of derivative-based solvers. However, no commercial solvers are available to generate surrogate models automatically although prototypes are being developed.[195,196] The other method is to apply derivative-free algorithms such as simulated annealing and genetic algorithms (GA). One of the most popular techniques to handle constraints is to use penalty function through which penalties are added to infeasible solutions. Despite their limitations, derivative-free algorithms are very easy to apply and can provide useful results at the design stage.[32]

In this work, GA is utilized to solve the grey-box design problem and Eq. 5.1-5.5 is reformulated as Eq. 5.6-5.10. Figure 5.4 illustrates the solution strategy that consists of two types of iterations: experimental iteration and GA iteration. Starting from the left, the historical sensorial

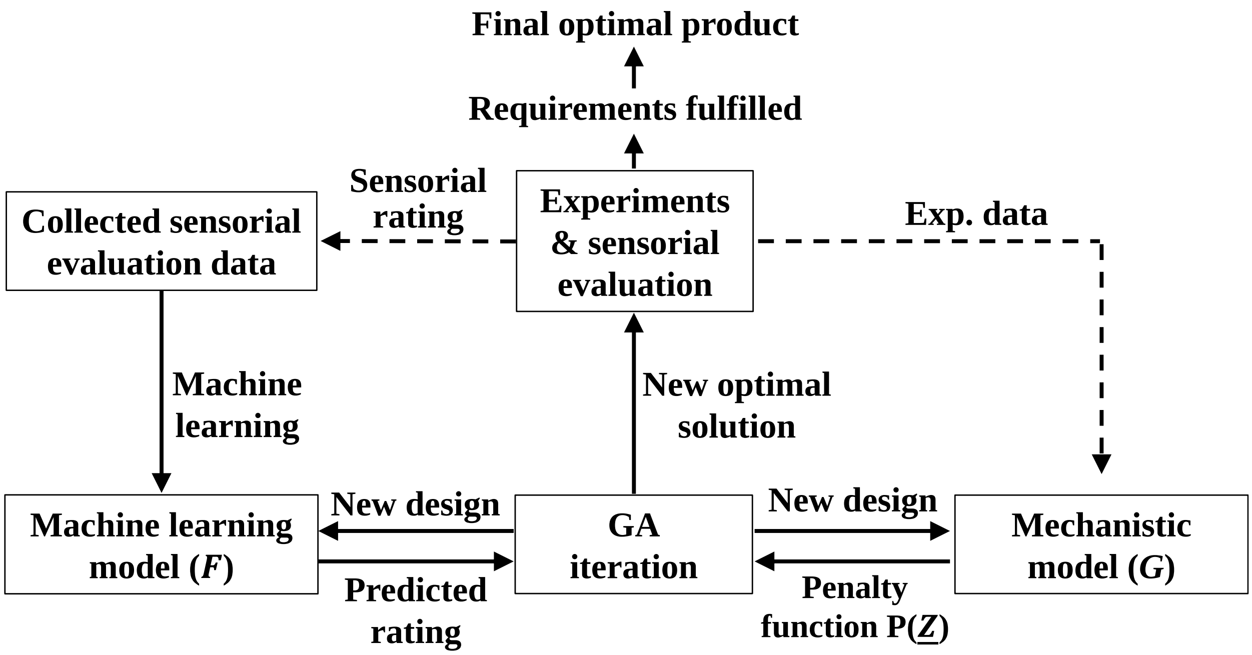


Figure 5.4. GA-based solution strategy for solving the grey-box food product design problem

ratings data is collected as training data for the machine learning model (F) to predict sensorial ratings. Design constraints calculated by mechanistic models are converted into penalty functions $P(\underline{Z})$ for use in the objective function in Eq. 5.6, which considers only a single overall rating q. If design constraints are fulfilled, the penalty function is equal to 0. Otherwise, it is equal to a large negative number ($-M$) in Eq. 5.8. The reformulated problem is solved by GA. After GA iteration, a new optimal solution can be obtained. Then, experiments should be conducted to validate the design constraints. Sensorial evaluation is performed to get the panelists' feedbacks and verify the predicted sensorial ratings. Once constraints are fulfilled and sensorial rating is confirmed, the final optimal product is obtained. Otherwise, the new data are added to the corresponding training dataset. Based on the feedback, a casual table can be used to rectify the design formulation. Table 5.4 provides the casual table for chocolate chip cookies. If the new design is considered to be too sweet, a new constraint on sugar content can be added. If the new design is too brown in color, a new constraint on the content of carbohydrate and protein can be added. Then, the revised design formulation is resolved by GA. Such an experiment iteration is stopped until the final optimal product is obtained.

$$\max_{\underline{x},\underline{pd}} \quad q + P(\underline{Z}) \qquad \text{(Objective function)} \qquad (5.6)$$

$$\text{s.t. } \underline{Z} = G(\underline{x}, \underline{pd}) \qquad \text{(Mechanistic model)} \qquad (5.7)$$

$$P(\underline{Z}) = \begin{cases} 0 & if\ \underline{Z}^L \leq \underline{Z} \leq \underline{Z}^U \\ -M & otherwise \end{cases} \qquad \text{(Penalty functions)} \qquad (5.8)$$

$$q = F(\underline{x}, \underline{pd}) \qquad \text{(Machine learning model)} \qquad (5.9)$$

$$\underline{c}^L \leq \underline{x}, \underline{pd} \leq \underline{c}^U \qquad \text{(Bounds)} \qquad (5.10)$$

Table 5.4. Casual table for designing chocolate chip cookie

Deviations/Problems	Possible Modifications
Too brown (pale)	• Reduce (increase) baking temperature or baking time • Increase (decrease) water content • Reduce (increase) the content of carbohydrate and protein (e.g., sugar, flour, milk, egg, etc.)
Too hard	• Reduce baking temperature or baking time • Reduce flour content or use another flour ingredients
Too greasy	• Reduce fat content • Select another fat ingredients • Consider new fat ingredient candidates
Too crumbly	• Reduce water content • Increase fat content
Too sweet	• Reduce sugar content • Consider new sugar and syrup ingredients
Taste is too simple	• Select multiple condiments and flavor additives
Taste is too old	• Consider new condiments and flavor additives
Chocolaty is too low (high)	• Increase (decrease) the chocolate content • Consider new chocolate ingredient candidates

For GA iteration, six parameters are specified: stopping criterion, selection method, number of GA iterations, the number of individuals in each iteration, and the probability of crossover and mutation operations. In general, a maximum number of GA iterations and roulette-wheel selection are used as the stopping criterion and selection method, respectively. The selection of these and other parameters depends on the tradeoff between solution quality and computational cost. For example, although an increase in the possibility of crossover and mutation may result in better solutions, it slows down the GA convergence.[197]

5.3. Case Study: Chocolate Chip Cookie

The proposed framework and algorithm are applied here to design new chocolate chip cookies with desired food characteristics. For simplicity, issues such as shelf life, packaging, and cost are not considered.

5.3.1. Scenario 1: Reduced-fat Chocolate Chip Cookies

5.3.2.1.Identify Preferred Sensorial Attributes and Constrained Food Characteristics

For cookies, the taste, sight, and touch are the most important sensorial attributes.[198] For taste, the new cookie is required to be chocolate-flavored and reduced-fat. For given shape and size, the color greatly affects the sight sensorial attribute. Typically, cookie should be baked to a brown (or yellow-gold) color. Note that the color on cookie surface does not include the color of additives such as edible dyes, and black chocolate.[198] Moreover, crumbliness and crispness affect the sensation of bite and chewing in the mouth. The cookie must be compact without crumb.[181] Also, a crispy cookie is desired. In summary, five design constraints are considered in this scenario: chocolate-flavored, reduced-fat, brown color, no-crumb, and crispy.

5.3.2.2.Identify Ingredient Candidates and Key Operating Conditions

Table 5.2 lists the typical ingredient types based on the cookie manufacturing manual.[186] Additionally, 43 ingredient candidates are generated based on the manual and databases, including brown sugar, butter, and baking soda. Each ingredient has different properties such as water content, fat content, and density. Their properties are given in Table A5.2 in Appendix. Cookie is made by four processes: mixing, cutting, baking, and coating (if applicable).[186] The liquid, semi-solid, and solid ingredients are well-mixed to form a dough. Then, the dough is cut into specific shapes and baked in an oven. After this, some ingredients can be coated on the surface to enhance the quality. It has been found that the baking time and temperature are the most critical variables for making cookies.[192] Therefore, the selection and composition of 43 ingredient candidates along with the baking time and temperature are regarded as design variables.

5.3.2.3.Build Machine Learning and Mechanistic Models

Machine learning is used to predict the single sensorial rating of cookies. The training data is given in an EXCEL file which is provided in https://github.com/zx2012flying/Thesis-Supporting-Information/blob/master/Data%20Samples%20In%20Chapter%205.xlsx. It contains 446 data samples extracted from recipe sharing websites. Every data sample consists of the selected ingredients, their volumetric quantities, baking temperature, baking time, average sensorial rating, and original website. For consistency, the rating is converted into [0, 100] with 100 representing the best quality. Taking algorithm performance and the number of data samples into account, random forests is selected as the learning algorithm based on the heuristics in Table A5.1. The algorithm is called from the Scikit-learn package in Python 3.6. The number of trees and max features are tuned to be 16 and 45, respectively. 10-fold cross validation is performed to evaluate model accuracy, which is measured by the mean average percentage error (MAPE). Figure 5.5 shows the validation results. The number of the data samples whose ratings are less than 85 accounts for 22% of the total dataset. The MAPE of these data is 14%. The MAPE for other samples is less than 6% and the overall MAPE is 5.7%. These results show that the machine learning model fits the training data well and can be used for prediction. Then, the single sensorial rating for cookie quality (q) is predicted by the model in Eq. 5.11-5.12.

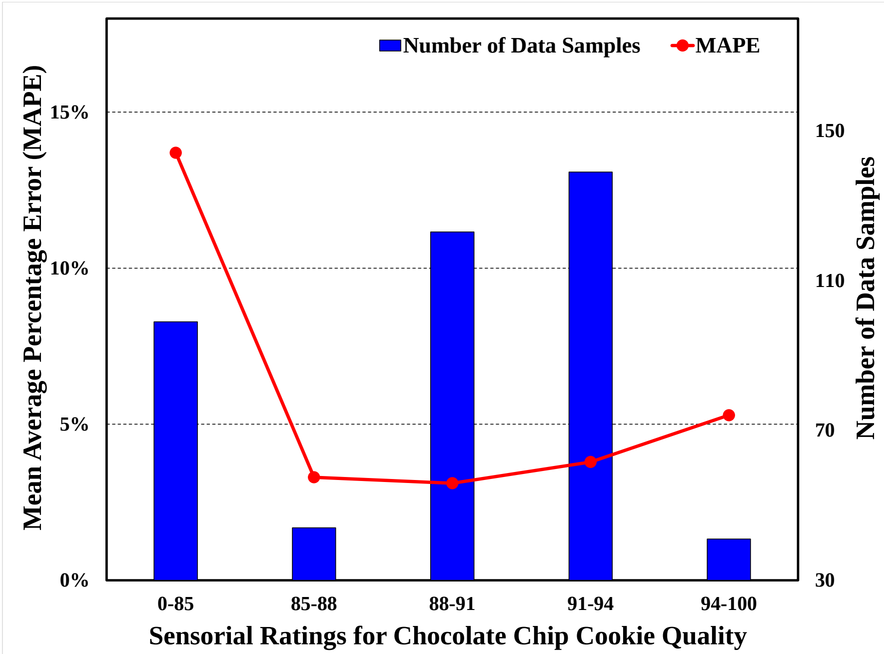


Figure 5.5. Ten-fold cross validation results obtained in Scenario 1

$$q = F(v_i, S_i, T_B, t_B) \tag{5.11}$$

$$v_i = \frac{V_i}{\sum_k V_k} \tag{5.12}$$

where i is the number given to an ingredient candidate in Table 5.2; v_i is the ingredient's volume fraction calculated based on the volumetric quantities of ingredients (V_i) in Eq. 5.12.

Moreover, the maximal volumetric quantity of ingredients are bounded by V_i^U in Eq. 5.13. Their values are given in Table A5.2. Ingredient selection is controlled by the binary variable, S_i. If i-th ingredient is selected, S_i is equal to 1 and V_i is larger than 0. Otherwise, S_i and V_i are equal to 0. The maximum number of ingredients is set to be less than or equal to 12. T_B and t_B are the baking temperature and time, respectively. Eq. 5.16-5.17 are the bounds for T_B and t_B, respectively.

$$0 \leq V_i \leq V_i^U \tag{5.13}$$

$$\begin{cases} S_i = 1, \;\; V_i > 0 & i\text{–}th\ ingredint\ selected \\ S_i = V_i = 0 & otherwise \end{cases} \tag{5.14}$$

$$\sum_i S_i \leq 12 \tag{5.15}$$

$$145 \leq T_B \leq 225\ ℃ \tag{5.16}$$

$$6.5 \leq t_B \leq 16.5 \text{ min} \tag{5.17}$$

The fat content (FC in kg fat/kg cookie) and chocolate content (CC in kg chocolate/kg cookie) are calculated based on mass balances. As a reduced-fat cookie, it must contain at least 25% less fat than the regular ones whose fat content is 0.28.

$$FC = \frac{M_{fat}}{M_{cookie}} \leq 0.28 \times 0.75 \tag{5.18}$$

where

$$M_{fat} = \sum_i m_i \cdot fc_i \tag{5.19}$$

where M_{fat} is the mass of fat in a cookie and M_{cookie} is the mass of cookie. During baking, it can be assumed that the water in the dough is totally evaporated while other constituents are retained.[199] Thus, M_{fat} is calculated based on the mass of used ingredients (m_i in kg) and their fat contents (fc_i in kg fat/kg ingredient). m_i depends on the mass fraction of the i-th ingredient (mf_i) which can be calculated based on the volumetric quantity in Eq. 5.20. M_{dough} is the mass of dough which is the summation of the mass of selected ingredients:

$$m_i = mf_i \cdot M_{dough} = \frac{V_i \cdot \rho_i}{\sum_i V_i \cdot \rho_i} \cdot M_{dough} \tag{5.20}$$

where

$$M_{dough} = \sum_i m_i \tag{5.21}$$

M_{cookie} is equal to the mass of dough subtracted by the mass of evaporated water (M_{water}). M_{water} depends on m_i and the water content of i-th ingredient (wc_i in kg water/kg ingredient).

$$M_{cookie} = M_{dough} - M_{water} \tag{5.22}$$

$$M_{water} = \sum_i m_i \cdot wc_i \tag{5.23}$$

Moreover, the chocolate content is assumed to be bounded to obtain strong chocolate flavor:

$$0.2 \le CC = \frac{M_{chocolate}}{M_{cookie}} \le 0.5 \tag{5.24}$$

where

$$M_{chocolate} = \sum_j m_j \qquad j \in \{19, 20, 21, 22,23,25\} \tag{5.25}$$

where $M_{chocolate}$ is the mass of chocolate in a cookie. The subscript j is the number given to an ingredient in Table 5.2.

Color, crispness, and crumbliness are determined by the mechanistic models that are derived based on the modeling of baking process. The process of color forming on cookie surface is known as browning. Color variation can be represented by the brownness index (BI) ranging from 0 to 1 (i.e., white to dark brown). Here, BI is bounded for representing a light brown to dark brown color.[181]

$$0.4 \le BI \le 0.8 \tag{5.26}$$

Browning is the result of the Maillard reaction producing the coloring compound melanoidin. This reaction can be initiated when the initial water activity (WA_0) is lower than 0.4.[198] It is assumed that the oven is pre-heated and the surface temperature of dough can reach the baking temperature instantly. Under the assumption, WA_0 can be calculated based on the Oswin model.[200]

$$WA_0 = \left[\left(\frac{100 \cdot M_{water}}{M_{dough} \cdot e^{-0.0056T_B+5.5}}\right)^{-2.63} + 1\right]^{-1} < 0.4 \tag{5.27}$$

The melanoidin gives a brown impression and BI is correlated with the mass of melanoidin (m_e). BI_0 is the initial brownness of dough which is assumed to be 0.05.

$$BI = 1 - (1 - BI_0) \cdot e^{-0.23 \cdot m_e} \tag{5.28}$$

The formation of melanoidin follows zero order kinetics:

$$\frac{dm_e}{dt} = k_0 \cdot e^{\left[\frac{-E_a}{R}\left(\frac{1}{T_B} - \frac{1}{T_R}\right)\right]} \tag{5.29}$$

After integration, the mass of melanoidin is

$$m_e = k_0 \cdot e^{\left[\frac{-E_a}{R}\left(\frac{1}{T_B} - \frac{1}{T_R}\right)\right]} \cdot t_B \tag{5.30}$$

where E_a is the activation energy for bakery products (around 100 kJ/mol). T_R is the reference temperature (363 K). The pre-exponential factor k_0 depends on the water activity. For simplicity, the mean water activity (WA_m) is used to calculate k_0

$$k_0 = 4.9 \times 10^{-3} \cdot \frac{e^{9 \cdot WA_m}}{2000 + e^{11.3 \cdot WA_m}} \tag{5.31}$$

$$WA_m = \frac{1}{2} WA_0 \tag{5.32}$$

Crumb is formed when the elastic dough is transformed into a fixed structure due to starch gelatinization. The degree of gelatinization (α) is regarded as a measure for crumbliness. To ensure that the cookie has no crumb, α should be equal to zero.[181]

$$crumbliness = 0 \qquad if\ \alpha = 0\ (no\ crumb) \tag{5.33}$$

To prevent gelatinization, the initial water content in the dough (WC_0) cannot exceed 50% of the total initial starch content (STC_0).

$$WC_0 < \frac{STC_0}{2} \tag{5.34}$$

$$STC_0 = \sum_i m_i \cdot stc_i \tag{5.35}$$

where stc_i is the starch content of ingredient i. The crispness depends on the relative mobility of its constituents and the glass transition temperature (T_g) of cookie can provide a measure of this relative mobility. Cookie is presumably consumed at room temperature (T_r = 25°C). Consumers obtain a crispy sensation when T_g is considerably larger than T_r.[201] Specifically, the temperature difference must be less than (-150K) to make a crispy cookie. The crispness index (CI) ranging from 0 to 1 (i.e., not crispy to highly crispy) is[181]

$$CI = \begin{cases} 0 & if\ \Delta T > 0\ (not\ crispy) \\ -\frac{\Delta T}{150} & if -150 < \Delta T < 0\ (moderate\ crispy) \\ 1 & if\ \Delta T < -150\ (crispy) \end{cases} \tag{5.36}$$

$$\Delta T = T_r - T_g < -150 \tag{5.37}$$

T_g depends on the sugar/starch ratio (r_{ss}) for cookies, which is determined using the initial content of sugar (SUC_0) and starch

$$T_g = 457.1 - 396.32 \cdot r_{ss} + 430.27 \cdot r_{ss}^2 \tag{5.38}$$

$$r_{ss} = \frac{SUC_0}{STC_0} \tag{5.39}$$

$$SUC_0 = \sum_i m_i \cdot suc_i \tag{5.40}$$

where suc_i is the sugar content of the i-th ingredient (in kg sugar/kg ingredient). In summary, the cookie design problem is formulated as:

$$\max_{V_i, S_i, T_B, t_B} \quad q \qquad \text{(A single sensorial rating as objective function)}$$

s.t. Eq. 5.19-5.23, 5.25, 5.27-5.32, 5.34-5.35, 5.38-5.40 (Mechanistic models)

Eq. 5.18, 5.24, 5.26, 5.33, 5.36-5.37 (Design constraints)

Eq. 5.11-5.12 (Machine learning model)

Eq. 5.13-5.17 (Bounds)

5.3.2.4.Results

This grey-box optimization problem is solved by GA (see Figure 5.4). The algorithm, models, bounds, and penalty functions are encoded in Python 3.6. The maximum number of GA iterations is set to be 500 and each iteration contains 100 individuals. The possibility of performing crossover and mutation is set to be 0.6. The penalty $(-M)$ is equal to (-50). Additionally, the best design of current generation is directly passed to the next generation to ensure that the best design does not deteriorate. Ten optimization runs are performed using random initial values. The CPU time per run is around 20 seconds. After 10 runs, the optimal solutions are in the range of [91.0, 92.8]. This shows that GA with penalty functions can solve the cookie design problem quickly with good convergence.

Table 5.5 shows the optimal cookie design with the largest sensorial rating (i.e., 92.8) for this scenario of making reduced-fat chocolate chip cookies. The volumetric quantities of selected ingredients and their mass fractions are given. The baking temperature and time are 195°C and 12.5 min, respectively. All five design constraints are fulfilled. For this run, Figure 5.6 shows the best at each GA iteration. If the new iteration does not provide an improved outcome, an additional 100 individual moves are performed until an improved result is obtained. The solutions produced in the first two generations are infeasible and thus penalized by (-50). Beginning with the 3th generation, feasible solutions are produced and then improved to the optimal solution.

This optimal result is different from the original 446 training data samples. For further validation, experiment and sensorial evaluation should be performed. The procedure for performing experimental validation is not elaborated here because it is not the objective of this chapter. Related discussions can be found elsewhere.[18]

Table 5.5. Optimal results for chocolate chip cookie example

		Scenario 1:		**Scenario 2:**	
		Recipes	MF (%)	Recipes	MF (%)
Ingredients	Corn syrup	1 tsp	0.4	1 tsp	0.3
	White sugar	2 cups	21.4	2 cups	18.2
	Peanut butter	1 cup	14.5	1 cup	12.4
	Egg	0.5 piece	1.4	0.5 piece	1.2
	All-purpose flour	1.5 cup	10.1	1.5 cup	8.7
	Whole wheat flour	3.5 cups	23.7	3.5 cup	20.2
	Baking soda	1.5 tsp	0.4	1.5 tsp	0.3
	Milk chocolate chip	0.5 cup	6.7	0.5 cup	5.7
	White chocolate chip	0.5 cup	4.5	0.5 cup	3.8
	Cocoa powder	0.5 cup	2.4	0.5 cup	2.1
	Melted milk chocolate candy for coating	1.5 cup	14.2	1.5 cup	12.1
	Salt	1 tsp	0.3	–	–
	Coconut	–	–	2 cup	8.2
	Vanilla extract	–	–	1.5 tsp	0.3
	Banana	–	–	0.6 cup	6.5
Operating conditions	Baking temperature (T_B)	195 °C		175°C	
	Baking time (t_B)	12.5 min		9.5 min	
Mechanistic model	Fat content (FC)	0.17		0.18	
	Chocolate content (CC)	0.26		0.24	
	Brownness index (BI)	0.57		0.49	
	Crumbliness	0		0	
	Crispness index (CI)	1		1	
Machine learning model	Sensorial rating (q)	92.8		93.3	

MF: mass fraction; tsp: teaspoon (5 mL); cup (237 mL)

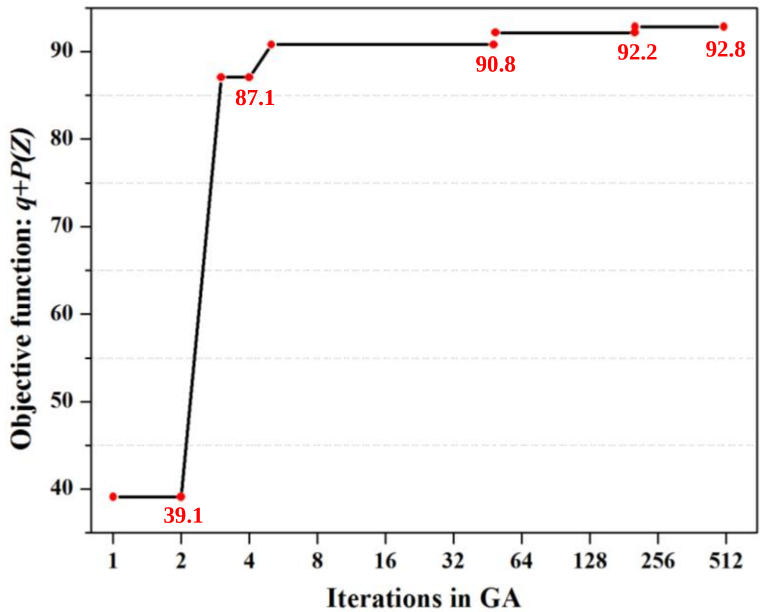


Figure 5.6. The evolution of the best solutions

5.3.2. Scenario 2: New Flavor Chocolate Chip Cookie

It is assumed that after sensorial evaluation, the panelists consider that the taste of the new cookie in scenario 1 is not sufficiently new to capture a larger market share.[173] Based on the casual table (Table 5.4), new ingredient candidates of condiments or flavor additives should be generated for selection.

5.3.2.1.Identify Preferred Sensorial Attributes and Constrained Food Characteristics

Brainstorming concludes that the compound isoamyl acetate ($C_7H_{14}O_2$) provides an 'edible' flavor.[202] In this scenario, the condiments and flavor additives of the new recipe in Scenario 1 is modified to design a new cookie.

5.3.2.2.Identify Ingredient Candidates and Key Operating Conditions

After searching isoamyl acetate in the database (http://foodb.ca), it is found that this compound is present in food aromas, and is especially rich in banana. It is decided to add mashed banana to the pool of the original flavor additive candidates for selection while keeping the basic recipe in scenario 1. In other words, 21 design variables (i.e., 8 condiment candidates, 11 flavor additive candidates, baking time, and baking temperature) are considered.

5.3.2.3.Build Machine Learning and Mechanistic Models

Since mashed banana is not included in the original 446 data samples, additional data samples are collected to augment the dataset. Another 16 new data samples with mashed banana are collected. Then, based on a total 462 data samples, random forest is applied to build a black-box model. The design constraints and mechanistic models identified in Scenario 1 are applied. The total number of ingredients in Eq. 5.15 is increased from 12 to 14. After 10-fold cross validation, the MAPE is equal to 6.3%. The content of mashed banana is assumed to be larger than 5%, but less than 20%.

$$0.05 \leq \frac{M_{banana}}{M_{cookie}} \leq 0.2 \tag{5.41}$$

5.3.2.4.Results

Again, GA is utilized to solve the design problem. Similar to Scenario 1, 10 optimization runs are performed. The maximum sensorial rating is equal to 93.3 and the optimal results are shown in the second column of Table 5.5. Compared with the results in Scenario 1, vanilla extract is added as condiment. Coconut and banana are selected as flavor additives. In addition, the operating conditions are different. Lower baking temperature and shorter baking time are preferred. The mass fraction of banana content is 6.5% and other design constraints are fulfilled.

5.4.Conclusion

This chapter presents a hybrid machine learning and mechanistic modeling approach for new food product design. A systematic framework is proposed to formulate food product design as a grey-box optimization problem. Knowledge-base, databases, heuristics, and screening experiments are properly applied to identify a set of ingredient candidates and key operating conditions as design variables. As the objective function, food quality is measured by sensorial ratings predicted by the black-box model generated through machine learning. Design constraints on food characteristics are represented by mechanistic models. Then, a GA-based algorithm is applied to solve the grey-box optimization problem. The framework is illustrated using a chocolate chip cookie design example which shows good efficiency and convergence of the algorithm.

This study can be expanded in many ways. In a society where healthy living is emphasized, it is natural to include nutritional values in food product design. As shown in Figure 5.1b, the Grand Product Design Model must consider aesthetics and human senses because all products have to include human factors in addition to functional attributes. The importance of the former increases as the product type changes from commodity chemicals to personal products, which demands hard-to-quantify attributes. By combining models that are based on chemical engineering principles and big data, the hybrid approach is ideally suited to performing this transition. Efforts to refine this approach and apply it to products such as cosmetic products are underway.

5.5. Appendix

Table A5.1. Heuristics for selecting training algorithms and tuning hyper-parameters

Training algorithms	Heuristics	Key hyper-parameters
Linear regression	• As the easiest method, linear model is always used as a baseline method before using other advanced models. • Linear model often under-fits in complex systems with many input variables.	None
K-nearest neighbors	• Easy to use without heavily tuning hyper-parameters. • For sparse datasets and large datasets with many input variables, this method often has poor performance in regression. • Using 3-5 neighbors and Euclidean distance metric are proper for most cases.[188]	Number of neighbors, distance metric

Random forest	• As one of the mostly used methods, random forest works very well for regression and classification, even in sparse and complex dataset. • Random forest can only be used for interpolation, instead of extrapolation. • Tuning the number of trees by testing 2, 4, 8, …, etc. and then do fine-tuning. • As good rule of thumb, max features for split is suggested as the number of features for regression problems.	Number of trees, max features for split
Support vector machine	• It is always used for classification such as tasty or not, smells good or not, etc. • For complex systems, non-linear kernel functions (e.g., polynomial, radial basis function, etc.) are preferred. • The performance is sensitive to the setting of hyper-parameters and the scaling of input data. The input data should be scaled (e.g., between 0-1). • Small regularization parameter may lead to under-fitting while large ones can result in overfitting. In general, it is tuned in a descending order.	Kernel function, regularization parameter
Neural network	• A large training dataset is required for using neural network. • Neural network often provides the best performance for large datasets and complex systems with many input variables and large variations. • Input features should be scaled to a mean of zero and a variance of one.[188] • Tuning hyper-parameters is difficult and overfitting often occurs with large network. • Using at most 2 hidden layers can work well for most datasets.[203] • The number of neurons in each layer is suggested between the number of input and output variables.[203]	Activation function, number of hidden layers, number of neurons

A Brief Introduction on K-fold Cross-validation

The *K*-fold cross-validation is elaborated here. *K* is the number of groups that the collected dataset is to be split into. There is no formal rule to specify the *K* and it is usually specified as 5 or 10. Figure A5.1 shows the mechanism of 5-fold cross validation. The dataset is split into 5 groups randomly. For one run, four data groups are used as training dataset to build a black-box model. The remaining data group is regarded as test dataset. Its input variables are imported into the black-box model to predict the outputs. The predicted outputs are compared with the true values to calculate the accuracy. This procedure is repeated five times. The average accuracy shows how the algorithm and hyper-parameters are suitably selected for the collected dataset. The desired accuracy varies in different cases. If the model is not accurate enough, the algorithm or hyper-parameter should be re-selected.

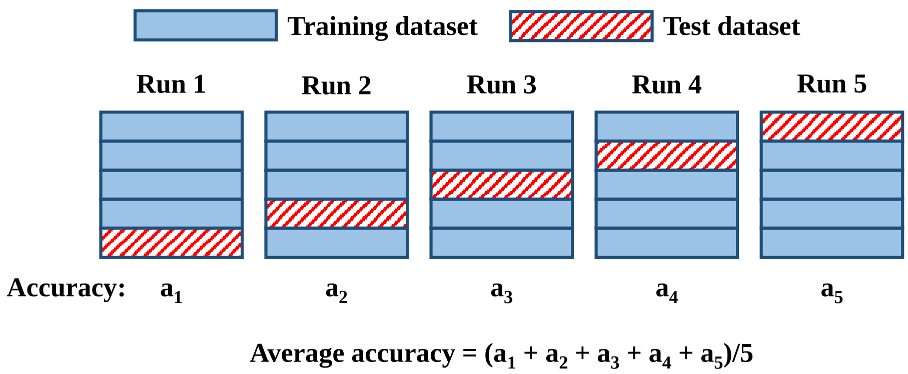


Figure A5.1. Five-fold cross validation for building black-box models

Table A5.2. Food ingredient properties and their volumetric bound

No.	Ingredient	Volumetric upper bound V^L	Volumetric unit	Density ρ (kg/ml)	Fat content fc (g/g)	Water content wc (g/g)	Starch content stc (g/g)	Sugar content suc (g/g)
1	Brown sugar	2	Cup	0.93	0.00	0.01	0.00	0.97
2	Corn syrup	4	Teaspoon	1.33	0.00	0.22	0.00	0.00
3	White sugar	2	Cup	0.80	0.00	0.00	0.00	1.00
4	Butter	2	Cup	0.96	0.81	0.16	0.00	0.00
5	Peanut butter	2	Cup	1.09	0.51	0.01	0.00	0.00
6	Melted semisweet chocolate	2	Cup	1.00	0.27	0.00	0.05	0.53
7	Shortening	2	Cup	0.86	1.00	0.00	0.00	0.00
8	Vegetable oil	2	Cup	0.93	1.00	0.00	0.00	0.00
9	Cream cheese	2	Cup	0.98	0.34	0.53	0.00	0.00
10	Egg	3	Piece	0.83	0.10	0.76	0.00	0.00
11	Milk	4	Tablespoon	1.29	0.09	0.27	0.00	0.54
12	Almond extract	2	Teaspoon	0.84	0.00	0.00	0.00	0.00
13	Cinnamon	2	Teaspoon	0.52	0.01	0.11	0.24	0.00
14	Instant vanilla pudding mix	2	Teaspoon	0.96	0.01	0.03	0.00	0.00
15	Instant coffee granules	2	Teaspoon	0.18	0.00	0.00	0.06	0.00
16	Nutmeg	2	Teaspoon	0.44	0.36	0.06	0.22	0.00
17	Orange zest	2	Teaspoon	0.95	0.00	0.00	0.00	0.00
18	Salt	2	Teaspoon	1.20	0.00	0.00	0.00	0.00
19	Vanilla extract	2	Teaspoon	0.84	0.00	0.53	0.00	0.00

20	All-purpose flour	4	Cup	0.51	0.03	0.00	0.68	0.00
21	Rice cereal	4	Cup	0.12	0.01	0.04	0.50	0.00
22	Whole wheat flour	4	Cup	0.51	0.03	0.11	0.68	0.00
23	Oats	4	Cup	0.42	0.08	0.00	0.14	0.00
24	Cake mix	4	Cup	0.97	0.12	0.00	0.68	0.46
25	Baking powder	2	Teaspoon	0.92	0.00	0.05	0.00	0.00
26	Baking soda	2	Teaspoon	0.92	0.00	0.00	0.00	0.00
27	Semisweet chocolate chips	2	Cup	1.00	0.27	0.00	0.05	0.53
28	White chocolate chips	2	Cup	0.67	0.27	0.00	0.05	0.80
29	Milk chocolate chips	2	Cup	1.00	0.27	0.00	0.05	0.00
30	Cocoa powder	2	Cup	0.36	0.14	0.03	0.06	0.00
31	Water	1	Cup	1.00	0.00	1.00	0.00	0.00
32	Dry cherry	2	Cup	0.68	0.00	0.00	0.01	0.00
33	Pumpkin puree	2	Cup	1.03	0.00	0.90	0.01	0.00
34	Raisin	2	Cup	0.70	0.00	0.15	0.00	0.00
35	Almond chip	2	Cup	0.61	0.53	0.05	0.00	0.00
36	Flaked coconut	2	Cup	0.36	0.28	0.15	0.00	0.00
37	Macadamia nut	2	Cup	0.57	0.76	0.01	0.01	0.00
38	Peanut	2	Cup	0.62	0.49	0.07	0.04	0.00
39	Peanut butter chip	2	Cup	0.67	0.27	0.00	0.04	0.00
40	Walnut	3	Cup	0.46	0.72	0.04	0.00	0.00
41	Melted milk chocolate candy (coating)	2	Cup	0.71	0.30	0.02	0.05	0.75
42	Confectioners' sugar (coating)	2	Tablespoon	0.50	0.00	0.00	0.00	0.00
43	Melted semisweet chocolate (coating)	2	Cup	1.00	0.27	0.00	0.05	0.53

*Data of density, fat content, water content, starch content, and sugar content are from United States Department of Agriculture Database (https://ndb.nal.usda.gov/ndb/)

Chapter 6: Conclusion and Future Work

6.1.Summary of Major Achievements

This research focuses on product design with the consideration of multiple influential business and management issues. Multi-scale modeling, heuristics, databases, etc. have been utilized properly at various places. The main contributions are summarized below.

In chapter 2, we study the influence of government policies (i.e., incentives and regulations) and corporate social responsibly on product design. Government-company-consumer relationship has been well studied. A multi-objective optimization framework is presented from the company's perspective in order to illustrate the trade-off between company profits and social responsibility. Different models as well as rule-based methods –quality, consumer utility, product demand, product cost, capital budgeting, social indices, and government policy –are employed. A solar photovoltaic case study is used to illustrate the framework. In principle, the framework can be applied for any product design project, particularly for those with great potentials for creating environmental and social benefits to the society.

In chapter 3, a new product design framework is presented with the simultaneous consideration of make-or-buy analysis and supplier selection. Consumer preference, ingredient selection, product pricing, make-or-buy analysis, and supplier selection are fully integrated in the framework. This framework tells designers when and how the important supply chain issues should be considered during the product design processes in order to maximize the profits. Two case studies consisting of light duty liquid detergent and controlled release granular herbicide are provided to illustrate the framework. In fact, this framework is applicable beyond the two examples. Particularly, it is useful for designing formulated and functional products since these products generally involves multiple ingredients and thus suppliers.

In chapter 4, we focused on sustainable chemical product design. A five-step design framework is proposed where the state-of-the-art LCSA methodology, rule-based methods, and general sustainable product design principles and knowledge are properly integrated for the development of more sustainability products. The economic, environmental, and social issues are simultaneously considered to provide a comprehensive view. Two case studies – composite bumper beam and lithium ion battery – are provided to illustrate the framework. It is clear that the generic framework can be applied to any product regardless of the availability of LCI data, especially those products needed to be recycled.

In chapter 5, a hybrid machine learning and mechanistic modeling approach is proposed to expedite the development of new food products. At present, food products are designed by trail-and-error and the sensorial ratings are determined by a tasting panel. By using machine learning, we can predict the sensorial rating reliably. In addition, with the aid of mechanistic models for calculating food characteristics, optimal food product can be obtained. Moreover, to solve this grey-box optimization problem, genetic algorithm is utilized where the design constraints (representing the desired food characteristics) are handled as penalty functions. A chocolate chip cookie example is provided to illustrate the applicability of the hybrid modeling framework and solution strategy. Clearly, this hybrid modeling approach can be applied beyond the considered cookie example. Its application is straightforward for general food product design problem.

6.2.Limitations

Despite the above achievements in product design and development, the proposed approaches still have many limitations. For instance,

- In Chapter 2, given certain government incentives, the framework is hard to cover the variations of product ingredients and manufacturing process design. Because no specific models exist to correlate the variations of ingredients or processes with product quality under certain government incentives. Another limitation is the definition of weight factors in Eq. 2.19. The weighting factors can greatly influence the optimization results. To reach a universal consensus on CSR, a more comprehensive and in-depth evaluation of the weighting factors is required.

- In Chapter 3, by using the framework, the resulted optimization problem is always complicated with a large number of variables and non-convex. When many ingredient candidates and suppliers are simultaneously considered, the complexity and search space increases. In this case, the computation efficiency is likely to become a limiting factor.
- In Chapter 4, although the framework can be used to generate a more sustainable product, much work is still needed before sustainability can be truly claimed. For instance, uncertainties are involved in the problem formulation and solutions due to the imprecise data, model assumptions, etc. In the literature, many approaches have been proposed to facilitate decision making under uncertainties such as probability simulation, interval numbers, and rigorous modeling. However, it is still not clear how those approaches can be employed to handle uncertainties in sustainable product design. Moreover, Eq. 4.17 assumed that the economic, environmental, and social aspects are equally important. In fact, the relative importance among the three metrics and their inter-connections still need to be studied in the future. For instance, the economy is nested inside society. Both the economic and society are nested in the environment.
- In this chapter, the application of the hybrid modeling approach actually depends on the availability of training data for building machine models and the understanding of underlying mechanisms in food processing. Without any of these, the approach cannot be used. Moreover, the GA-based solution strategy still suffer many limitations. For instance, it cannot guarantee

optimality. In addition, as the number of design variable increases, the computational reliability drops significantly.

6.3.Future Work

Despite the above important achievements, it is clear that these are theoretical and conceptual improvements in the area of product design and development, instead of designing new products in practice. Therefore, the design of a few specific real chemical products is worth to be considered in the future. The potential products can be

Cosmetics

Like the food products, cosmetics are the products with high profit margin and the entire cosmetic industry is quite competitive. In this case, cosmetic companies are seeking to reduce the time to market and develop better products for commercialization. The former always requires efficient and effective design framework and procedures with proper tools, models, and heuristics for many products. The latter can be achieved through the innovation of new ingredients and new combinations of existing ingredients. Clearly, the synthesis of new materials rely on the understanding of material science and chemistry. The new combination of existing ingredients should be always optimized so that new products with desired quality can be obtained. Accordingly, two research problems should be considered in the future: systematic design framework for cosmetics product; reliable models and tools for cosmetics products.

Lubricant oil

As an important formulated product, lubricant oil is made up of two types of ingredients: base oil and additives. The base oil can be derived from three sources: petroleum, synthetic, and biological. At present, petroleum base oil is the mainstream in the lubricant industry. However, with the awareness of the damage to the environment, the trend for designing new synthetic and biological lubricant oil is inevitable. Moreover, additives are used to modify and enhance the properties of lubricant oil such as rheology, flammability, and freezing point. How to select additives with proper composition is always a problem. Accordingly, it is worth to study how the synthetic and biological base oil should be designed and what additives should be selected.

Reference

1. Ng KM, *A Multidisciplinary Hierarchical Framework for the Design of Consumer Centered Chemical Products*, in *Computer Aided Chemical Engineering*, K.V. Gernaey, J.K. Huusom, and R. Gani, Editors. 2015, Elsevier. p. 15-24.
2. Fung KY, Ng KM, Zhang L, Gani R. A grand model for chemical product design. *Computers & Chemical Engineering*. 2016;91:15-27.
3. Zhang L, Babi DK, Gani R. New vistas in chemical product and process design. *Annual Review of Chemical and Biomolecular Engineering*. 2016;7(1):557-582.
4. Cussler EL, Wei J. Chemical product engineering. *AIChE Journal*. 2003;49(5):1072-1075.
5. Costa R, Moggridge GD, Saraiva PM. Chemical product engineering: An emerging paradigm within chemical engineering. *AIChE Journal*. 2006;52(6):1976-1986.
6. Hill M. Chemical product engineering—The third paradigm. *Computers & Chemical Engineering*. 2009;33(5):947-953.
7. Gani R, Ng KM. Product design – Molecules, devices, functional products, and formulated products. *Computers & Chemical Engineering*. 2015;81:70-79.
8. Wibowo C, Ng KM. Product-Centered Processing: Manufacture of Chemical-Based Consumer Products. *AIChE Journal*. 2002;48(6):1212-1230.
9. Wibowo C, Ng KM. Product-oriented process synthesis and development: Creams and pastes. *AIChE Journal*. 2001;47(12):2746-2767.
10. Fung KY, Ng KM. Product-centered processing: Pharmaceutical tablets and capsules. *AIChE Journal*. 2003;49(5):1193-1215.
11. Bagajewicz MJ. On the role of microeconomics, planning, and finances in product design. *AIChE Journal*. 2007;53(12):3155-3170.
12. Whitnack C, Heller A, Frow MT, Kerr S, Bagajewicz MJ. Financial risk management in the design of products under uncertainty. *Computers & Chemical Engineering*. 2009;33(5):1056-1066.
13. Street C, Woody J, Ardila J, Bagajewicz M. Product design: A case study of slow-release carpet deodorizers/disinfectants. *Industrial & Engineering Chemistry Research*. 2008;47(4):1192-1200.
14. Bagajewicz MJ, Hill S, Robben A, Lopez H, Sanders M, Sposato E, Baade C, Manora S, Hey Coradin J. Product design in price-competitive markets: A case study of a skin moisturizing lotion. *AIChE Journal*. 2011;57(1):160-177.
15. Cheng YS, Lam KW, Ng KM, Ko RKM, Wibowo C. An integrative approach to product development-A skin-care cream. *Computers and Chemical Engineering*. 2009;33(5):1097-1113.
16. Bernardo FP, Saraiva PM. A conceptual model for chemical product design. *AIChE Journal*. 2015;61(3):802-815.
17. Conte E, Gani R, Ng KM. Design of formulated products: A systematic methodology. *AIChE Journal*. 2011;57(9):2431-2449.
18. Conte E, Gani R, Cheng YS, Ng KM. Design of formulated products: Experimental component. *AIChE Journal*. 2012;58(1):173-189.
19. Mattei M, Kontogeorgis GM, Gani R. A comprehensive framework for surfactant selection and design for emulsion based chemical product design. *Fluid Phase Equilibria*. 2014;362:288-299.

20. Korichi M, Gerbaud V, Floquet P, Meniai AH, Nacef S, Joulia X. Computer aided aroma design I–Molecular knowledge framework. *Chemical Engineering and Processing: Process Intensification*. 2008;47(11):1902-1911.
21. Ng KM. MOPSD: a framework linking business decision-making to product and process design. *Computers & Chemical Engineering*. 2004;29(1):51-56.
22. Stephanopoulos G. Invention and Innovation in a Product-Centered Chemical Industry: General Trends and a Case Study. In AIChE Conference. 55th Institute Lecture, San Francisco. 2003.
23. Smith BV, Ierapepritou M. Framework for consumer-integrated optimal product design. *Industrial & Engineering Chemistry Research*. 2009;48(18):8566-8574.
24. Dupont. https://s2.q4cdn.com/752917794/files/doc_downloads/2015/DuPont_2015_DataBook-FINAL.pdf *(accessed in March 2017)*. 2015.
25. Seider WD, Lewin DR, Seader JD, Widegado S, Gani R, Ng KM. *Product and process design principles: Synthesis, analysis and evaluation*. 4 ed. New York: Wiley. 2017.
26. Kraslawski A, *Product Development*, in *Computer Aided Process and Product Engineering*. 2006, Wiley-VCH Verlag GmbH. p. 419-442.
27. Smith BV, Ierapepritou MG. Modeling and optimization of product design and portfolio management interface. *Computers & Chemical Engineering*. 2011;35(11):2579-2589.
28. Lee CKH, Choy KL, Chan YN. A knowledge-based ingredient formulation system for chemical product development in the personal care industry. *Computers & Chemical Engineering*. 2014;65:40-53.
29. Tam SK, Fung KY, Poon GSH, Ng KM. Product design: Metal nanoparticle-based conductive inkjet inks. *AIChE Journal*. 2016;62(8):2740-2753.
30. Sundaram A, Ghosh P, Caruthers JM, Venkatasubramanian V. Design of fuel additives using neural networks and evolutionary algorithms. *AIChE Journal*. 2001;47(6):1387-1406.
31. Sahinidis NV, Tawarmalani M, Yu M. Design of alternative refrigerants via global optimization. *AIChE Journal*. 2003;49(7):1761-1775.
32. Dahmen M, Marquardt W. Model-based design of tailor-made biofuels. *Energy & Fuels*. 2016;30(2):1109-1134.
33. Martín M, Martínez A. A methodology for simultaneous process and product design in the formulated consumer products industry: The case study of the detergent business. *Chemical Engineering Research and Design*. 2013;91(5):795-809.
34. Almeida-Rivera C, Jain P, Bruin S, Bongers P, *Integrated product and process design approach for rationalization of food products*, in *Computer Aided Chemical Engineering*, V. Pleşu and P.Ş. Agachi, Editors. 2007, Elsevier. p. 449-454.
35. Heflin L, Walsh S, Bagajewicz M. Design of medical diagnostics products: A case-study of a saliva diagnostics kit. *Computers & Chemical Engineering*. 2009;33(5):1067-1076.
36. Chan YC, Fung KY, Ng KM. Product design: A pricing framework accounting for product quality and consumer awareness. *AIChE Journal*. 2018;64(7):2462-2471.
37. Pigosso CD, Ferraz M, Teixeira EC, Rozenfeld H. The Deployment of Product-Related Environmental Legislation into Product Requirements. *Sustainability*. 2016;8(4):332-346.
38. Marshall KP, Piper WS. *Government Policy and Program Impacts on Technology Development, Transfer, and Commercialization: International Perspectives*. Vol. 13. Routledge. 2005.

39. Record SC. Statements on introduced bills and joint resolutions: Sec.846. Procurement of photovoltaic devices. https://www.congress.gov/111/plaws/publ383/PLAW-111publ383.pdf *(assessed in June2018)*. 2017.
40. You F, Tao L, Graziano DJ, Snyder SW. Optimal design of sustainable cellulosic biofuel supply chains: Multiobjective optimization coupled with life cycle assessment and input–output analysis. *AIChE Journal*. 2012;58(4):1157-1180.
41. McWilliams A, Siegel D. Corporate Social Responsibility: A Theory of the Firm Perspective. *Academy of Management Review*. 2001;26(1):117-127.
42. Baumann H, Boons F, Bragd A. Mapping the green product development field: engineering, policy and business perspectives. *Journal of Cleaner Production*. 2002;10(5):409-425.
43. NDRC. Feed in tariff in Mainland China. http://www.ndrc.gov.cn/xwzx/xwfb/201512/t20151224_768534.html *(accessed in March 2017)*. 2011.
44. Koehler J. Detergent Phosphates: an EU Policy Assessment. *Journal of business chemistry*. 2006;31(2):15-30.
45. Coren MJ. Tax incentives might run out on Tesla, but electric cars will be just fine. https://qz.com/1025713/teslas-tsla-drop-in-hong-kong-sales-after-the-expiration-of-tax-incentives-wont-really-matter-for-electric-vehicles-in-the-long-run/ *(accessed in January 2018)*. 2017.
46. Yoo T. Tesla sales stopped dead in Hong Kong after a tax break for electric cars was scrapped. http://www.businessinsider.com/tesla-sales-stopped-in-hong-kong-tax-break-for-electric-cars-scrapped-2017-7 *(accessed in January 2018)*. 2017.
47. Varian H. *Microeconomic Analysis*. Third Edition ed. New York: W.W. Norton & Company, Inc. . 1992.
48. Hanemann WM. Discrete/continuous models of consumer demand. *Econometrica: Journal of the Econometric Society*. 1984;52(3):541-561.
49. Lancaster KJ. A new approach to consumer theory. *The Journal of Political Economy*. 1966;74:132-157.
50. Armstrong JS, Brodie RJ, *Forecasting for Marketing*, in *Quantitative Methods in Marketing*. 1999. p. 92-120.
51. Train KE. *Discrete choice methods with simulation*. Cambridge university press. 2009.
52. Walker J, Ben-Akiva M. Generalized random utility model. *Mathematical Social Sciences*. 2002;43(3):303-343.
53. McFadden D, *Conditional logit analysis of qualitative choice behavior*, in *Frontiers in Econometrics*, P. Zarembka, Editor. 1973, Academic Press: Cambridge, MA. p. 105-142.
54. Commission JRC-E. *Handbook on constructing composite indicators: Methodology and user guide*. OECD publishing. 2008.
55. GRI. *Available at:* https://www.globalreporting.org */resourcelibrary/GRIG4-Part1-Reporting-Principles-and-Standard-Disclosures. pdf (accessed in March 2017)*. 2015.
56. Curran MA. *Life cycle assessment*. Wiley Online Library. 2008.
57. Lehmann A, Russi D, Bala A, Finkbeiner M, Fullana-i-Palmer P. Integration of social aspects in decision support, based on life cycle thinking. *Sustainability*. 2011;3(4):562-577.
58. Miller RE, Blair PD. *Input-output analysis: foundations and extensions*. Cambridge University Press. 2009.
59. Van den Bossche F, Rogge N, Devooght K, Van Puyenbroeck T. Robust Corporate Social Responsibility investment screening. *Ecological Economics*. 2010;69(5):1159-1169.

60. Capelle-Blancard G, Petit A. The Weighting of CSR Dimensions: One Size Does Not Fit All. *Business & Society*. 2015;56(6):919-943.
61. Hsu A, Zomer A. Environmental Performance Index. *Wiley StatsRef: Statistics Reference Online*. 2016.
62. Goedkoop M, Spriensma R. The eco-indicator 99—a damage oriented method for life cycle assessment: methodology annex. https://www.pre-sustainability.com/download/EI99_annexe_v3.pdf *(accessed in June 2018)*. 2004.
63. OECD. Composite leading indicator (CLI). https://data.oecd.org/leadind/composite-leading-indicator-cli.htm *(accessed in June 2018)*. 2018.
64. Sen A. Human Development Index: Methodology and Measurement. 1994.
65. Rangaiah GP. *Multi-objective optimization: techniques and applications in chemical engineering*. Vol. 5. World Scientific. 2016.
66. Goodrich AC, Powell DM, James TL, Woodhouse M, Buonassisi T. Assessing the drivers of regional trends in solar photovoltaic manufacturing. *Energy & Environmental Science*. 2013;6(10):2811-2821.
67. Wang Y, Zhou S, Huo H. Cost and CO2 reductions of solar photovoltaic power generation in China: Perspectives for 2020. *Renewable and Sustainable Energy Reviews*. 2014;39:370-380.
68. Branker K, Pathak MJM, Pearce JM. A review of solar photovoltaic levelized cost of electricity. *Renewable and Sustainable Energy Reviews*. 2011;15(9):4470-4482.
69. Peng J, Lu L. Investigation on the development potential of rooftop PV system in Hong Kong and its environmental benefits. *Renewable and Sustainable Energy Reviews*. 2013;27:149-162.
70. Benthem Av, Gillingham K, Sweeney J. Learning-by-Doing and the Optimal Solar Policy in California. *The Energy Journal*. 2008;29(3):131-151.
71. Nemet GF. Beyond the learning curve: factors influencing cost reductions in photovoltaics. *Energy Policy*. 2006;34(17):3218-3232.
72. Hong J, Chen W, Qi C, Ye L, Xu C. Life cycle assessment of multicrystalline silicon photovoltaic cell production in China. *Solar Energy*. 2016;133:283-293.
73. Fritzmann C, Löwenberg J, Wintgens T, Melin T. State-of-the-art of reverse osmosis desalination. *Desalination*. 2007;216(1):1-76.
74. Di X, Nie Z, Yuan B, Zuo T. Life cycle inventory for electricity generation in China. *The International Journal of Life Cycle Assessment*. 2007;12(4):217-224.
75. Administration NE. http://www.nea.gov.cn/2015-03/09/c_134049519.htm *(accessed in June2018)*. 2014.
76. Administration NE. http://www.nea.gov.cn/2016-02/05/c_135076636.htm *(accessed in June 2018)*. 2015.
77. NE21. http://www.ne21.com/news/show-51365.html *(accessed in June 2018)*. 2013.
78. Wang Z, Rangaiah GP. Application and Analysis of Methods for Selecting an Optimal Solution from the Pareto-Optimal Front obtained by Multiobjective Optimization. *Industrial & Engineering Chemistry Research*. 2017;56(2):560-574.
79. Smith BV, Ierapepritou MG. Integrative chemical product design strategies: Reflecting industry trends and challenges. *Computers & Chemical Engineering*. 2010;34(6):857-865.
80. Edwards MF. Product engineering: some challenges for chemical engineers. *Chemical Engineering Research and Design*. 2006;84(4):255-260.

81. Mattei M, Hill M, Kontogeorgis GM, Gani R. Design of an emulsion-based personal detergent through a model-based chemical product design methodology. *Computer Aided Chemical Engineering*. 2013;32:817-822.
82. Dahmen M, Marquardt W. Model-based formulation of biofuel blends by simultaneous product and pathway design. *Energy & Fuels*. 2017;31(4):4096-4121.
83. Omidbakhsh N, Duever TA, Elkamel A, Reilly PM. Systematic statistical-based approach for product design: Application to disinfectant formulations. *Industrial & Engineering Chemistry Research*. 2010;49(1):204-209.
84. Omidbakhsh N, Duever TA, Elkamel A, Reilly PM. A systematic computer-aided product design and development procedure: Case of disinfectant formulations. *Industrial & Engineering Chemistry Research*. 2012;51(45):14925-14934.
85. Mata VG, Gomes PB, Rodrigues AE. Engineering perfumes. *AIChE Journal*. 2005;51(10):2834-2852.
86. Teixeira MA, Rodríguez O, Rodrigues S, Martins I, Rodrigues AE. A case study of product engineering: Performance of microencapsulated perfumes on textile applications. *AIChE Journal*. 2012;58(6):1939-1950.
87. Li J, Xiao J, Huang Y, Lou HH. Integrated process and product analysis: A multiscale approach to paint spray. *AIChE Journal*. 2007;53(11):2841-2857.
88. Xiao J, Huang Y. Microstructure–property–quality-correlated paint design: An LMC-based approach. *AIChE Journal*. 2009;55(1):132-149.
89. Kalakul S, Eden MR, Gani R. The chemical product simulator – ProCAPD. *Computer Aided Chemical Engineering*. 2017;40:979-984.
90. Zhang X, Zhang L, Fung KY, Rangaiah GP, Ng KM. Product design: Impact of government policy and consumer preference on company profit and corporate social responsibility. *Computers & Chemical Engineering*. 2018;118:118-131.
91. Moschuris SJ. Organizational participants in the make-or-buy process. *Industrial Marketing Management*. 2008;37(2):143-153.
92. Geyskens I, Steenkamp JEM, Kumar N. Make, buy, or ally: A transaction cost theory meta-analysis. *Academy of management journal*. 2006;49(3):519-543.
93. Van de Water H, Van Peet HP. A decision support model based on the Analytic Hierarchy Process for the Make or Buy decision in manufacturing. *Journal of Purchasing and Supply Management*. 2006;12(5):258-271.
94. Platts KW, Probert DR, Cáñez L. Make vs. buy decisions: A process incorporating multi-attribute decision-making. *International Journal of Production Economics*. 2002;77(3):247-257.
95. Amorim P, Curcio E, Almada-Lobo B, Barbosa-Póvoa APFD, Grossmann IE. Supplier selection in the processed food industry under uncertainty. *European Journal of Operational Research*. 2016;252(3):801-814.
96. Ware NR, Singh SP, Banwet DK. Supplier selection problem: A state-of-the-art review. *Management Science Letters*. 2012;2(5):1465-1490.
97. Knowles A. *Chemistry and technology of agrochemical formulations*. Netherlands: Kluwer Academic Publishers. 1998.
98. Fung HK, Wibowo C, Ng KM, *Product-centered process synthesis and development: Detergents*, in *Chemical Product Design: Toward a Perspective through Case Studies*, K.M. Ng, R. Gani, and K. Dam-Johansen, Editors. 2007, Elsevier: Amsterdam. p. 239-274.
99. Baki G, Alexander KS. *Introduction to cosmetic formulation and technology*. New Jersey: John Wiley & Sons. 2015.

100. Showell M. *Handbook of Detergents, Part D: Formulation*. Vol. 128. Florida: Taylor & Francis. 2006.
101. Davis G, Dickey P, Duxbury D, Griffith B, Oakley B, Cornell K. *Household cleaners: Environmental evaluation and proposed standards for general purpose household cleaners*. Knoxville: Center for Clean Products and Clean Technologies, University of Tennessee. 1992.
102. Müller B, Poth U. *Coatings Formulation: An International Textbook*. 2 ed. Hannover: Vincentz Network GmbH & Co. KG. 2011.
103. Fishburn AG. *An Introduction to Pharmaceutical Formulation: The Commonwealth and International Library: Pharmacy and Pharmaceutical Chemistry*. London: Pergamon Press Ltd. 1965.
104. Petrie EM. *Handbook of adhesives and sealants*. New York: McGraw-Hill. 2000.
105. Magdassi S. *The chemistry of inkjet inks*. Singapore: World Scientific Publishing Co. Pte. Ltd. 2010.
106. Leach R, Pierce RJ, Hickman EP, Mackenzie MJ, Smith HG. *The printing ink manual*. 5 ed. Netherlands: Springer. 1993.
107. Mortier RM, Fox MF, Orszulik ST. *Chemistry and technology of lubricants*. 3 ed. Vol. 107115. Springer. 2010.
108. Maravelias CT, Sung C. Integration of production planning and scheduling: Overview, challenges and opportunities. *Computers & Chemical Engineering*. 2009;33(12):1919-1930.
109. Calfa BA, Grossmann IE. Optimal procurement contract selection with price optimization under uncertainty for process networks. *Computers & Chemical Engineering*. 2015;82:330-343.
110. Gambogi J, Arvanitidou ES, Lai K, *Light-duty liquid detergents*, in *Liquid detergents*, K.Y. Lai, Editor. 2006, Taylor & Francis: New Jersey. p. 171-238.
111. Chan KY, Kavanagh PE. The application of linear programming and regression analysis to light duty liquid detergent formulation. *Journal of the American Oil Chemists' Society*. 1988;65(12):1971-1976.
112. Uhrich KE, Cannizzaro SM, Langer RS, Shakesheff KM. Polymeric systems for controlled drug release. *Chemical Reviews*. 1999;99(11):3181-3198.
113. Fung KY, Ng KM, Nakajima S, Wibowo C. A systematic iterative procedure for determining granulator operating parameters. *AIChE Journal*. 2006;52(9):3189-3202.
114. Ennis BJ, Tardos G, Pfeffer R. A microlevel-based characterization of granulation phenomena. *Powder Technology*. 1991;65(1):257-272.
115. Cussler EL, Moggridge GD. *Chemical product design*. 2 ed. Cambridge, UK: Cambridge University Press. 2011.
116. Wei J. *Product engineering: molecular structure and properties*. New York: Oxford University Press. 2007.
117. Wesselingh JA, Kiil S, Vigild ME. *Design & development of biological, chemical, food and pharmaceutical products*. England: John Wiley & Sons, Ltd. 2007.
118. Ge S, Wang N, Fung KY, Wong KW, Chan CT, Ng KM. Product design: Nanoparticle-Loaded polyvinyl butyral interlayer for solar control. *AIChE Journal*. 2018;64(10):3614-3624.
119. Daoutidis P, Zachar M, Jogwar SS. Sustainability and process control: A survey and perspective. *Journal of Process Control*. 2016;44:184-206.

120. Azapagic A, Perdan S. Sustainable chemical engineering: Dealing with “wicked” sustainability problems. *AIChE Journal*. 2014;60(12):3998-4007.
121. Stouffer DB, Ng CA, Amaral LAN. Ecological engineering and sustainability: A new opportunity for chemical engineering. *AIChE Journal*. 2008;54(12):3040-3047.
122. Bakshi BR, Fiksel J. The quest for sustainability: Challenges for process systems engineering. *AIChE Journal*. 2003;49(6):1350-1358.
123. Jaafar I, Venkatachalam A, Joshi K, Ungureanu A, De Silva N, Dillon Jr O, Rouch K, Jawahir I. Product design for sustainability: a new assessment methodology and case studies. *Environmentally conscious mechanical design*. 2007;5:25-65.
124. Kloepffer W. Life cycle sustainability assessment of products. *The International Journal of Life Cycle Assessment*. 2008;13(2):89.
125. Ciroth A, Finkbeier M, Hildenbrand J, Klöpffer W, Mazijn B, Prakash S, Sonnemann G, Traverso M, Ugaya CML, Valdivia S, *Towards a live cycle sustainability assessment: making informed choices on products*. 2011, United Nations Environment Programma (UNEP).
126. Schöggl J-P, Baumgartner RJ, Hofer D. Improving sustainability performance in early phases of product design: A checklist for sustainable product development tested in the automotive industry. *Journal of Cleaner Production*. 2017;140:1602-1617.
127. Van Boeijen A, Daalhuizen J, Zijlstra J, van der Schoor R, *Part 2: Design method*, in *Delft design guide: Design strategies and methods*. 2014, BIS Publishers.
128. Charter M, Tischner U, *Sustainable product design*, in *Sustainable Solutions*. 2017, Routledge. p. 167-187.
129. Ramani K, Ramanujan D, Bernstein WZ, Zhao F, Sutherland J, Handwerker C, Choi J-K, Kim H, Thurston D. Integrated sustainable life cycle design: A review. *Journal of Mechanical Design*. 2010;132(9):091004.
130. Chiu M-C, Chu C-H. Review of sustainable product design from life cycle perspectives. *International Journal of Precision Engineering and Manufacturing*. 2012;13(7):1259-1272.
131. Go TF, Wahab DA, Hishamuddin H. Multiple generation life-cycles for product sustainability: the way forward. *Journal of Cleaner Production*. 2015;95:16-29.
132. Ahmad S, Wong KY, Tseng ML, Wong WP. Sustainable product design and development: A review of tools, applications and research prospects. *Resources, Conservation and Recycling*. 2018;132:49-61.
133. Heintz J, Belaud J-P, Pandya N, Teles Dos Santos M, Gerbaud V. Computer aided product design tool for sustainable product development. *Computers & Chemical Engineering*. 2014;71:362-376.
134. Badurdeen F, Aydin R, Brown A. A multiple lifecycle-based approach to sustainable product configuration design. *Journal of Cleaner Production*. 2018;200:756-769.
135. Ljungberg LY. Materials selection and design for development of sustainable products. *Materials & Design*. 2007;28(2):466-479.
136. Babi DK, Holtbruegge J, Lutze P, Gorak A, Woodley JM, Gani R. Sustainable process synthesis–intensification. *Computers & Chemical Engineering*. 2015;81:218-244.
137. Guillen-Cuevas K, Ortiz-Espinoza AP, Ozinan E, Jiménez-Gutiérrez A, Kazantzis NK, El-Halwagi MM. Incorporation of safety and sustainability in conceptual design via a return on investment metric. *ACS Sustainable Chemistry & Engineering*. 2018;6(1):1411-1416.
138. Hanes RJ, Bakshi BR. Sustainable process design by the process to planet framework. *AIChE Journal*. 2015;61(10):3320-3331.

139. Martínez-Guido SI, González-Campos JB, del Río RE, Ponce-Ortega JM, Nápoles-Rivera F, Serna-González M, El-Halwagi MM. A multiobjective optimization approach for the development of a sustainable supply chain of a new fixative in the perfume industry. *ACS Sustainable Chemistry & Engineering*. 2014;2(10):2380-2390.
140. Zore Ž, Čuček L, Kravanja Z. Syntheses of sustainable supply networks with a new composite criterion – Sustainability profit. *Computers & Chemical Engineering*. 2017;102:139-155.
141. Seay JR. Education for sustainability: Developing a taxonomy of the key principles for sustainable process and product design. *Computers & Chemical Engineering*. 2015;81:147-152.
142. Wang X, Guo M, Koppelaar RHEM, van Dam KH, Triantafyllidis CP, Shah N. A nexus approach for sustainable urban energy-water-waste systems planning and operation. *Environmental Science & Technology*. 2018;52(5):3257-3266.
143. Cui J, Forssberg E. Mechanical recycling of waste electric and electronic equipment: a review. *Journal of Hazardous Materials*. 2003;99(3):243-263.
144. Kaya M. Recovery of metals and nonmetals from electronic waste by physical and chemical recycling processes. *Waste Management*. 2016;57:64-90.
145. Schrijvers DL, Loubet P, Sonnemann G. Developing a systematic framework for consistent allocation in LCA. *The International Journal of Life Cycle Assessment*. 2016;21(7):976-993.
146. Organization IS. *ISO 14040: Environmental management-Life cycle assessment-Principles and framework*. 1997.
147. Andrews ES. *Guidelines for social life cycle assessment of products*. UNEP/Earthprint. 2010.
148. Huijbregts M, Steinmann Z, Elshout P, Stam G, Verones F, Vieira M, Hollander A, Zijp M, R vZ. ReCiPe 2016, a life cycle impact assessment method which comprises harmonised category indicators at the midpoint and the endpoint level-Report I: Characterization. 2016. https://www.rivm.nl/bibliotheek/rapporten/2016-0104.pdf (access in June 2019).
149. Zampori L, Saouter E, Schau E, Cristóbal Garcia J, Castellani V, Sala S, *Guide for interpreting life cycle assessment result*. 2016, EUR.
150. Fernandes PT, Canciglieri Júnior O, Sant'Anna ÂMO. Method for integrated product development oriented to sustainability. *Clean Technologies and Environmental Policy*. 2017;19(3):775-793.
151. Kalakul S, Zhang L, Fang Z, Choudhury HA, Intikhab S, Elbashir N, Eden MR, Gani R. Computer aided chemical product design – ProCAPD and tailor-made blended products. *Computers & Chemical Engineering*. 2018;116:37-55.
152. Bocken NMP, de Pauw I, Bakker C, van der Grinten B. Product design and business model strategies for a circular economy. *Journal of Industrial and Production Engineering*. 2016;33(5):308-320.
153. Halim I, Carvalho A, Srinivasan R, Matos HA, Gani R. A combined heuristic and indicator-based methodology for design of sustainable chemical process plants. *Computers & Chemical Engineering*. 2011;35(8):1343-1358.
154. Tula AK, Babi DK, Bottlaender J, Eden MR, Gani R. A computer-aided software-tool for sustainable process synthesis-intensification. *Computers & Chemical Engineering*. 2017;105:74-95.

155. Gopalakrishnan V, Bakshi BR. Ecosystems as unit operations for local techno-ecological synergy: Integrated process design with treatment wetlands. *AIChE Journal*. 2018;64(7):2390-2407.
156. Liu Z, Lu J, Zhu P. Lightweight design of automotive composite bumper system using modified particle swarm optimizer. *Composite Structures*. 2016;140:630-643.
157. Kim D-H, Kim H-G, Kim H-S. Design optimization and manufacture of hybrid glass/carbon fiber reinforced composite bumper beam for automobile vehicle. *Composite Structures*. 2015;131:742-752.
158. Pastore CM, Gowayed YA. A self-consistent fabric geometry model: modification and application of a fabric geometry model to predict the elastic properties of textile composites. *Journal of Composites, Technology and Research*. 1994;16(1):32-36.
159. Witik RA, Teuscher R, Michaud V, Ludwig C, Månson J-AE. Carbon fibre reinforced composite waste: An environmental assessment of recycling, energy recovery and landfilling. *Composites Part A: Applied Science and Manufacturing*. 2013;49(Supplement C):89-99.
160. Li X, Bai R, McKechnie J. Environmental and financial performance of mechanical recycling of carbon fibre reinforced polymers and comparison with conventional disposal routes. *Journal of Cleaner Production*. 2016;127:451-460.
161. Mallick PK. *Fiber-reinforced composites: materials, manufacturing, and design*. CRC press. 2007.
162. Laboratory AN, *BatPac Version 3.0*. 2015. http://www.cse.anl.gov/batpac/index.html (accessed in August 2018).
163. Nelson PA, gallagher KG, Bloom I, DW D. Modeling the performance and cost of lithium-ion batteries for electric-drive vehicles. 2011. http://www.cse.anl.gov/batpac/about.html (accessed May 2019).
164. Li Q, Fung KY, Xu L, Wibowo C, Ng KM. Process synthesis: Selective recovery of lithium from lithium-ion battery cathode materials. *Industrial & Engineering Chemistry Research*. 2019.
165. Cai G, Fung KY, Ng KM, Wibowo C. Process development for the recycle of spent lithium ion batteries by chemical precipitation. *Industrial & Engineering Chemistry Research*. 2014;53(47):18245-18259.
166. Chong J, Xun S, Zheng H, Song X, Liu G, Ridgway P, Wang JQ, Battaglia VS. A comparative study of polyacrylic acid and poly(vinylidene difluoride) binders for spherical natural graphite/LiFePO4 electrodes and cells. *Journal of Power Sources*. 2011;196(18):7707-7714.
167. Cai ZP, Liang Y, Li WS, Xing LD, Liao YH. Preparation and performances of LiFePO4 cathode in aqueous solvent with polyacrylic acid as a binder. *Journal of Power Sources*. 2009;189(1):547-551.
168. Chou S-L, Pan Y, Wang J-Z, Liu H-K, Dou S-X. Small things make a big difference: binder effects on the performance of Li and Na batteries. *Physical Chemistry Chemical Physics*. 2014;16(38):20347-20359.
169. Huijbregts MAJ. Application of uncertainty and variability in LCA. *The International Journal of Life Cycle Assessment*. 1998;3(5):273.
170. Ren J, Ren X, Dong L, Manzardo A, He C, Pan M. Multiactor multicriteria decision making for life cycle sustainability assessment under uncertainties. *AIChE Journal*. 2018;64(6):2103-2112.

171. Bakshi BR, Gutowski TG, Sekulic DP. Claiming sustainability: Requirements and challenges. *ACS Sustainable Chemistry & Engineering*. 2018;6(3):3632-3639.
172. Norton I, Fryer P, Moore S. Product/Process integration in food manufacture: Engineering sustained health. *AIChE Journal*. 2006;52(5):1632-1640.
173. Costa AIA, Jongen WMF. New insights into consumer-led food product development. *Trends in Food Science & Technology*. 2006;17(8):457-465.
174. Arrieta-Escobar JA, Bernardo FP, Orjuela A, Camargo M, Morel L. Incorporation of heuristic knowledge in the optimal design of formulated products: Application to a cosmetic emulsion. *Computers & Chemical Engineering*. 2018.
175. Meeuse FM, *Chapter 6 - Process Synthesis for structured food products*, in *Computer Aided Chemical Engineering*, K.M. Ng, R. Gani, and K. Dam-Johansen, Editors. 2007, Elsevier. p. 167-179.
176. Dubbelboer A, Janssen J, Krijgsman A, Zondervan E, Meuldijk J, *Integrated Product and Process Design for the Optimization of Mayonnaise Creaminess*, in *Computer Aided Chemical Engineering*, K.V. Gernaey, J.K. Huusom, and R. Gani, Editors. 2015, Elsevier. p. 1133-1138.
177. Zhang X, Zhang L, Fung KY, Ng KM. Product design: Incorporating make-or-buy analysis and supplier selection. *Chemical Engineering Science*. 2019;202:357-372.
178. Ng KM, Gani R. Chemical Product Design: Advances in and Proposed Directions for Research and Teaching. *Computers & Chemical Engineering*. 2019.
179. Carpenter RP, Lyon DH, Hasdell TA. *Guidelines for sensory analysis in food product development and quality control*. Springer Science & Business Media. 2012.
180. Lawless HT, Heymann H. *Sensory evaluation of food: principles and practices*. Springer Science & Business Media. 2010.
181. Hadiyanto, Asselman A, Straten Gv, Boom RM, Esveld DC, Boxtel AJBv. Quality prediction of bakery products in the initial phase of process design. *Innovative Food Science & Emerging Technologies*. 2007;8(2):285-298.
182. Costell E, Tárrega A, Bayarri S. Food Acceptance: The Role of Consumer Perception and Attitudes. *Chemosensory Perception*. 2010;3(1):42-50.
183. Hu R. *Food Product Design : A Computer-Aided Statistical Approach*. Lancaster, Pa: Routledge. 1999.
184. Bower JA. *Statistical methods for food science: introductory procedures for the food practitioner*. John Wiley & Sons. 2013.
185. Types of Food Ingredients. https://foodingredientfacts.org/facts-on-food-ingredients/type-of-ingredients/ *(access in May 2019)*.
186. Manley D. *Manley's technology of biscuits, crackers and cookies*. Elsevier. 2011.
187. Berk Z. *Food process engineering and technology*. Academic Press. 2018.
188. Müller AC, Guido S. *Introduction to machine learning with Python: a guide for data scientists*. " O'Reilly Media, Inc.". 2016.
189. Tijskens L, Hertog M, Nicolaï BM. *Food process modelling*. Vol. 59. Woodhead Publishing. 2001.
190. Bakalis S, Knoerzer K, Fryer PJ. *Modeling food processing operations*. Elsevier. 2015.
191. Datta AK. Status of Physics-Based Models in the Design of Food Products, Processes, and Equipment. *Comprehensive Reviews in Food Science and Food Safety*. 2008;7(1):121-129.
192. Trystram G. Modelling of food and food processes. *Journal of Food Engineering*. 2012;110(2):269-277.

193. Devahastin S, Niamnuy C. Invited review: Modelling quality changes of fruits and vegetables during drying: a review. *International Journal of Food Science & Technology*. 2010;45(9):1755-1767.
194. Sam Saguy I, Marabi A, Wallach R. New approach to model rehydration of dry food particulates utilizing principles of liquid transport in porous media. *Trends in Food Science & Technology*. 2005;16(11):495-506.
195. Eason JP, Biegler LT. Advanced trust region optimization strategies for glass box/black box models. *AIChE Journal*. 2018;64(11):3934-3943.
196. Boukouvala F, Floudas CA. ARGONAUT: AlgoRithms for Global Optimization of coNstrAined grey-box compUTational problems. *Optimization Letters*. 2017;11(5):895-913.
197. Zhou T, Zhou Y, Sundmacher K. A hybrid stochastic–deterministic optimization approach for integrated solvent and process design. *Chemical Engineering Science*. 2017;159:207-216.
198. Purlis E. Browning development in bakery products – A review. *Journal of Food Engineering*. 2010;99(3):239-249.
199. Hadiyanto, Esveld DC, Boom RM, van Straten G, van Boxtel AJB. Product quality driven design of bakery operations using dynamic optimization. *Journal of Food Engineering*. 2008;86(3):399-413.
200. Purlis E, Salvadori VO. Bread baking as a moving boundary problem. Part 2: Model validation and numerical simulation. *Journal of Food Engineering*. 2009;91(3):434-442.
201. Piazza L, Masi P. Development of Crispness in Cookies During Baking in an Industrial Oven. *Cereal Chemistry*. 1997;74(2):135-140.
202. Keller A, Vosshall LB. Olfactory perception of chemically diverse molecules. *BMC Neuroscience*. 2016;17(1):55.
203. Heaton J. *Introduction to neural networks with Java*. Heaton Research, Inc. 2008.