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**LIFE CYCLE BASED SUSTAINABILITY ASSESSMENT AND
DECISION MAKING FOR INDUSTRIAL SYSTEMS**

by

HAO SONG

DISSERTATION

Submitted to the Graduate School

of Wayne State University,

Detroit, Michigan

in partial fulfillment of the requirements

for the degree of

DOCTOR OF PHILOSOPHY

2017

MAJOR: CHEMICAL ENGINEERING

Approved By:

Advisor

Date

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DEDICATION

To my wife Zhe,
my son Brandon,
and my parents.

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I would like to thank my doctoral advisor, Dr. Yinlun Huang, for all he has taught me about process systems engineering and engineering sustainability, his steady guidance, and his encouragement to forge my own path. Without his support and invaluable didactic guidance, such a dissertation would not have been completed.

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CHAPTER 1 INTRODUCTION

The improvement of living condition, medical innovations and preventive care, in the last 50 years provides effective prevention of communal and contagious diseases, advance health treatments, increase life expectancy, and improve gender equality which inevitably result in the substantial growth of global human population (Livinggreen, 2013). According to U.S. Census Bureau (Census, 2016), total population in the world is more than 7.3 billion and increases at a very fast speed, 1 person every 15 seconds. In the meanwhile, human population growth and overconsumption have been causing many pressing environmental issues such as the species extinction crisis, resource depletion, environmental degradation and climate change.

Energy poverty is becoming a critical variable for economic, social, and global welfare due to the fact that most of energy is produced and consumed in unsustainable ways (Yüksel, 2008). More than 90% of global commercial energy production comes from the consumption of nonrenewable fossil fuels including petroleum oil, coal, and natural gas. According to the technical report from Organization of the Petroleum Exporting Countries (OPEC, 2016), the demand of fossil fuels will continuously soar in the following decades. Thus, the depletion of energy supply inevitably becomes one of the major issues in the development of human society.

Another major challenge that we have to address is associated with water which is one of the most important elements in human's lives. Although the freshwater resource in the whole world is only 3% of the total volume, the amount that is accessible for human consumption such as drinking, agriculture, and industrial manufacturing activities is only

one third of the total freshwater while the remaining is frozen in glaciers (Postel, 1997). In addition, the water resource that human beings have been using, freshwater, rather scarce, expensive, and unevenly distributed. As population growth continues to soar, the finite amount of fresh water continues to be extracted at a faster rate than the hydrologic cycle can recharge. Water usage has risen three times from 1950 to 2000 while the U.S. population nearly increases 100% at the same time period. At least 36 states encounter local, regional or statewide water shortages, even under non-drought conditions (EPA, 2013). Beside the water consumption by human beings' daily living, nearly all industrial manufacturing activities that produce metals, wood and paper products, chemicals, gasoline and oil use water during some production processes such as fabricating, processing, washing, diluting, cooling, or transporting a product; incorporating water into a product; or for sanitation needs within the manufacturing facility. Therefore, the expected economy growth and rising population will inevitably lead to the continuation of conflicts over this vital resource.

In addition to the shrinkage of scarce freshwater resource, water quality might be an even bigger issue. According to the report from United Nations Environment Programme (UNEP), intensifying degradation of water quality of surface waters is a critical issue in many parts of the world due to the economic development (UNEP, 2012). Water contamination typically results from the direct discharge of wastewater from industrial manufacturing sites without sufficient treatment, runoff from land including sediment, fertilizer and pesticides, and deposition from air pollution. Inadequate wastewater treatment facilities and poor government regulations lead to the contamination of potable water supplies by untreated sewage and industrial wastes. Water pollution could pose a great risk

to public health, food security, and livelihoods. Meanwhile, the climate change in the past several decades also significantly affects the water temperature which also poses great threat to environmental ecological system. As the global population is expected to double by 2050, it is urgent to take proper actions to prevent the exacerbation of water resource issues.

In the meanwhile, the industrial activities are always accompanied by emissions such as carbon dioxide, sulfur dioxide, nitrogen oxides, particulate matter and other chemicals which contribute to global warming and air pollution. Greenhouse gas (GHG) emission leads to the climate change which has tremendous environmental impact to global ecosystem. The gas phase chemicals released due to industrial activities also result in another serious problem, Ozone depletion. The main function of stratospheric ozone is to block incoming ultraviolet (UV) radiation which could lead to skin cancer. The thinning and disappearing protective ozone layer will certainly put the health of human beings in danger, increase in skin cancer, increase in the lethality of malaria and influenza, increase in the spread and/or severity of a number of diseases, and decrease in the effectiveness of immunization in humans.

The limited land resource is another big issue that people are facing. Although 30% of earth surface is land, the amount of land that is suitable for living and working is significantly limited largely due to the terrain and climate. The recent economic development in most of the countries especially in developing countries occupies more and more land source that should be used for agriculture and human living. All kinds of waste generated due to human activities also significantly affects the quantity of usable land.

The essential resources available for human development are diminishing and the natural generation of these key resources cannot keep up with world population growth. The fast growing pollution could inevitably intensify the challenge that we have been facing. Appropriate actions must be taken to handle these issues in order to pursue long-term present of human beings on earth. Improvement toward sustainable manner is the ultimate way. It is of great importance to tackle these issues to meet the development need of human beings globally in a sustainable manner (Demirbaş, 2001). Luckily, increasing concern with the environmental impact resulted from human activities has led to a rising interest in sustainable development that will not only meet the needs of current development but also protect the natural environment without compromising the needs of future generations (Carvalho *et al.*, 2008).

1.1 Definition of Sustainability

Sustainability science and associated studies has grown rapidly due to the increasing concern that the modern, interconnected global economy and rising population is moving far away from expectation and is pushing natural environment and ecosystem to their limits where they are not able to support the human prospect in the future. It is of great importance to know what sustainability is and how people can make everything to be sustainable.

The word “sustainability” means to “hold up” or “maintain”. The concept of sustainability emerged in the 1960s in response to concern about environmental degradation. As of today, there is no universal definition of sustainability although numerous attempts have been made to define sustainability and many of them are contrasting perspectives and views as to exactly what “sustainability” is. The Organization for Economic Cooperation

and Development (OECD) defines sustainability as “the efficiency with which ecological resources are used to meet human needs” (OECD, 1960) and represents it as a ratio of an output (the value of products and services produced by a firm, sector or economy as a whole) divided by the input (the sum of environmental pressures generated by the firm, the sector or the economy) (Kopnina and Shoreman-Ouimet, 2015). In the World Conservation Strategy, the International Union for the Conservation of Nature and Natural Resources (IUCN) interpreted the concept of sustainable development as a strategic approach to integrating conservation and development (IUCN, 1980). However, the most widely referred definition of sustainability is from the report of UN-sponsored World Commission on Environment and Development (WCED) (WCED 1987), *Our Common Future*. WCED defines sustainability as: “meets the needs of the present without compromising the ability of future generations to meet their own needs.” It consists of two parts: the concept of 'needs', in particular the essential needs of human development; and the idea of limitations imposed by the state of technology and social organization on the environment's ability to meet present and future needs. Figure 1.1 denotes the definition of sustainability from WCED. Gibson and Hassan interpreted WCED’s sustainability definition as: “Environment and development had to be addressed together because they are interdependent” (Gibson and Hassan, 2005). The development of human beings cannot be accompanied by the ecological decline and resource depletion. Thus, it is substantially important to allow people to sustain themselves while also sustaining the environment which is the foundation for human’s livelihoods through the development of proper conditions and capabilities.

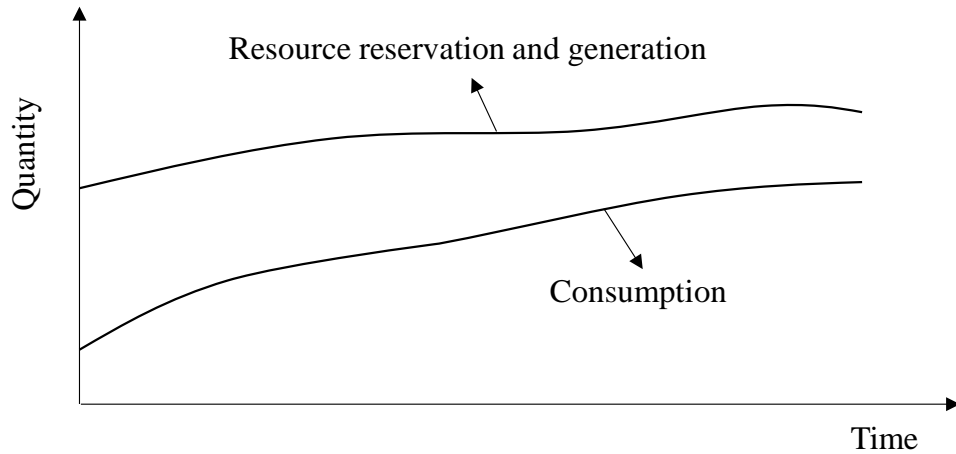


Figure 1.1. The definition of sustainability from WCED (Gibson and Hassan, 2005).

Although the WCED definition of sustainable development has been highly instrumental in developing a “global view” with respect to our planet’s future, this definition is still very vague and ambiguous. Most of existing studies on sustainability science and sustainable development agree that sustainability is widely considered a subjective concept. Soule and Terborgh noted that sustainability and sustainable development are seldom rigorously defined, and thus everyone could introduce the definition of these two terms (Soulé and Terborgh, 1999).

The goal of sustainability is to improve the quality of human life within the limitations of the natural resources and global ecology. It involves the development of human welfare without compromising the natural environment and the well-being of other people. The subjective concept “sustainability” involves complicated relationship among economic growth, ecological integrity, and justice around the world. This can be elaborated as: living within certain limits of the earth’s capacity to maintain life; understanding the interaction among economy, society, and environment; and maintaining a fair distribution

of resources and opportunity for this generation and the next. Thus, sustainability can be defined based on the view of “need” and “limitation” with the consideration of people, planet, and profit. For instance, from environmental expert’s point of view, sustainability is to preserve natural ecology while maintaining necessary economic improvement. From the perspective of business operation, sustainability can be interpreted as maximizing the economic performance with minimum environmental and social repercussion.

1.2 Sustainability Assessment

Assessment of sustainability rests on the understanding of the main contents within the framework of sustainability. The interpretation of sustainability bases on a number of interconnected pillars. The Brundtland Commission indicates a two-pillar sustainability which consists of environment and human development (WCED, 1987). Figure 1.2 depicts the structure of sustainability defined by WCED.

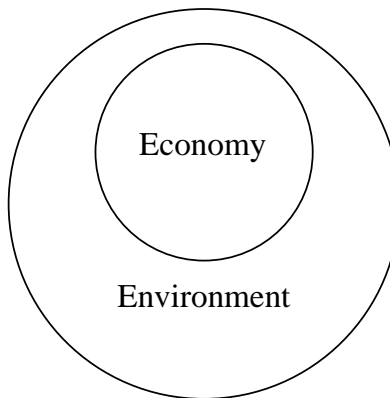


Figure 1.2. WCED sustainability circle (Gibson and Hassan, 2005).

People or society becomes the third important element of sustainability as the development of sustainability continues. Figure 1.3 denotes the relationship of the three

elements of sustainability. However, the most popular version is the sustainability with three distinct and interdependent elements (Pope *et al.*, 2004). Elkington established the sustainability framework of “Triple Bottom Line” (TBL) as people, planet, and profit which present the three pillars of sustainability, economy, environment, and society (Elkington, 1994). Figure 1.4 elaborates the equal importance and inherent interdependent nature of the three elements and the cross-section area demonstrates the concept of desired sustainability. This interpretation implies that investigation of sustainability must take into account of sustainability in three categories: economic sustainability, environmental sustainability, and social sustainability.

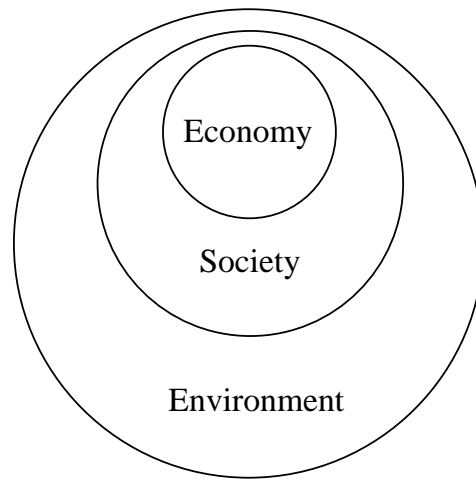


Figure 1.3. Circles of sustainability (Gibson and Hassan, 2005).

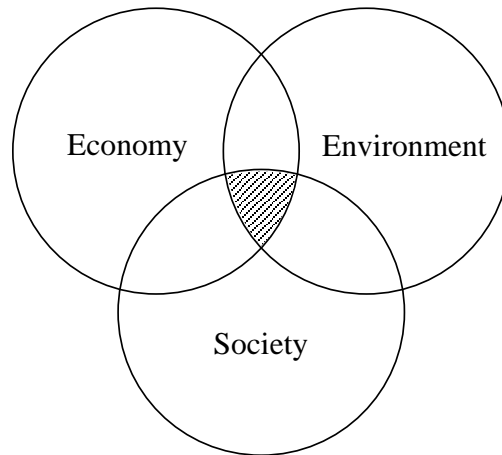


Figure 1.4. Modern structure of sustainability.

Given the well-established structure of sustainability, it is essential to create a set of criteria that could represent the core interests of economic, environmental, and social sustainability. Such a set of criteria is called sustainability metrics system which consists of three different groups of sustainability indicators. Due to the fact that sustainability is a complex and multifaceted goal, it is required that the metrics system should contain multiple indicators which can quantitatively analyze the state of system sustainability.

Increasing awareness of the importance of sustainability assessment stimulates the development of sustainability metrics systems which is regarded as the most significant progress in sustainability study. Interest has grown in creating sustainability metrics systems to evaluate sustainability over the past several decades. As of today, a number of sustainability metrics systems have already been created and used for performing sustainability assessment. For instance, the IChemE and AIChE sustainability metrics are widely adopted in the chemical and allied industries; each contains three sets of metrics for assessing economic, environmental, and social sustainability separately. The assessment

utilizes the system information provided by sustainability models or other means (e.g., direct and/or indirect measurements). Other metrics systems can be assembled on need basis. For instance, net profit analysis is frequently adopted for economic sustainability assessment (Möller and Schaltegger, 2005); for environmental sustainability, the EPA's WAR Algorithm is often preferred, which is based on potential environmental impact balance (Cardona *et al.*, 2004), measuring the potentials of chemicals about adverse effect on human health and the environment (e.g., aquatic eco-toxicology, global warming, etc.). Social sustainability is usually referred to the treatment of employees, suppliers, and customers, its impact on society at large, and industrial safety (Docherty *et al.*, 2008). Many other types of sustainability metrics are also available. The Dow Jones Sustainability Indices is for assessing corporate business sustainability, which creates global indexes tracking the financial performance of leading sustainability-driven companies. BASF has created and implemented eco-efficiency sustainability metrics which mainly focuses on economic and environmental performances (Saling *et al.*, 2002; Shonnard *et al.*, 2003). Sustainable manufacturing metrics, product sustainability index, sustainable water metrics, and business sustainability index are among the others.

In general, the selection of sustainability indicators has to follow these requirements:

(1) The selected indicators must be highly relevant to the defined analyzing target and reflect the interest of stakeholders, environment, and society. Sustainability assessment involves the evaluation from three different aspect, economy, environment, and society. The selected indicators are capable of providing a comprehensive analyzing result.

(2) Key aspects must be evaluated. Note that sustainability interest in different scenarios are generally not the same as each other, it is of great importance to concentrate the evaluation on critical issues rather than cover as much detail as possible.

(3) The selected indicators must be quantifiable based on data availability of analyzing target. Quantitative result can clearly demonstrate the sustainability status and the potential for improvement. Qualitative variables or linguistic variables involved in some indicators can be evaluated and transformed to quantitative result for further analysis.

Interpretation of sustainability related information is one key step of the sustainability assessment. Prior to the involvement of sustainability indicators, system based information are collected, managed, and integrated together. Sustainability assessment can then be conducted based on the selected sustainability indicators as well as the corresponding system knowledge. Figure 1.5 elaborates the interpretation process of system information during sustainability assessment.

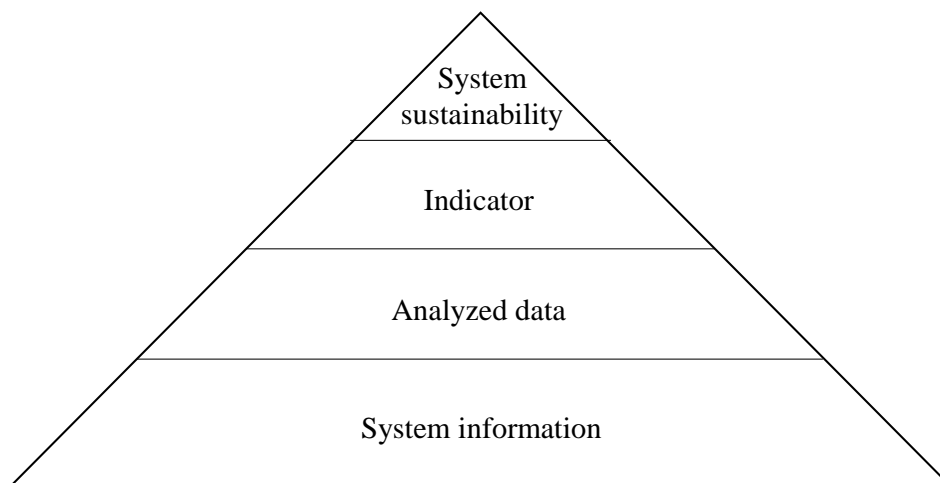


Figure 1.5. The process of sustainability assessment.

Note that at the different layers of a sustainability management hierarchy, the levels of details of needed information could be quite different (Mayer, 2008). For instance, at the process or plant level, specific indices need to be used; at the corporate level, more valuable information should be categorized in economic, environmental, and social sustainability; at the industrial regional level, possibly the overall sustainability data of each member is sufficient. The quality of the selected data must be validated in order to obtain reliable analyzing result of sustainability status.

Given that sustainability assessment covers a wide range of indicators which evaluate data from a variety of disciplines, it is of great importance to present the result of sustainability assessment in a clear and brief manner to facilitate the effort toward sustainable development. Therefore, construction of composite values of sustainability becomes the primary choice. Effective methodologies must be developed to characterize the information interpretation and integration process.

Recently, a sustainability-cube-based approach to show triple-bottom-line assessment is introduced which make much easier the comparison of different scenarios in each of three pillars or overall sustainability (Piluso and Huang, 2009). The sustainability cube can also be used to compare sustainability development paths involving different capital investments. Figure 1.6 shows an example of sustainability cube.

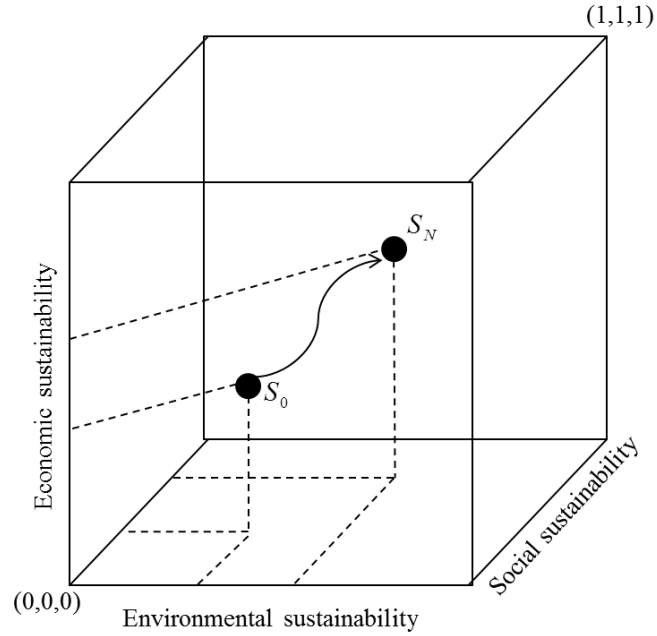


Figure 1.6. An example of sustainability assessment cube (Piluso and Huang, 2009).

The sustainability of an industrial process can be evaluated using a set of three-dimensional (3D) indicators that represent all three dimensions of sustainability: economic, environmental, and societal. For an industrial system named P, we assume that a set of sustainability metrics, namely set S , is selected by the decision maker. The set of metrics contains three subsets, each of which can have a number of specific indices:

$$S = \{E, V, L\} \quad (2.1)$$

where

$E = \{E_i \mid i = 1, 2, \dots, F\}$, the set of economic sustainability indices

$V = \{V_i \mid i = 1, 2, \dots, G\}$, the set of environmental sustainability indices

$L = \{L_i \mid i = 1, 2, \dots, H\}$, the set of social sustainability indices

Generally, most studies evaluate the sustainability indices by using normalized values in order to simplify the process. Therefore, it is required that in application, all the data be normalized first. By using selected sustainability indices, the status quo of the sustainability of system could be evaluated using available data collected from the system. The sustainability cube can effectively quantify the overall sustainability. By that approach, we can evaluate the overall sustainability (S) using the normalized, categorized sustainability.

In summary, computing aggregated values requires the following steps: (1) Evaluate the relationships among the categorized economic, environmental, and social sustainability and that among selected indicators in each group, i.e., economic group, environmental group, and social group; (2) normalize and weighting of the indicators; (3) test for robustness and sensitivity; and (4) compute composite values using weighted summation.

1.3 Navigating towards Sustainability

To address the growing environmental crisis and to reduce social inequalities in global development, adoption of sustainable development as a leading development model becomes the primary target of world political leadership (Kopnina and Shoreman-Ouimet, 2015). In the World Conservation Strategy (IUCN, 1980), the International Union for the Conservation of Nature and Natural Resources (IUCN) interpreted the concept of sustainable development as a strategic approach to integrating conservation and development. The strategy illustrates that sustainable development must take account of social and ecological factors, as well as economic ones; of the living and non-living resource base; and of the long term as well as the short term advantages and disadvantages of alternative actions.

Sustainable development is the route towards complete sustainability of all human activity (Figure 1.7).

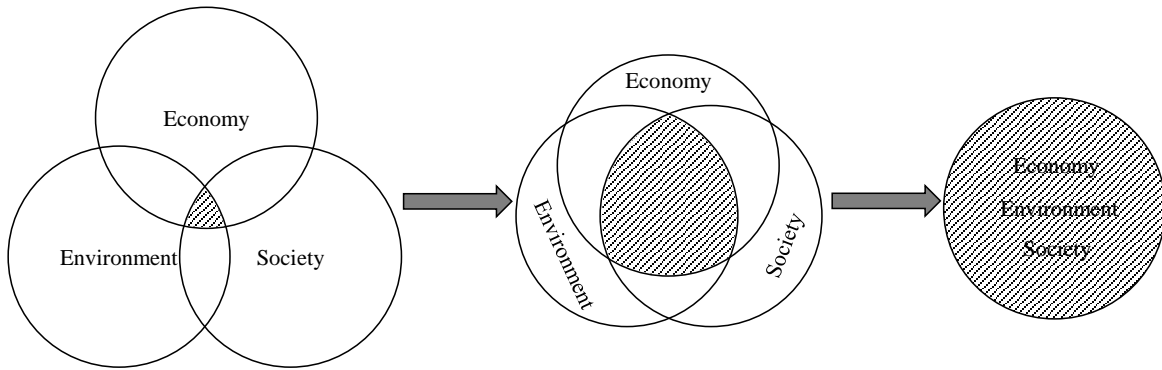


Figure 1.7. General scheme of sustainable development.

Industrial, social, and ecological systems are closely linked, and their time-variant correlations are extremely complicated and pose great challenges to sustainable development. Therefore, decision-making methods toward sustainable development should be systems based. It is necessary to gain deep understanding of the dynamic, adaptive behavior of complex systems, as steady-state sustainability models are too simplistic. It becomes clear that the quest for sustainability and sustainable development requires: (i) integrating economic, environmental and social factors simultaneously, (ii) constructive articulation of top-down approaches to development with bottom-up of grassroots initiatives, (iii) simultaneous consideration of local and global dimensions and of the way they interact, and (iv) broadening spatial and temporal horizons to accommodate the need for intra-generational as well as inter-generational equity. In dealing with these issues, systems approaches can offer a perspective more useful than other analytical approaches, because the systems view is a way of thinking in terms of connectedness, relationships, and context.

In 1992, EPA established the Design for the Environment (DfE) Program, targeting pollution prevention (P2) to meet stringent criteria for human and environmental health. That helped the industries tremendously in source (waste) reduction. As sustainable development (SD) becomes a goal of the human society, DfE has been naturally extended to Design for Sustainability (DfS), aiming at a simultaneous achievement of economic prosperity, environmental friendliness, and social responsibility (Sherwin, 2004; Crul and Diehl, 2010).

Today, sustainable design of products and processes is considered one of the most suitable areas for sustainability enhancement (Mendler and Odell, 2000; Szokolay, 2008). Such design activities are a typical multi-objective optimization task. Note that if the problem scope is large, then the optimization problem could be highly nonlinear with various types of constraints, making the solution search very difficult. A practical approach is to incorporate appropriate heuristics in problem formulation and/or solution search. It is also possible that the optimization problem is decomposed into a few tasks, and then localized optimizations are coordinated at the upper level using the large-scale system theory. An important note is that since DfS chiefly focuses on “static” design, the designed processes or products may be not or less sustainable in the (near) future. This should be an area of research in advancement of DfS, but again a difficulty is how to incorporate uncertainty into design models.

1.4 Main Challenges

The 21st century is a time of perpetual, environmental, technological and social change. To move beyond the rhetoric and to implement the concept of sustainability and

sustainable development, a number of challenges must be addressed despite existing effort on promoting sustainable development.

The first challenge is associated with the development of effective sustainability metrics systems. As sustainability is a complex and multidisciplinary topic, the core sustainability interests are not always the same as the analyzing target could be substantially distinct from each other. An effective sustainability metrics system should provide deep insights about the current sustainability performance of the targeting system. Therefore, it is vital to establish an appropriate sustainability metrics system that can address the stakeholder's economic interest, severe environmental concerns as well as social impact simultaneously. The development of objective and quantitative economic sustainability indicators requires the least effort. The derivation of environmental sustainability indicators also has less difficulty. Nevertheless, it is substantially challenging to acquire proper and effective social sustainability indicators due to intangible quality of life issues.

In addition to the necessity of appropriate sustainability metrics system, most of existing research may conduct results based on one or only a few stages of the manufacturing process without considering all the stages of a product's life (Onstad and Gould, 1998). Therefore, the results could be bias and sometimes not feasible for the whole life-cycle (Gourinchas and Parker, 2002). In the meanwhile, life cycle analysis (LCA) which has been widely adopted in a variety of industries does provide an effective approach to evaluate the environmental impact. The lack of life-cycle based economic and social sustainability assessment results in the difficult to conduct more comprehensive sustainability assessment. Life-cycle based sustainable decision-making approach has the advantage to study the

industrial system and could offer a more comprehensive view toward sustainable decision-making. It is of great importance to develop an effective framework that could guide the sustainability assessment and decision-making toward sustainable development from the life cycle perspective.

The third challenge is absence of a systematic methodology for long-term multistage sustainability development. Although current studies provide a variety of different methodologies to address sustainability assessment and decision-making (Busemeyer and Townsend, 1993; Hersh, 1999; NILSSON and Dalkmann, 2001; Antunes *et al.*, 2006), the increasing size and complexity of industrial systems results in the necessity to develop more comprehensive systems approaches to ensure the sustainable development over a long time period for industrial systems. This leads to the necessity of a systems approach to long-term multistage decision-making in which economic, environmental and social factors are integrated together to ensure the triple bottom lines of sustainability.

In addition, the sustainability assessment of industrial systems is always a very challenging task due to the existence of various types of uncertainties that are associated with the available data, assessable information, possessed knowledge, and problem understanding, etc. In addition to the data uncertainty, sustainability investigation also involves a variety of subjective judgement which can contribute to the uncertainty results. In sustainability study, data and information uncertainty arises from the complex nature of industrial systems (Dovers and Handmer, 1992; Howarth, 1995). For example, the multifaceted makeup of the inter-entity dynamics, dependencies, and relationships, the prospect of forthcoming environmental policies, and the interrelationship among the triple-

bottom-line aspects of sustainability are always uncertain. Moreover, the data about material or energy consumption, toxic/hazardous waste generation, and market fluctuation, etc., of an industrial system are often incomplete and imprecise. Uncertainties also appear in the activities for future planning, such as regulation changes, supply chain structures, etc.

According to Parry (Parry, 1996), the uncertainties can be classified into two types: aleatory and epistemic. The aleatory uncertainty refers to the inherent variations associated with physical systems and the environment; it is objective and irreversible. By contrast, the epistemic uncertainty is carried by the lack of knowledge and/or information; it is subjective and reducible. Piluso *et al* (2010) illustrates that both the aleatory and epistemic uncertainties appear in industrial sustainability problems. Four different approaches suitable for investigating uncertainty within the scope of sustainability and sustainable development are: (i) Probability Bounds Analysis (PBA); (ii) Information Gap Theory (IGT); (iii) Interval Parameter (IP) based approaches; and (iv) Fuzzy Arithmetic (FA). Therefore, it is crucial to explore different methodologies to handle the complex uncertainty issues due to the vastly different investigating scenarios.

1.5 Objectives and Significance

Great attention on sustainable development must be paid in order to achieve the harmonious interaction among the economic, environmental and societal aspects of the systems of interest. In order to achieve a sustainable development which is a multi-objective and interdisciplinary task, effort is needed for the identification, design and implementation of appropriate products, processes, supply chains, planning strategies and even policies under various types of uncertainty. Thus, it is necessary to develop systems methods and

tools, which enable the generation of sustainable design and decisions to adapt to the short-to long-term needs into the future (Carvalho *et al.*, 2008).

The main interests of this research are to propose a series of methodologies to investigate the sustainability problems and optimize the systems approach toward sustainable development. By taking into account of the main challenges mentioned earlier, attention will be focused on: (i) the development of life cycle based sustainability assessment approach; (ii) the development of life cycle based decision-making framework toward sustainability assessment at life cycle level; (iii) the generation of multistage decision-making methodology for long-term sustainable development with uncertainty.

In this dissertation, three fundamental frameworks are to be developed, that is life cycle based sustainability assessment (LCBSA), life cycle based decision-making (LCBDM) and fuzzy dynamic programming (FDP) based multistage decision-making methodology. LCBSA can offer a profound insight of status quo of the sustainability performance over the whole life cycle. LCBSA is then applied to assess the industrial system of automotive coating manufacturing process from raw material extraction, material manufacturing, product manufacturing to the recycle and disposal stage. Consequently, LCBDM could render a comprehensive decision-making strategy that combines the evaluation of sustainability status with life cycle perspective, the analysis of development priorities, and allocation of the effort for sustainable development together. FDP based multistage decision-making methodology offers an effective way to ascertain the achievement of long time sustainable development goal of complex and dynamic industrial systems by combining

decision-making and sustainability assessment of complex industrial systems with uncertainty issue involved together.

1.6 Organization of Dissertation

The dissertation body mainly consists of five key chapters. The first section, Chapter 2 and 3, describes the development of life cycle based sustainability assessment framework and life cycle based decision-making framework. Chapter 4 is a supportive chapter for Chapter 2 and 3. The second section, Chapter 5 and 6, focuses on the design of practical sustainability metrics system and the development of FDP based multistage sustainable development methodology.

In Chapter 2, the life cycle based sustainability assessment (LCBSA) framework is developed. A general hierarchical LCBSA framework includes four consecutive steps which contribute to the achievement of sustainability assessment at life cycle level. Parameter identification, selection of sustainability indicators, stage-based sustainability assessment and final information integration are involved in the methodology. The applicability of the methodology is demonstrated with a case study on the life cycle of a new automotive nanocoating material.

In Chapter 3, the efforts made towards the life cycle based decision-making (LCBDM) framework are described. Based on the preceding framework of LCBSA, LCBDM involves the two-phase prioritization of sustainability development and resource allocation. The first phase concentrates on the urgent improvement of stage-based “must-be” system variables and the second one prioritizes the sustainability development needs from the life cycle point of view. Priority order can then be used to guide the resource

allocation for sustainability enhancement to achieve life cycle based sustainability improvement. A case study which follows the investigation in Chapter 2 is applied to elaborate the methodology.

Chapter 4 provides the details of the multiscale modeling and simulation of paint application process (automotive paint curing process). The modeling of paint curing oven is performed in order to study the effects of nanoparticles addition into coating matrix on the process dynamics, energy consumption and coating film quality. The energy transfer process, solvent removal process, and polymer network formation process are investigated. An energy efficient operational setting is obtained based on with the consideration of coating quality requirement. The data obtained in these chapters could be used for the quantification of some of the sustainability indicators described in Chapter 2 and 3.

Chapter 5 describes a practical sustainability assessment and performance improvement for electroplating processes in which a systematic method for designing sustainability metrics system from the supply chain perspective is involved. With the selected sustainability metrics system, the sustainability status and possible improvement technology candidates are evaluated accordingly. An effective methodology for identifying optimal decisions for sustainability improvement is also introduced in this work. An electroplating process case study is employed to outline the proposed evaluation method, which prioritizes improvement measures to guide advances toward sustainability.

Chapter 6 presents a FDP based multistage decision-making framework designed for long-term development of industrial sustainability. By this methodology, data uncertainty, qualitative sustainability indicators, and subjective judgement are addressed with fuzzy set

theory. Decision constraints including budget, time, and improvement achievement are evaluated based on fuzzy set theory as well. A comprehensive fuzzy dynamic programming approach is applied to identify the optimal route to achieve preset long-term sustainability goal.

Finally, the concluding remarks and possible directions to extend this work in the future are outlined in Chapter 7.

CHAPTER 2 LIFE CYCLE BASED SUSTAINABILITY ASSESSMENT OF NANOCOMPOSITE COATING MATERIALS

Since World Commission on Environment and Development (WCED) defined the terms “sustainability” and “sustainable development” in the book, *Our Common Future*, sustainability is nowadays accepted by all stakeholders as a guiding principle (Mebratu, 1998; Sikdar, 2003; Bansal, 2005). Typical sustainability assessment is to evaluate impacts in three dimensions - economic, environmental, and social aspects with respect to closely associated products, processes, and systems (Sikdar, 2003). Comparing to the traditional economy or environment driven enhancement, integration of the analyzing result can then provide a comprehensive view of the studied system which can be used to systematically improve the sustainability status (Morrison-Saunders and Therivel, 2006). Great effort related to sustainability and sustainable development has been made in a variety of fields including academia, industry, government, and other organizations (Mehta, 2002; Kemp *et al.*, 2005; Lafferty, 2006). In return, sustainability guided improvement is becoming the mainstream of the development of human being on economy, environment, and society.

There are still a number of challenges to be addressed. Firstly, the challenge to unambiguously determine and measure sustainability performance does remain, especially for products and processes. The maturity of methods and tools is different for the three sustainability dimensions. While the economic and environmental dimension can be covered quite well today, the social indicators and evaluation methods still need fundamental scientific progress (Diener and Suh, 1997; Veenhoven, 2002). Economic sustainability concentrates on the aspect that is highly associated with the economic interest of stakeholders. Many financial tools together with scientific analysis can well characterize

the economic sustainability. Investigation of environmental sustainability is also a relatively easy task as numerous studies have been conducted for that purpose. However, social sustainability involves a highly subjective evaluation. There has been some attempt to study the social sustainability. A series of industry-specific sustainability assessment tools is offering some support. The effort on studying social sustainability in many well-known sustainability evaluation tools including AIChE sustainability metrics system, IChemE sustainability metrics system and BASF's eco-efficiency metrics system are still not sufficient (Saling *et al.*, 2002; Schwarz *et al.*, 2002; Labuschagne *et al.*, 2005).

Another major challenge is the restricted scope of sustainability assessment. Most current studies only focus on a specific stage of product life cycle. The results cannot provide a holistic view of product sustainability performance over its life cycle. Although lots of attention has been paid to the analysis of the product sustainability for a while, it is agreeable that sustainability assessment of product should integrate the analysis throughout the life cycle (Anastas and Warner, 1998; Finkbeiner *et al.*, 2010; Guinee *et al.*, 2010). When developing a new product, engineers who should have the complete product life cycle in mind must have a decisive impact on all phases of the product life cycle-from the extraction of raw materials through the material and energy generation to assembly, and product use to its end-of-life phase when developing a product. In order to avoid problem shifting in the product system, it is of great importance to extend the study to whole life span and investigate the product sustainability from a life cycle perspective.

With the increasing awareness of “sustainability” and “sustainable development”, it is required that modern sustainability assessment can provide deep insight upon not only the

current status of sustainability related fields but also the preceding and succeeding life cycle stages with a life cycle thinking (LCT). As a qualitative concept, LCT represents the fundamental concept of involving the product life cycle from cradle to grave (Kloepffer, 2008; Finkbeiner *et al.*, 2010). Rather than concentrating on the traditional production processes and manufacturing systems, the main goal of LCT is to mitigate the environmental impact by reducing the emission of waste and consumption of raw materials and energy while improving its socio-economic performance through the life cycle. LCT is expected to strengthen the interaction among economy, environment, and society within an organization and the lifespan.

There are a number of obvious advantages for pursuing sustainability with life cycle perspective (Finkbeiner *et al.*, 2010). It could provide guidance for practitioners to manage complex sustainability related information and data in a structured form. A more comprehensive structure of the positive and negative impacts along the product life cycle can help decision makers to address the trade-offs among the three sustainability pillars, life cycle stages and products (Badurdeen *et al.*, 2009). The result of sustainability assessment from the life cycle perspective could clearly elaborate the involvement and interaction of the sustainability status of life cycle stages. Stakeholders or decision makers are also benefited from the assessment as it could provide holistic analysis of the implications of a product's life cycle for the environment and the society. The evaluation result could help decision makers in prioritizing resources and capital investment and selecting sustainable technologies and products to achieve sustainable development with a big picture. It could also encourage enterprises to become more responsible and proactive for their business by

considering the full spectrum of impacts associated with the product life cycle. It will offer guidance to reduce the use of natural resources and waste emission in their production practices and increase the environmental, economic and social benefits for society and local communities.

In general, it is very challenging to perform complete sustainability assessment of emerging or developing products (e.g. nanocomposite coatings) due to insufficient data availability for inputs and outputs of the system at each stage of life cycle. However, if succeeded, it can provide significant amount of supplementary information to support decisions related to the future development (Finkbeiner *et al.*, 2010). The development of a comprehensive life-cycle based sustainability assessment methodology can significantly assist in directing the research and sustainable development of products.

The life cycle perspective is inevitable for all sustainability dimensions in order to achieve reliable and robust results. The inherent complexity of an approach that is supposed to allow a valid measurement of the sustainability performance is a challenge for decision-makers. Therefore, effective and efficient ways to present sustainability assessment from life cycle point of view are needed. This is a prerequisite for the communication of analyzing results to the non-expert audience of real world decision-makers in public and private organizations. This holistic approach should respect the product life cycle and should be in the position to cover potential trade-offs and synergies between the three dimensions of sustainability. The desired approach must take into account the principles of comprehensiveness and life cycle perspectives in order to achieve reliable and robust sustainability assessment results. The life cycle perspective considers all life cycle stages

for products, and for organizations the complete supply or value chains, from raw material extraction and acquisition, through energy and material production and manufacturing, to use and end-of-life treatment and final disposal. Apart from challenges with regard to indicators and weighting issues, LCSA has to deal with the trade-off between validity and applicability. Through such a systematic overview and perspective, the performance of economic, environmental, and social sustainability among all of the life cycle stages can be identified. Another important principle is comprehensiveness, because it considers all attributes or aspects of environmental, economic and social performance and interventions. By considering all attributes and aspects within one assessment in a cross-media and multi-dimensional perspective, potential trade-offs can be identified and assessed.

In this study, we first review the development of life cycle based studies toward sustainable development. After the evaluation of pros and cons of current methods, this work introduces a novel and practical framework, life cycle based sustainability assessment (LCBSA), to evaluate the sustainability performance for sustainable development of product throughout its life cycle by incorporating life cycle into general sustainability assessment. A case study focusing the automotive nanocoating materials will be used to illustrate the efficacy of LCBSA techniques.

2.1 Review of Existing Sustainability Concepts with Life Cycle Perspective

The need to provide a methodological framework for LCSAs and the urgency of addressing increasingly complex systems are acknowledged globally. According to Finkbeiner (Finkbeiner *et al.*, 2010), “Product Line Analysis” proposed by the German Oeko-Institute is the first attempt to contribute to the conceptual idea of life cycle

sustainability assessment (LCSA) (Oeke-Institut). According to UNEP's "Toward Life Cycle Sustainability Assessment" (UNEP, 2012), LCSA can be defined as "the evaluation of all environmental, social and economic negative impacts and benefits in decision-making processes towards more sustainable products throughout their life cycle."

Recently, a framework for LCSA was suggested linking life cycle sustainability questions to knowledge needed for addressing them, identifying available knowledge and related models, knowledge gaps, and defining research programs to fill these gaps. Kloepffer (2008) proposed life cycle sustainability assessment of products based on the extension of the LCA concept. Life cycle costing (LCC) and social life cycle assessment (SLCA) are studied similar to LCA. The foundation of this LCSA approach is based on one of the widely used life cycle tool, life cycle assessment (LCA). The framework of LCSA can consist of three different and independent life cycle approaches which are correlated to the triple bottom line of sustainability, that is, economic, environmental and social sustainability. Kloepffer stated that the technique of LCSA contributed to an assessment of product, providing more relevant results in the context of sustainability if combining LCA, LCC and SLCA together. The conceptual formula of LCSA framework can be expressed as:

$$\text{LCSA} = \text{LCC} + \text{LCA} + \text{SLCA} \quad (2.1)$$

where LCC, LCA, and SLCA denote Life Cycle Costing, Life Cycle Assessment, and Social Life Cycle Assessment, respectively.

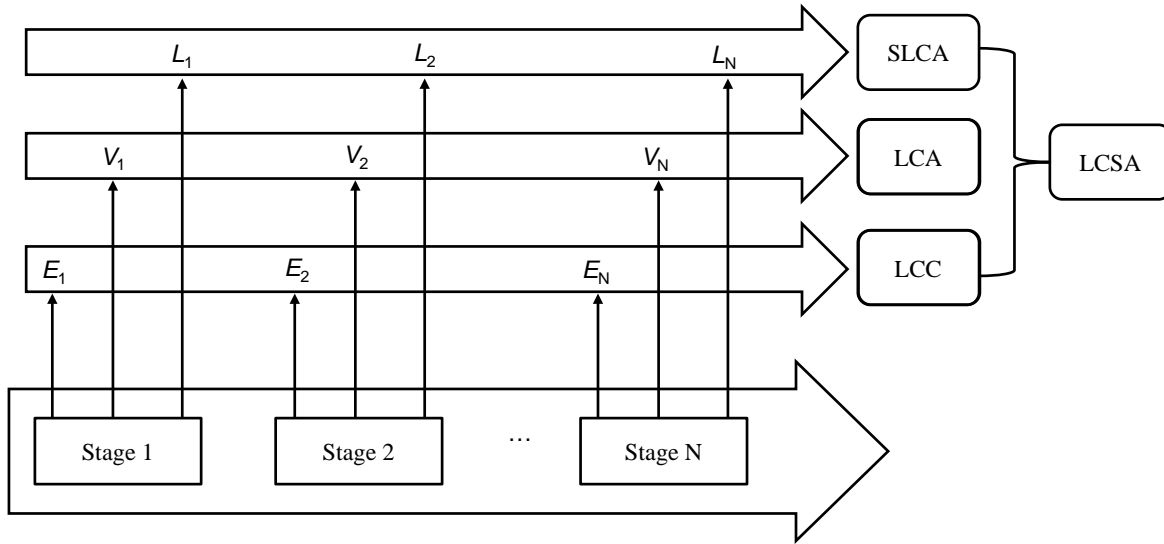


Figure 2.1. General framework of LCSA.

Kloepffer's LCSA framework relies on three fundamental life cycle techniques depicted in Figure 2.1. As the first and oldest of the three life cycle techniques, LCC is an aggregation of all cost and benefits for all internal and external systems that are directly related to a product over its entire life cycle developed to address a strict financial cost accounting situation (Asiedu and Gu, 1998).

Although there has been many attempt to study the product from a life cycle perspective, LCA or environmental life cycle assessment (LCA) which has developed fast over the last three decades is the dominant approach. LCA is an emerging powerful tool to assess the potential environmental impacts and resources used in manufacturing processes throughout a product's life cycle, i.e., from raw material acquisition, via material and product manufacturing, use and maintenance phase, to waste management. Many of the more recent developments were initiated to broaden traditional environmental LCA to a more

comprehensive Life Cycle Sustainability Analysis (LCSA) (White and Shapiro, 1993; Curran, 2008).

The final element of LCSA, SLCA, was developed by extending the fundamental concept of LCA into social field due to the increasing need for the integration of social criteria into LCA (Benoît *et al.*, 2010; Jørgensen *et al.*, 2010; Muthu, 2015). SLCA technique is expected provide important information for managing ‘social responsibility’ of an organization and its value chain – from the ‘cradle to the grave’ – taking into account all social sustainability related system variables at every life cycle stage.

LCSA integrates different life cycle assessment techniques to allow individuals and enterprises to assess the impact of their purchasing decisions and production methods along different aspects of this value chain. An environmental life cycle assessment (LCA) looks at potential impacts to the environment as a result of the extraction of resources, transportation, production, use, recycling and discarding of products; life cycle costing (LCC) is used to assess the cost implications of this life cycle; and social life cycle assessment (S-LCA) examines the social consequences.

Despite that LCSA framework developed by Kloepffer aims at providing the desired results of sustainability assessment with life cycle thinking, there are a number of drawbacks associated with this framework. Although LCA has been proven to be an effective approach and applied to many studies, the weakness of LCA is apparent. LCA focuses on the classification of environmental impact and integration of available information based on that. Decision-making has been a major challenge with such analyzing result. In addition, while using (environmental) LCA to measure the environmental dimension of sustainability is

widespread, similar approaches for the economic (LCC) and the social (S-LCA) dimensions of sustainability have still limited application worldwide.

Another concern associated with LCSA is that there is so far no international standard for measuring the sustainability of a product. Effective methodology to apply this LCSA approach has not been developed yet. In addition, it investigates LCSA based on three one-dimension studies which highly rely on the integrated information. However, product life cycle has a series of stages which can be distinct spatially and temporally. The interests of stakeholders, government, manufacturing companies, and local communities are also very distinct. This poses a great challenge on information integration at each dimension. Economic aspects can be evaluated together as revenue and cost. Environmental aspects can only be added together by focusing on the major impact categories. However, some issues which may be omitted overall actually play a major role in a specific life cycle stage. Social life cycle assessment aims to evaluate the social impact throughout life cycle together use a single number. The interest of social aspect in each life cycle stage is distinct from that in other life cycle stages. The methodology to address such a challenge has yet to be explored.

The analyzing result of this LCSA approach also increases the complexity of decision-making. It is a common understanding that decisions taken during each individual phase of product life cycle have an important impact on the life cycle costs as well as the environmental and social aspects. Due to the fact that the economic, environmental, and social interests in different life cycle stages are merged separately, the decision making process will be challenging as it could not elaborate the correlation among the three sustainability aspect in each individual stages.

2.2 Goal and Scope of the Study

In this study, we introduced a novel framework, life cycle based sustainability assessment (LCBSA), to evaluate the sustainability performance for sustainable development of product throughout its life cycle by incorporating life cycle into general sustainability assessment. Comparing to LCSA framework, LCBSA is more practical and easy to use for experts and non-experts. LCBSA could lead to a much more composite result with less effort in data gathering and information integration. The final result can reveal the sustainability status much more clearly. To achieve LCBSA, a heuristic rule to divide product life cycle into a series of proper stages is firstly presented to promote the analysis. The approach to obtain LCBSA is evaluation of the stage-based sustainability followed by integration of stage-based sustainability performance to life cycle level. The following section elaborates the detailed methodology for LCSA. The methodology, life cycle based decision-making to enhance sustainability performance, is then introduced to optimize the sustainability performance of product in its whole life cycle to obtain an optimal status. The proposed methodology is then applied to the analysis of automotive nanocoating materials. The case study is used to demonstrate the efficacy of this methodology on product.

2.3 Framework of Life Cycle Based Sustainability Assessment

A general framework of LCBSA which consists of four steps is presented Figure 2.2. The first step is to effectively divide the product life cycle into multiple stages for detail analysis. A closer examination of stage-based system evaluation can then be achieved after the first step. The third step is to assess stage-based sustainability performance of the involved systems based on the proper sustainability metrics system for each life cycle stage.

Finally, LCBSA can be achieved based on the characterization of stage-based sustainability status.

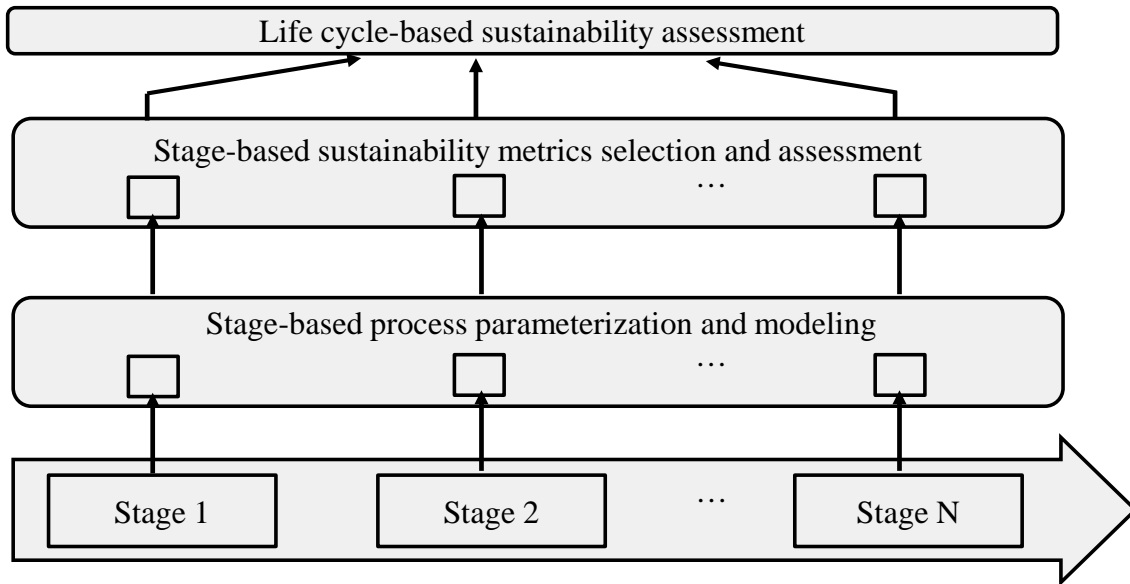


Figure 2.2. General framework of LCBSA.

2.4 Categorization of Product Life Cycle

The product life cycle which covers the span from cradle to grave, typically crosses a long lifespan at temporal level and exists at various spatial level. The flow of material, energy, and money are involved in the life cycle of a product. Nonetheless, the analysis of product is not complete unless all factors along the 'life cycle chain' are evaluated with a holistic view of sustainability. To achieve this goal, it is essential to divide the whole lifespan of product into a number of different life cycle stages to promote the study. Existing studies categorize product life cycle purely based on the researchers' interest. There is yet a lack of

general rule to guide the process. In this study, we propose a general heuristic rule to determine the proper separation of product life cycle.

The first and foremost task is to define the concept “product”. Product life cycle (PLC) is the cycle through which every product goes through from introduction to withdrawal or eventual demise. Materials are transformed from the original form to a series of other appearances within the life cycle. The product of the preceding life cycle stage can be considered the input material of current life cycle. Although there are many different forms of products in the life cycle, the name of “product” should be defined by the product appeared in the stage of use and maintenance.

A specific life cycle stage consists of a number of different and consecutive processes which can be systematically investigated together. Such processes should contribute same interest either at temporal or spatial level. With the defined concept “product life cycle”, the categorization of product life cycle can be accomplished based on the change of product, that is, transformation process from the spatial and temporal perspective. In this chapter, the change of product includes:

1. The presenting form of product is substantially distinct from the input materials. For instance, a number of different raw material input are integrated together to form a new form of product which has different physical and chemical properties.

2. The geographic location of the product has a major change. For example, the product is transported from one plant to another plant at different regions. Therefore, the entire life cycle of product is divided into a number of different stages based on existing regions.

The stage of product life cycle can then be established based on the two different changes of product with the special interest from investigator. In general, the number of product life cycle stage ranges between 3 and 8.

2.5 System Parameter Analysis

Given that the life cycle of product is divided into N different stages. The whole life cycle involves a number of input parameters (X) which can be divided into two distinct categories, process-based parameter (X^C) and product-based parameter (X^D).

$$X = \{X^C, X^D\} \quad (2.2)$$

Product-based parameter represents the inherent quantifiable properties such as the size and composition of a specific content.

$$X^D = \{X_1^D, X_2^D, \dots\} \quad (2.3)$$

These parameters are determined at the early stage of product life cycle and keep constant in the following stages. Process-based parameter mainly includes the ones that exist during the production and use of product in its lifespan. Typically, each life cycle has its own process-based parameters which may or may not occur in the rest stages. Therefore, it is essential to differentiate these parameters:

$$X^C = \{X^C(s_1), X^C(s_2), \dots, X^C(s_N)\} \quad (2.4)$$

For i -th stage (s_i) in the life cycle, the quantifiable parameters can be expressed as:

$$X^C(s_i) = \{x_{i,j} \mid j = 1, 2, \dots, n_i\} \quad (2.5)$$

2.6 Stage-Based Sustainability Assessment

In this chapter, the life cycle based sustainability can be evaluated through two consecutive steps: (i) stage-based sustainability evaluation; (ii) life cycle based integration of stage-based sustainability performance. In this section, a stage-based sustainability assessment method is presented.

2.6.1 Selection of Stage-based Sustainability Metrics System

Product life cycle consists of a number of consecutive stages of which sustainability interests might be distinct from each other. It is impossible to apply one universal sustainability metrics system to assess the sustainability related system performance. Therefore, stage-based sustainability evaluation indicators must be selected individually at the first place.

In general, the selection of sustainability indicators has to follow these requirements: (1) the selected indicators must be highly relevant to the defined analyzing target; (2) key aspects must be evaluated; (3) indicators must be quantifiable; and (4) duplication and needless complexity should be avoided.

For i -th stage (s_i), it is assumed that a set of sustainability metrics is selected by stage-based decision makers, which contains three subsets, each of which can have a number of specific indicators:

$$S_i = \{E(s_i), V(s_i), L(s_i)\}, \quad (2.6)$$

where

$$E(s_i) = \{E_j(s_i) \mid j = 1, 2, \dots, N_A\}, \text{ the set of economic sustainability indicators,}$$

$V(s_i) = \{V_j(s_i) \mid j = 1, 2, \dots, N_B\}$, the set of environmental sustainability indicators,

$L(s_i) = \{L_j(s_i) \mid j = 1, 2, \dots, N_C\}$, the set of social sustainability indicators.

where N_A , N_B , and N_C are the number of identified sustainability indicators for evaluating economic, environmental, and social aspects.

2.6.2 Stage-based Sustainability Evaluation

Analysis of the selected indicators are not only based on the parameters involved in current stages but also the parameters in other stages. The calculation of each indicator can be expressed as:

$$E_j(s_i) = f_E(X^C(s_i), X^D) \quad (2.7)$$

$$V_j(s_i) = f_V(X^C(s_i), X^D) \quad (2.8)$$

$$L_j(s_i) = f_L(X^C(s_i), X^D) \quad (2.9)$$

where X^D denotes the associated product-based parameters.

Estimation of categorized sustainability for the system, i.e., $E(s_i)$, $V(s_i)$, and $L(s_i)$, which are called the composite sustainability indices and can be evaluated using the following formulas:

$$E(s_i) = \frac{\sum_{j=1}^{N_A} a_j(s_i) E_j(s_i)}{\sum_{j=1}^{N_A} a_j(s_i)}, \quad (2.10)$$

$$V(s_i) = \frac{\sum_{j=1}^{N_B} b_j(s_i) V_j(s_i)}{\sum_{j=1}^{N_B} b_j(s_i)}, \quad (2.11)$$

$$L(s_i) = \frac{\sum_{j=1}^{N_C} c_j(s_i) L_j(s_i)}{\sum_{j=1}^{N_C} c_j(s_i)}, \quad (2.12)$$

where $a_j(s_i)$, $b_j(s_i)$, and $c_j(s_i) \in [1, 10]$ are the weighting factors associated with indices, reflecting the relative importance of an individual index against others in overall assessment.

Therefore, the stage-based sustainability can be expressed as:

$$S_i = \frac{\|(\alpha(s_i) E(s_i), \beta(s_i) V(s_i), \gamma(s_i) L_i(s_i))\|}{\|(\alpha(s_i), \beta(s_i), \gamma(s_i))\|} \quad (2.13)$$

where $\alpha(s_i)$, $\beta(s_i)$, and $\gamma(s_i)$ each has a value of 1 (default) to 10. All of the weight factors in this work follow the same rule.

2.7 Assessment of Life Cycle-based Sustainability Performance

Life cycle based sustainability performance can be obtained by integrating the sustainability performance of all life cycle stages. A number of approaches are proposed.

2.7.1 Arithmetic Calculation

Overall sustainability performance can be directly calculated based on stage-based sustainability evaluation result:

$$S_i = F \{S_1, S_2 \cdots S_N\} \quad (2.14)$$

There are two different means to address this integration. One is to obtain the final value by using a set of weighting factors $M = \{m_i | i = 1, 2 \cdots N\}$. This approach might be suitable to

the life cycle that the results of stage-based sustainability assessment are deterministic with little uncertainty and subjective. Thus Eq. (2.14) can be interpreted as

$$S_t = \frac{\|(m_1 S_1, m_2 S_2, \dots, m_N S_N)\|}{\|(m_1, m_2, \dots, m_N)\|} \quad (2.15)$$

Overall LC based sustainability status can also be represented by the sustainability performance of a specific stage. Thus Eq. (2.14) can be interpreted as

$$S_t = \min(S_1, S_2, \dots, S_N) \quad (2.16)$$

$$S_t = \max(S_1, S_2, \dots, S_N) \quad (2.17)$$

Equation (2.16) can show the LC stage that needs stake holders to take immediate action on the improvement of its sustainability performance. On the contrary, Eq. (2.17) indicates the LC stage that requires take holders take least action.

2.7.2 Comprehensive Elaboration

This approach is not to obtain a single composite number to represent the overall life cycle-based sustainability performance. It illustrates the life cycle-based sustainability status as a set:

$$S_t = (S_1, S_2 \dots S_N) \quad (2.18)$$

Comparing to the composite result obtained through arithmetic calculation, this approach could provide a comprehensive and straightforward view of life cycle based sustainability performance.

2.8 Case Study

The remarkable development on nanocoating materials brings a wide range of potential applications in the automotive, aerospace, and pharmaceutical industries. Despite

the obvious technical benefits of nanocoating such as anti-scratch and corrosion prevention, the unintended health and environmental risks as well as the economic and social benefit associated with the use of nanoproducts are not yet fully understood. The proactive and deep understanding of nanocoating materials requires a comprehensive assessment over each stage of its life cycle in order to develop nanocoating systems with improved product performance and reduced impact on environment and society. It becomes urgent to develop systems approaches for comprehensive evaluation of performance of nanocoating products and assurance of sustainability performance over their life cycle.

The life cycle of nanocoating materials consists of the stages ranging from (nano)material selection and processing, through nanopaint/nanocoating manufacturing, to product use and disposal. In this chapter, a life cycle based sustainability assessment LCBSA methodology is introduced. It can be used to assess the economic, environmental, and social aspects in every life cycle stage. To perform a comprehensive assessment, different sets of sustainability metrics have been identified for use in different life cycle stages. These metrics are analyzed to ensure the consistency of the assessment. The methodology has been used to study the sustainability performance of nanopaint and its application to automotive coatings. A comprehensive case study will highlight critical issues concerning the material's development and nanoparticles emission to the environment and health impact, economic incentive and social satisfaction.

In this research, an automotive paint system was selected for the case study. Nanocoating material is considered the next generation coating material as it could not only bring outstanding improvement of coating properties and even introduce new functionalities

comparing to conventional coating materials. However, the implications of nanomaterials and products on the environmental safety and human health are often either ignored or not highlighted. There is a major knowledge gap existing between the applicability of nano-size materials into consumer products and their effects on health and environment. Presumably, nanocoating material should be sustainable in terms of economy, resource and energy efficiency and health care. However, so far only the economic prospect of nanotechnology has been highlighted and a very little attention is given to its social and environmental implications. The various types of nanoparticles that are incorporated in nanocoating formulations possess serious health concerns. The potential to develop systems with smart and newer functionalities significantly inspires competitiveness among different companies which use nanotechnology based coatings to avail all its economic benefits. Currently, the economic growth of the nanocoatings market and corresponding research and development gives very little attention to the assessment of social and ecological risks which are a part of complete holistic sustainability assessment of nanocoating products. Thus, it is important to stress on benefits and risks of this technology during the life cycle to detect all hidden short and long term adverse effects and to support all the decisions related to its future development (Uttarwar, 2013).

With the proposed methodology, a comprehensive study on the life cycle of nanocoating material can analyze, evaluate and address all the issues related to the environmental and health effects of nanoparticle induced coating materials. It can also identify and optimize ways to develop a sustainable nanocoating system with minimal

environmental implications and improved societal safety and health care while preserving all the economic benefits of this novel technology.

2.8.1 Categorization of the Life Cycle of Nanocoating Materials

The life cycle of nanocoating technology is divided into five stages which encompass ‘cradle-to-grave’ continuum: (1) automotive nanocoating manufacturing process, (2) paint spray process, (3) coating curing process, (4) use and maintenance, and (5) end of use. First three stages account for nanopaint film development, and remaining two stages account for its use and disposal. Figure 2.3 represents the pathway that connects all the stages of life cycle of nanocoatings.

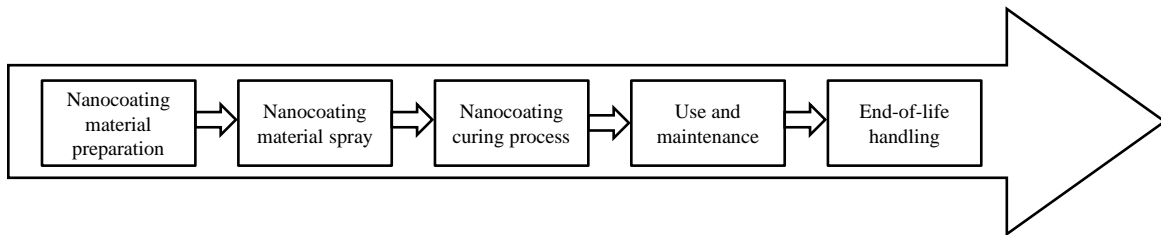


Figure 2.3. The life cycle of nanocoating material.

2.8.2 Assessment of the Sustainability Interest in Each Life Cycle Stage

System parameters and key sustainability interest must be identified in order to assess the sustainability status of each life cycle stage. Characterization of system parameters in the involved industrial systems in each life cycle stage is essential for the selection of proper sustainability indicators. Note that sustainability assessment of the automotive nanocoating materials is proactive and there is little deterministic information during material design and

selection stage, the selected indicators are either quantitative or qualitative and the evaluation could be subjective.

2.8.2.1 Life cycle stage 1: automotive nanocoating manufacturing process

The main goal of this life cycle stage is to manufacture paint that is suitable for generating automotive coating systems. In this case, a paint manufacturing process aiming at producing solvent-borne automotive nanocoat is investigated. The raw materials used in the modern paint manufacturing process consists of resins, pigments, fillers, solvents, and additives. Resins form a film and bind the raw materials in the paint to each other. They are chosen according to the requirement of paint properties and can thus greatly affect the weatherability and durability of the paint. Pigments mainly provide the desired color and coverage. For solvent-borne nanopaint, nanoparticles are mixed into the paint as a pigment. Fillers are used to give paint its required opacity and application properties. The viscosity of the paint is adjusted by the added solvents so that it can be applied sparingly to a substrate. Paint also consists of a small amount of additives which are used to add special functionalities to the paint or affect the paint-making process flow.

The paint industry is essentially a chemical manufacturing sector. Paint manufacturing process typically includes a series of batch production processes. Figure 2.4 depicts a general paint manufacturing process which involves mixing, milling, thinning, filtering, and packing operations (Wikipedia). Note that facilities which manufacture pigments, resins, additives, nanoparticles, fillers, and solvent are not considered in this life cycle stage. The manufacturing process of solvent-borne and waterborne, high solids products includes the following process steps: (i) dissolution of solid materials; (ii) mixing

of different liquids or liquids with solid materials; (iii) further mixing to fulfil required specifications regarding viscosity, color, etc; and (iv) sieving and filtering of base materials, intermediate and end products.

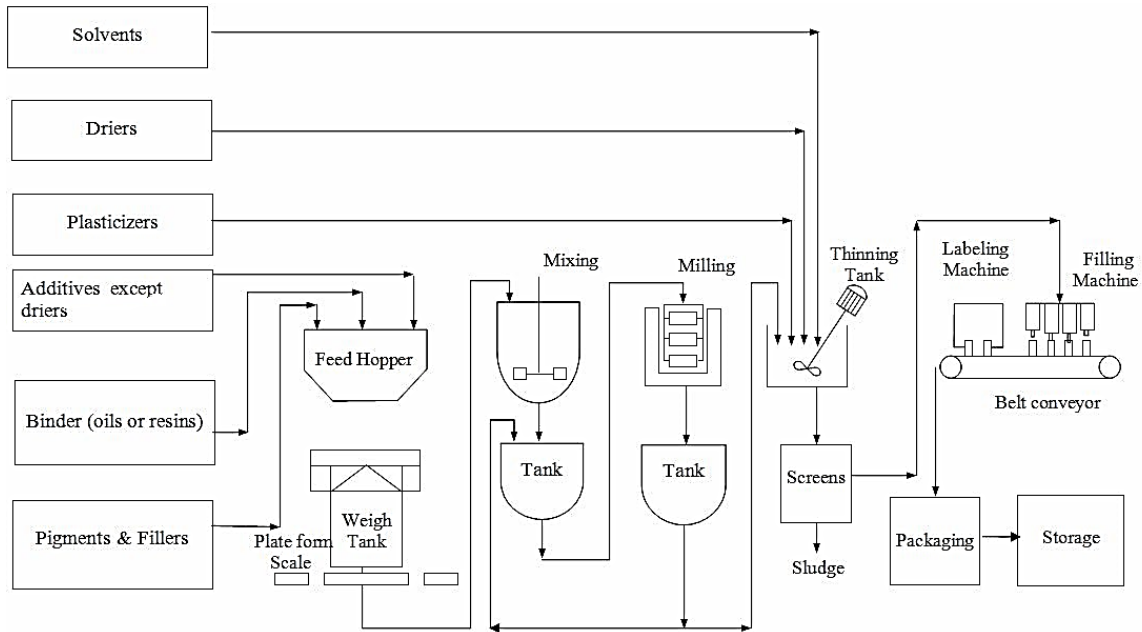


Figure 2.4. Paint manufacturing process (Wikimedia Commons, 2012).

The key system variables in this life cycle stage can be determined based on the analysis of paint manufacturing system (Table 2.1). The selection of these parameters is based on the availability of the data for analysis. It is worth noting that certain parameters are neglected at this stage due to the limitation of the data although they also contribute to the performance of the system.

Table 2.1. Key system variables of the first life cycle stage.

Index	Variable
V1-1	Types of additives selected for the paint formulation
V1-2	Nanoparticles size, shape and orientation
V1-3	Volatile Organic Content (VOC)
V1-4	Toxicity of each of the formulation ingredient
V1-5	Raw materials cost
V1-6	Paint system composition
V1-7	Concentration of nanoparticles released/exposed to the surrounding during manufacturing of the paint
V1-8	VOC emission during manufacturing
V1-9	Amount of energy consumed for all the processes

The main concern associated with economic sustainability is the design difficulty of paint materials and the effectiveness of manufacturing process. With the specific requirement from automotive manufacturers, the nanocoating material must provide sufficient protection and appealing appearance for automotive vehicles. Appropriate components and their composition must be well designed and tested. Economic sustainability needs the manufacturing process use effective approaches to maximize the raw material efficiency and minimize the energy consumption.

The use of toxic components could lead to a significant impact on environmental sustainability. Volatile organic compounds can pose significant threat to human health. On the other hand, many existing studies have shown that exposure to high concentrations of nanoparticles may result in possible acute symptoms to workers, including headache, dizziness, and exposure to suspected carcinogens, and sometimes this can also affect the

central nervous system. Therefore, these components should be carefully applied during manufacturing processes. During paint manufacturing, proper sealing of the equipment, ventilation, and employee protection are critical to the environment and human's health.

With the consideration of all key issues in this life cycle stage, the indicators to evaluation sustainability performance is proposed in Table 2.2.

Table 2.2. Sustainability indicators of the first life cycle stage.

Category	Indicator	
Economic sustainability	E1	Cost of raw materials per kg paint
	E2	Cost of energy consumption per kg paint
Environmental sustainability	V1	Energy consumption per kg paint
	V2	VOC consumption per kg paint
	V3	The quantity of nanoparticle released during manufacturing
	V4	Health impact of nanoparticles in the plant
Social sustainability	L1	Customer satisfaction of paint quality
	L2	Manufacturing process safety

2.8.2.2 Life cycle stage 2: automotive coating spray process

The goal of this life cycle is to provide a uniformly wet layer of nanoclearcoat with a specific thickness to the vehicle surface. The raw materials of this life cycle stage are obtained directly from the previous life cycle stage, paint manufacturing process.

Modern automotive paint spray process which typically takes place in a spray booth consists of spray guns/bells, ventilation system, tools, appliances, and equipment, such as pump, compressor, conveyor belt, and personal protective gear, which are necessary for an operator to apply paint on the object surface to be coated. Figure 2.5 illustrates the general spray process in an automotive manufacturing plant. In operation, the pretreated vehicle

body is firstly delivered into the spray booth by carrier. The vehicle body then stays stationary when automated robotic spray equipment applies certain amount of clearcoat in the form of paint particles to the surface of the vehicle at a high speed. Most of the paint droplets could land on the vehicle panel while the rest stays in the ambient air. The overspray released during the painting operation is then removed by the downdraft air that flows through the booth geometry and is absorbed by the water flowing underneath the exhaust grid.

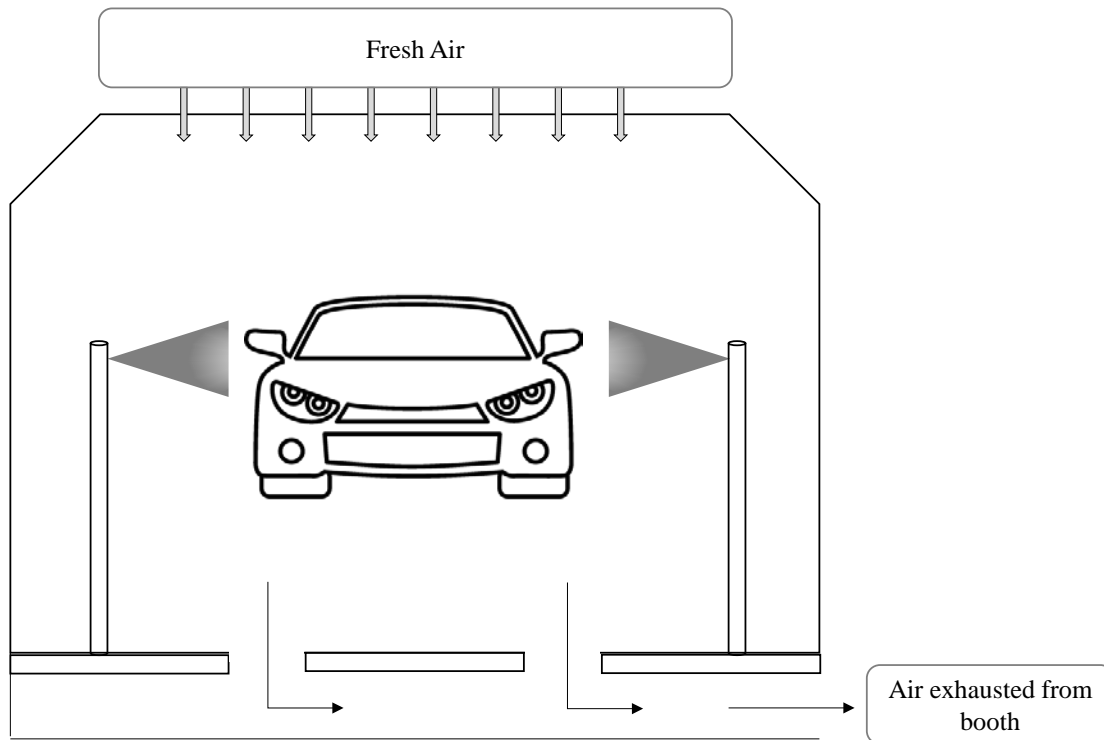


Figure 2.5. Schematic of paint spray booth.

Automotive coating spray process consumes significant amount energy due to the ventilation system. Robotic spray guns apply paint materials to the vehicle panel with high pressure after rotary atomizer transforming bulk liquid paint materials into tiny paint droplets.

The overspray paint must be effectively removed by ventilation air with a higher downdraft velocity. In the meanwhile, high air flow velocity could also have a negative impact on paint transfer efficiency as the efficiency of paint spray and the final coating film quality largely depend on several factors including the paint flow rate, paint injection velocity, atomization method, ventilation air velocity, spray angle, distance between gun and substrate. The existence of nanoparticle in the paint could also inevitably lead to nanoparticle emission which is a serious health and safety hazard. The paint droplets not landing on the receiving panels are emitted into the surrounding atmosphere resulting in contamination of the air inside the spray booth. This contamination could include a noticeable concentration of nanoparticles and VOCs. In addition to the economic and environmental concerns, the quality of wet paint film is also one of the critical variables that largely affect the aesthetic appearance of the automotive product which could play an important role on future sale and customer satisfaction. Thus, automotive paint spray process must deliver a satisfactory wet film for next life cycle stage, automotive curing process.

Given the process concerns, critical system variables and sustainability metrics system for this life cycle stage are identified as shown in Table 2.3 and Table 2.4 respectively.

Table 2.3. Key system variables of the second life cycle stage

Index	Variable
V2-1	Film surface topology parameters
V2-2	Emission of VOC's and nanoparticles during paint application through spray technique
V2-3	Wet film defects
V2-4	Paint transfer efficiency
V2-5	Paint film thickness data
V2-6	Energy efficiency of the paint-spray system
V2-7	Concentration of nanoparticles released/exposed to the surrounding during paint spray
V2-8	VOC emission during spray process
V2-9	Amount of energy consumed for all the processes

Table 2.4. Sustainability indicators of the second life cycle stage

Category	Indicator	
Economic sustainability	E1	Paint transfer efficiency
	E2	Cost of energy consumption per vehicle
Environmental sustainability	V1	Energy consumption per vehicle
	V2	VOC emission per vehicle
	V3	Density of nanoparticles in the spray booth
	V4	The quantity of nanoparticle released during spray
Social sustainability	L1	Satisfaction of coating thickness
	L2	Satisfaction of film surface topology

2.8.2.3 Life cycle stage 3: automotive coating curing process

The goal of this life cycle is to transform the wet nanoclearcoat film into a cured transparent hard coating through various heating processes. In general, automotive manufacturers use a baking oven with substantial length to complete the paint curing task.

Figure 2.6 illustrates a general curing process. Oven wall radiation and hot convection air are typical heating sources. Two key phenomena takes place in the curing oven, solvent evaporation, and cross-linking reaction. In operation, conveyor carries the vehicle body covered with wet film slowly move through the oven. To better curing the coating film, the curing oven is divided into different heating zones with different temperature settings. The zones in the front aims at removing all of the solvent content in the coating film while the rest zones provide sufficient heat to cure the coating film. The oven operational settings such as wall temperature and air temperature settings and convection air flow rate should be carefully selected.

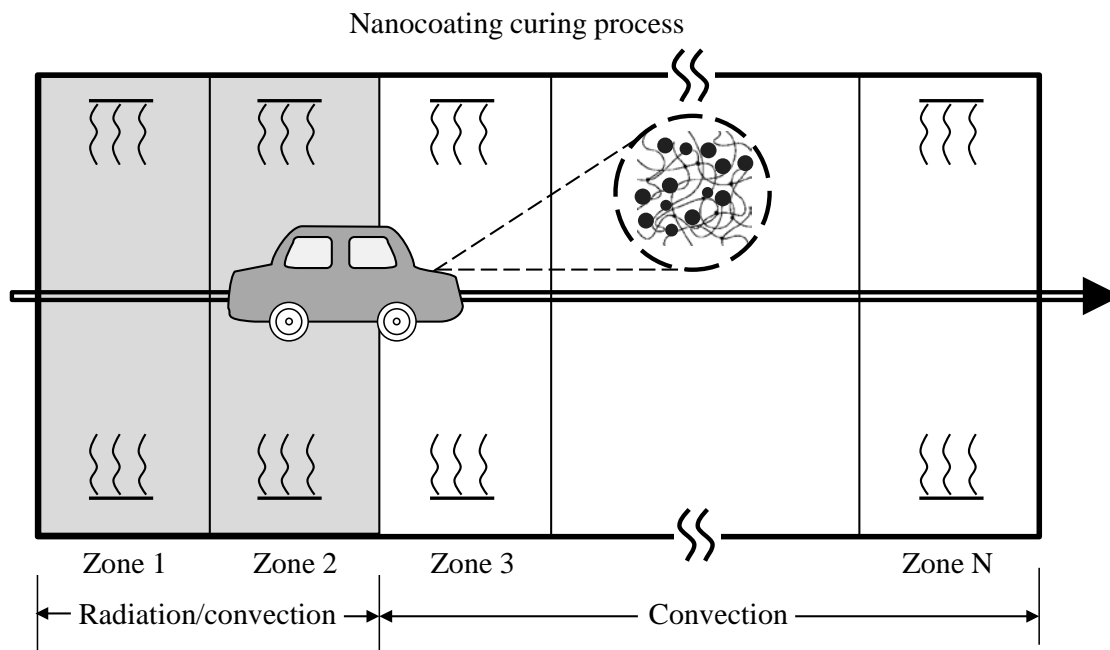


Figure 2.6. Schematic of paint curing oven (Song and Huang, 2016).

Automotive coating curing oven is the most energy intensive unit in automotive manufacturing plant. Huge amount energy is required for removal of solvent residual and

completion of cross-linking reaction. The main economic sustainability concern is the cost of energy consumed in the curing process. The amount of energy used in the process, VOC emission, and CO₂ emission due to the natural gas combustion and electricity consumption are the key environmental impacts. As the wet film is set on the vehicle surface, it is significantly difficult for nanoparticle emitted to the air. The quality of cured coating film must meet the requirement of end user in the next life cycle stage. Therefore, the essential system variables in this life cycle stage are determined as shown in Table 2.5.

Table 2.5. Key system variables of the third life cycle stage.

Index	Variable
V3-1	Crosslinking reaction conversion
V3-2	Net energy consumption by ovens
V3-3	VOC and nanoparticles emission
V3-4	Film thickness and uniformity
V3-5	Oven operation settings and parameters
V3-6	Coating mechanical properties

Given the sustainability concerns, sustainability metrics system for this life cycle stage consists of the following indicators:

Table 2.6. Sustainability indicators of the third life cycle stage.

Category	Indicator	
Economic sustainability	E1	Cost of energy consumption per vehicle
Environmental sustainability	V1	Energy consumption per vehicle
	V2	The quantity of nanoparticle released during curing
Social sustainability	L1	Cured coating mechanical performance
	L2	Cured coating quality

2.8.2.4 Life cycle stage 4: use and maintenance

This life cycle is highly associated with the automobile users. The coating performance at this stage is essentially decided by the performance of previous stages. The assessment of Stage 4 includes majority of the parameters related coating quality, performance and toxicity issues and key variables related to daily use and maintenance. These parameters are enlisted below (Table 2.7).

Table 2.7 Key system variables of the fourth life cycle stage.

Index	Variable
V4-1	Gloss retention
V4-2	Coating film functionalities
V4-3	Cost of coating maintenance
V4-4	Coating maintenance frequency
V4-5	Energy used during maintenance
V4-6	Water consumption during normal usage
V4-7	Amount of chemical emitted due to coating degradation

The economic sustainability concern is due to the cost that end users spend on the regular maintenance of the automotive coating. Environmental sustainability concerns consists of the impact brought by the coating degradation. Long-term coating performance is the key to customer satisfaction. Thus, the sustainability metrics system for this life cycle stage is as follows:

Table 2.8. Sustainability indicators of the fourth life cycle stage.

Category	Indicator	
Economic sustainability	E1	Cost of maintenance per vehicle
Environmental sustainability	V1	Energy consumption per vehicle in the life time of vehicle
	V2	Water consumption per vehicle per year
	V3	Total nanoparticle emission in the life time of vehicle
Social sustainability	L1	Average amount of maintenance per year
	L2	Gloss retention rate
	L3	Coating degradation rate
	L4	Anti-scratch performance

2.8.2.5 Life cycle stage 5: end of life

The end of life is the stage of disposal and recycle of automotive body. It is worth noting that automotive coating is disposed rather than recycled. The cost to remove automotive coating material from the disposed vehicle body is the main concern of economic sustainability. Environmental sustainability concerns consists of the impact brought by the coating degradation. The easiness of coating separated from vehicle body is the key to social sustainability. Thus, critical system variables and sustainability metrics system for this life cycle stage are identified as shown in Table 2.9 and Table 2.10 respectively.

Table 2.9. Key system variables of the fifth life cycle stage.

Index	Variable
V5-1	Process complexity for removing coating from metal surface
V5-2	Energy used during disposal
V5-3	The amount of coating materials that can be recycled
V5-4	Amount of chemical emitted during disposal

Table 2.10. Sustainability indicators of the fifth life cycle stage.

Category	Indicator	
Economic sustainability	E1	Cost of energy consumption per vehicle during disposal
Environmental sustainability	V1	Energy consumption per vehicle used during disposal
	V2	Percentage of material recycled
	V3	The quantity of waste generated during disposal
	V4	The quantity of nanoparticle released during disposal
Social sustainability	L1	Easiness of coating material separated from metal surface

2.8.3 Stage-based Sustainability Assessment

In this work, an examples of automotive nanocoating materials was selected. This coating materials for automotive clearcoat was a solventborne paint system while the additive nanoparticle is nano-silica (20nm). The quantities of raw materials given in Table 2.11 are in weight percent of the total paint weight.

Table 2.11. Automotive nanocoating formulation.

Material	Quantity (w.t. %)
Naptha	3
Xylene	16
Methanol	2
Melamine formaldehyde	11
Ethylbenzene	1
N-butyl alcohol	11
Cumene	1
MTS*	5
Butyl acetate	3
PMMA*	40
Silicon dioxide (20nm)	6

* MTS: 3-methacryloxypropyl-trimethoxy-silane; PMMA: Polymethylmethacrylate

For the stage 1-paint manufacturing process, the selected plant has an annual production capacity of 2.54×10^7 kg for this nanocoating material and the total annual material cost is \$ 1.2×10^8 . Annual energy consumption for the production plant is 1.5×10^8 kWh and the cost is equivalent to \$ 1.65×10^7 . Annual VOC consumption is 1.27×10^7 kg for this specific paint material. About 5% of total nanomaterials is released to the manufacturing environment which leads to a very high health impact and low safety rating. Based on the feedback from downstream customer, the satisfaction of paint quality is rated as high.

The fact of coating manufacturing system can then be converted to the sustainability status based on the defined sustainability metrics system for stage 1 based on Eqs. (2.7)-(2.9). The result of sustainability assessment is shown in Table 2.12. The actual sustainability performance is normalized based on the current best and worst industrial practice. In this

case, all of the weighting factors are considered equally important and set to 1. Therefore, the economic, environmental, social and overall sustainability status can be obtained as 0.49, 0.42, 0.39, and 0.44, respectively by following Eqs. (2.10)-(2.13).

Table 2.12. Sustainability assessment of life cycle stage 1.

Category	Indicator	Current status	Normalized value	Worst	Best
Economic sustainability	E1 (\$/kg)	4.72	0.48	6.5	2.8
	E2 (\$/kg)	0.65	0.50	0.9	0.4
Environmental sustainability	V1 (kWh/kg)	5.9	0.50	8.3	3.5
	V2(kg/kg)	0.5	0.71	0.75	0.4
	V3 (%)	5	0.17	6	0
	V4	0.7	0.30	1	0
Social sustainability	L1	0.75	0.50	0.5	1
	L2	0.35	0.28	0.1	1

The evaluation of stage 2 - coating spray process is based on the results of computational modeling (Uttarwar and Huang, 2013). The selected nanocoating spray process has the same design as traditional spray booth and a center spray pattern is applied to the spray robotic nuzzle. Given that the production line has an annual production capacity of 4.1×10^4 vehicles, the annual energy consumption due to paint spray and air ventilation in the spray process is 2.1×10^6 kWh and the cost is equivalent to $\$ 2.2 \times 10^5$. During spray, the concentration of nanoparticles in booth air is 2.3×10^{12} per m^3 . An estimated 25% paint material is carried out to the sludge by down drafting air. 2% total amount of nanoparticles will be released to the environment. VOC emission is 1.3 kg for each spray job. The average

film thickness when coating is partially wet is 29.7 μm and the film surface topology is rated as average based on expert's knowledge.

Such information can be used to evaluate the status of selected sustainability indicators. Table 2.13 describes the result of sustainability assessment. The actual sustainability performance is normalized based on the current best and worst industrial practice. By applying Eqs. (2.10)-(2.13), the economic, environmental, social and overall sustainability status can be obtained as 0.55, 0.53, 0.59, and 0.56, respectively.

Table 2.13. Sustainability assessment of life cycle stage 2.

Category	Indicator	Current status	Normalized value	Worst	Best
Economic sustainability	E1 (%)	75	57	55	90
	E2 (\$/vehicle)	5.4	0.54	6.1	4.8
Environmental sustainability	V1 (kWh/vehicle)	49.1	0.54	55.5	43.6
	V2 (kg/vehicle)	0.9	0.60	1.5	1
	V3 ($\times 10^{12}$ per m^3)	2.3	0.38	3.7	0
	V4 (%)	2	0.60	5	0
Social sustainability	L1	0.7	0.63	0.2	1
	L2	0.6	0.56	0.1	1

The evaluation of stage 3 - coating curing process is obtained from multiscale computational modeling (Song *et al.*, 2016). It is expected that the curing oven setting follows the one for conventional clearcoat baking process. Thus, the heating source for the selected nanocoating curing process consists of radiation and convection air heating. Given that the production line has an annual production capacity of 4.1×10^4 vehicles, the annual energy consumption due to in the curing process is 2.87×10^6 kWh and the cost is equivalent to $\$ 3.15 \times 10^5$. It is expected that 1% total amount of nanoparticles in the wet film will be

released to the environment. The conversion rate of cross-linking reaction in the coating film could reach 90%. In the meanwhile, coating mechanical performance could improve 40% over conventional clearcoat after curing and the coating thickness might be 2 μm thicker than what is expected due to the solvent residual remaining in the film.

Such information can be used to evaluate the status of selected sustainability indicators. Table 2.14 describes the result of sustainability assessment. The actual sustainability performance is normalized based on the current best and worst industrial practice. By applying Eqs. (2.10)-(2.13), the economic, environmental, social and overall sustainability status can be obtained as 0.83, 0.71, 0.56, and 0.71, respectively.

Table 2.14 Sustainability assessment of life cycle stage 3.

Category	Indicator	Current status	Normalized value	Worst	Best
Economic sustainability	E1 (\$/vehicle)	7.7	0.83	9.35	7.35
Environmental sustainability	V1(kWh/vehicle)	70	0.75	85	65
	V2	0.01	0.67	0.03	0
Social sustainability	L1	1.4	0.57	1	1.7
	L2	0.9	0.55	0.85	0.94

Note that this study is only for demonstrative purpose of the proposed LCBSA framework. To simplify the case study, stage 4 (use and maintenance) and stage 5 (end of life) are not studied in this work due to the insufficient knowledge about the coating performance in the long-term and disposal techniques.

2.8.4 Life Cycle Based Sustainability Assessment

In this work, Eq. (2.18) is applied to evaluate the overall life cycle based sustainability performance due to the subjective, uncertainty, and data scarcity issue associated with the study. Therefore, a sustainability vector denoting the desired result is expressed as:

$$S_i = (0.44, 0.56, 0.71)$$

Figure 2.7 depicts the life cycle based sustainability performance of studied automotive nanocoating materials.

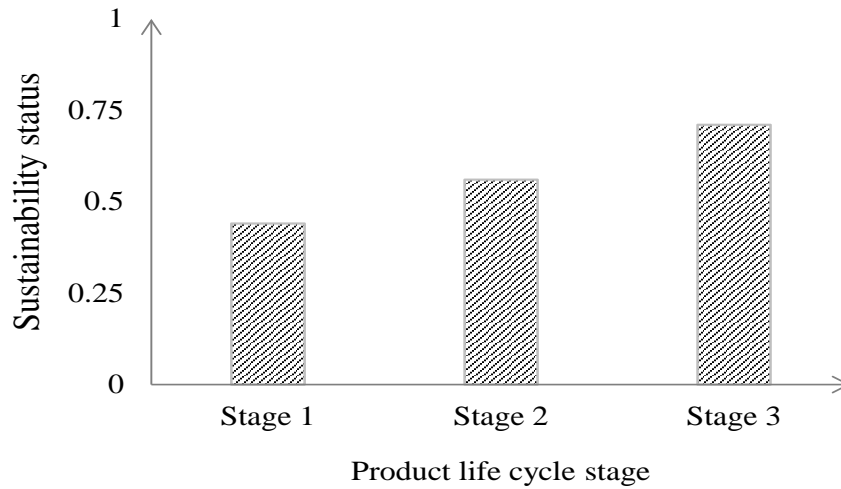


Figure 2.7. Life cycle based sustainability performance of automotive nanocoating materials.

2.9 Conclusions

Sustainability assessment with life cycle thinking has significant potential to be used by enterprises, governments, agencies for international cooperation and other organizations in their efforts to produce and consume more sustainable products. This chapter introduces a novel and practical LCBSA framework to promote the life cycle based analysis. LCBSA framework is superior to the LCSA framework proposed by Kloepffer.

The demonstrative case study on automotive nanocoating material was applied in this work. Five consecutive life cycle stages were categorized based on the heuristic rules proposed in the analysis. The sustainability indicator metrics systems for all the stages of life cycle were developed based on the interests of each individual life cycle stage parameter sets. The case studies were generated and the economic, environmental and social performance was studied and integrated toward the overall life cycle based sustainability status. The evaluation result concludes that LCBSA is capable of providing convincing sustainability assessment of product throughout the life cycle and it can be useful for not only the researchers but also industries to analyze the performance of nanocoatings and ensure the sustainable development of this novel and promising coating technology.

CHAPTER 3 LIFE CYCLE BASED DECISION MAKING FOR SUSTAINABLE DEVELOPMENT OF INDUSTRIAL SYSTEMS

Ever since the WCED emphasized the importance of sustainable development, it has been adopted as a core business value by many companies. Sustainable development must take account of social and ecological factors, as well as economic ones; of the living and non-living resource base; and of the long term as well as the short term advantages and disadvantages of alternative actions. Given that modern sustainability means economic well-being is inextricably linked to the health of the environment and the success of the world's communities and citizens. Sustainability decision-making process requires to use systems thinking to evaluate and identify a balanced strategy to promote sustainability status at three different directions.

Sustainable development planning and decision making are not an easy tasks as they require effective decision making approaches to utilize limited amount of resources to integrate new technology developments based on social, economic, environmental, and cultural well-being dimensions of sustainability assessment. Decision making may become more challenging when the objective is to promote life cycle based sustainability performance. Decision making for sustainability improvement over the life cycle includes the trade-off within each life cycle stage and across the life cycle stage. It should be noted here that life cycle based decision making (LCBDM) for sustainable development requires special consideration of the economy, environment, and society at each life cycle stage since the life cycle stages are interlinked. LCBDM is typically determined by the highest level planning group (decision maker at life cycle level), and interests of the life cycle stage (stage-based decision maker). Both groups of decision makers play significant roles in shaping the

final outcome of the sustainable development plans. The need for promoting a new approach for sustainability improvement from life cycle perspective has required a new methodology for LCBDM. Concept of this methodology comprises prioritization of the urgency of sustainability improvement, distribution of limited amount of sustainability enhancement efforts selection of the indicators, and identification of effective strategies to achieve sustainability goals at different level. Also, it is of paramount importance of the new methodology to adapt multi-criteria approach for its application. Global optimization of the strategies of sustainable development in the whole product life cycle could render an optimal solution if all involved system parameters are deterministic. However, the uncertainty issues and objective considerations involved in the LCBDM make it not an effective method.

The above discussions highlight two important issues of LCBDM. These are: (i) consideration of multiple criteria, and (ii) accommodation of diversified interests at economic, environmental, and social level in each life cycle stage. A number of system variables and distinct criteria are involved in the planning for sustainability improvement at life cycle level. It is often necessary to consider several aspects at the same time. Therefore, it is of great importance to employ effective method in the evaluation of complex system based on multiple criteria analysis. The task of LCBDM is essentially a multi-criteria decision making (MCDM) problem.

MCDM is developed to help decision makers to make complex decisions in a systematic and structured way. There are two categories of MCDM problems: multiple criteria discrete alternative problems and multiple criteria optimization problems. A variety of extensive mathematical approaches have been developed to solve multi-criteria decision

making problems, such as the analytic hierarchy process (AHP), analytic network process (ANP), case-based reasoning (CBR), data envelopment analysis (DEA), fuzzy set theory, genetic algorithm (GA), mathematical programming, simple multi-attribute rating technique (SMART), Outranking Methods such as ELECTRE or PROMETHEE or the TOPSIS (Technique for Order Preference by Similarity to Ideal Solution). It must be pointed out that all MCDM techniques have their advantages and drawbacks in evaluating complex problems. Therefore, the selection effective MCDM methods highly depends on the context.

The number of scientific publications related to AHP grows a lot in past several decades and stands out from the other techniques mentioned. The Analytic Hierarchy Process (AHP) which is developed by Saaty (1980) is a theory of relative measurement with absolute scales of both tangible and intangible criteria based on the experts' judgment. Decisions for the best outcome are determined by integrating multidimensional criteria into one dimensional information.

In this chapter, a two-phase decision making methodology is proposed. In the first phase, the managing board at each life cycle stage must determine and solve the urgent issues associated with sustainability performance with minimum amount improvement effort. The second phase consists of establishing a priority order among the life cycle stages that have specific improvement goal and limited effort. A decision-making approach based on the AHP is applied to help the managing board at the life cycle level to decide the priority order of sustainability improvement effort.

3.1 Decision Making Methodology toward Sustainability Improvement

The goal of LCBDM methodology is to provide a systematic framework to identify optimal decision to achieve the best overall sustainability status rather than individual stage sustainability achievement with the availability of finite resources. There will be trade-off among stage-based sustainability performance. In general, the sustainability among different stages are equally important. The sustainability performance at a specific stage remains independent from the performance of other stages and doesn't have significant difference from the rest stages. It is essential that the sustainability status related system parameters must satisfy all existing restrictions.

In this work, the task of decision-making is divided into two main steps. The first step is to address the “must-be” improved category in every life cycle stage. It is also essential to re-evaluate the stage based sustainability assessment after the first set of improvement actions. The second step is to prioritize the effort and necessity to enhance stage based sustainability improvement through prioritization matrix. A general framework is depicted in Figure 3.1.

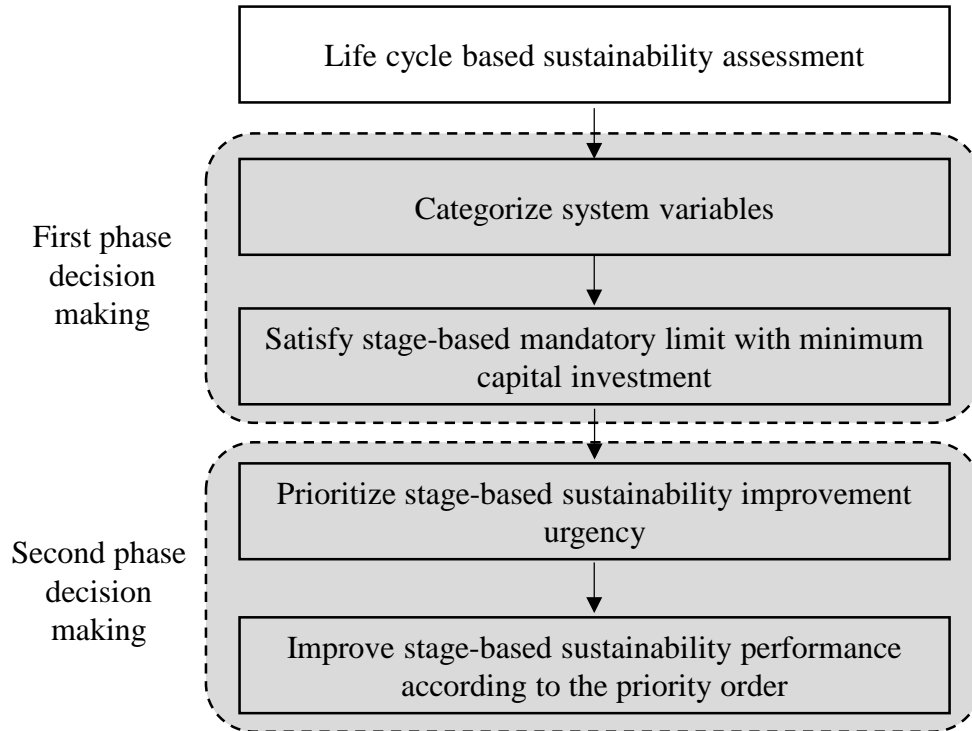


Figure 3.1. General framework of LCBDM.

3.2 First Phase Decision Making

Given that sustainability assessment is a comprehensive analysis of all key aspects associated with process and product variables. General sustainability consists of three aspects, economic sustainability, environmental sustainability, and social sustainability, which represent the interest and requirement of different groups. Stakeholders, environmental agency, and society may have distinct requirements for specific system variables. Such requirement can be mandatory which means it must reach the mandatory level or soft expectation which denotes. It is assumed that the selected sustainability indicators for evaluating stage-based sustainability performance have direct relationship

with all key system variables. Therefore, the first step of LCBDM is to ensure that all of the sustainability status related system parameters must satisfy all existing restrictions which can be posed by business interest, environmental crisis, or social demand.

3.2.1 Categorization of Stage-based System Variables

It is assumed that all of the selected sustainability indicators to evaluate sustainability status is highly relevant to the corresponding life cycle stage and the indicators are directly linked to the corresponding system parameters. In this study, the first step is to categorize the critical process and product variables associated with selected sustainability indicators into two different groups: must-be and satisfier (Figure 3.2).

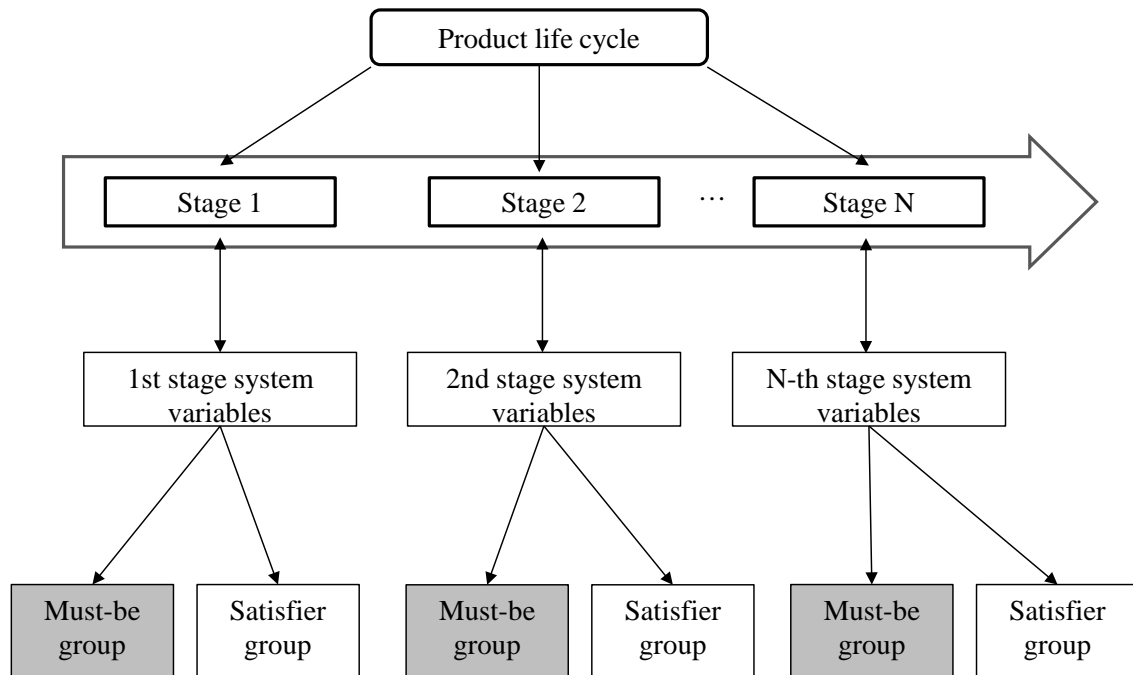


Figure 3.2. Categorization of the performance of stage-based system variables.

The system variables in must-be group have the attribute of must-be quality and indicate that the associated system variables have clear mandatory level defined by government regulations, investor's requirement, etc. However, the practical performance of the indicator or variable has not met the preset limit yet based on the initial analysis of sustainability status. Figure 3.3 denotes the description of system variables in must-be group. It is substantially important to implement appropriate decision to fulfill the requirement immediately.

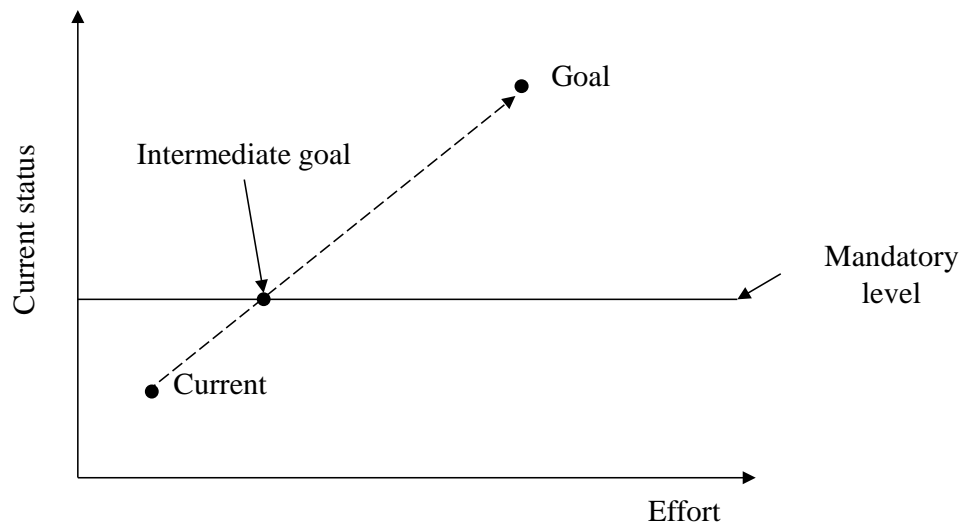


Figure 3.3. Property of system variables in must-be group.

The system variables in satisfier group have the attribute of one-dimensional quality. The process variables associated with the indicator either has no clear limit or has met the preset limit and the limit will be continuously satisfied in the future development (Figure 3.4). The more effort is invested, the higher the performance is.

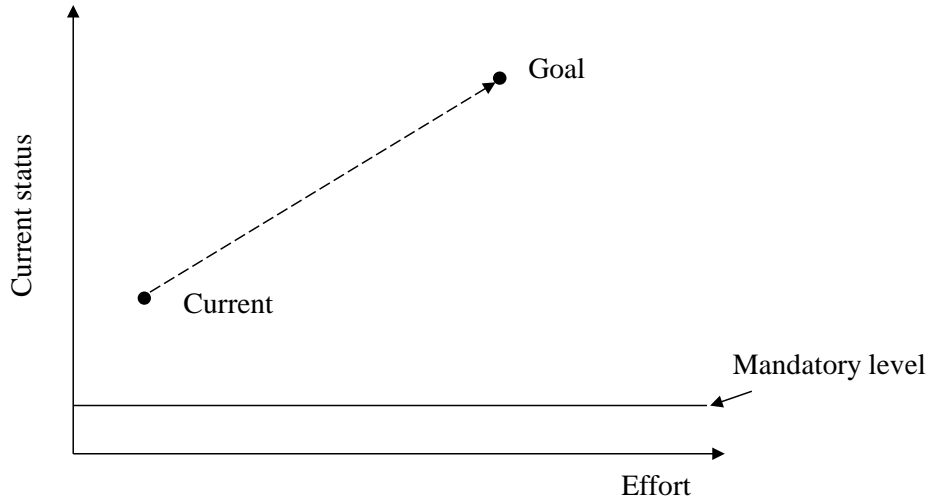


Figure 3.4. Property of system variables in satisfier group.

3.2.2 Evaluation of Stage-based Sustainability Improvement Strategy

It is comprehensible that industrial systems have to implement effective technologies to modify or optimize process, product and materials to improve its sustainability performance and therefore achieve overall life cycle based sustainable development. Thus, a thorough investigation of the sustainability improvement potential by implementing candidate technologies is essential to sustainable decision-making. Identification of candidate technologies requires the process characterization, experts' knowledge and stakeholder's preference. The selected sustainability metrics system for assessing system sustainability performance should also be used to evaluate the sustainability improvement potential of candidate technologies. A technology evaluation and decision making for sustainability enhancement methodology proposed by Liu and Huang is applied in this chapter (Liu and Huang 2012).

To interpret the sustainability assessment of technology candidate, the following methodology is presented for addressing the system variables associated with indicators in must-be group for i -th life cycle stage s_i . For the application of j -th sustainability improvement technology, system variables in i -th life cycle stage X_i is expected to change as follows:

$$\Delta X_i(T_j) = X_i(T_j) - X_i(0) \quad (3.1)$$

where $X_i(T_j) = \{x_{i,1}(T_j), x_{i,2}(T_j), \dots\}$; $X_i(0)$ is the initial value of system parameters; $X_i(T_j)$ is the performance of corresponding system parameters after the use of j -th sustainability improvement technology.

Given that the system parameters directly reflect the performance of associated sustainability indicators. Correspondingly, the evaluation can also provide the improvement potential for k -th economic sustainability indicator ($\Delta E_{i,k}(T_j)$), l -th environmental sustainability indicator ($\Delta V_{i,l}(T_j)$), m -th social sustainability indicator ($\Delta L_{i,m}(T_j)$), and capital cost ($B_i(T_j)$). Based on the available data of each technology, the sustainability improvement potential of each indicator with respect to each technology can be obtained in the following way:

$$\Delta E_{i,k}(T_j) = f_{E_i}(\Delta X_i(T_j)); \quad i = 1, 2, \dots, N; \quad k = 1, 2, \dots, N_A \quad (3.2)$$

$$\Delta V_{i,l}(T_j) = f_{V_i}(\Delta X_i(T_j)); \quad i = 1, 2, \dots, N; \quad l = 1, 2, \dots, N_B \quad (3.3)$$

$$\Delta L_{i,m}(T_j) = f_{L_i}(\Delta X_i(T_j)); \quad i = 1, 2, \dots, N; \quad m = 1, 2, \dots, N_C \quad (3.4)$$

where f_{E_i} , f_{V_i} , and f_{L_i} are the input-output evaluation model of economic, environmental, and social sustainability indicators.

The above evaluation results can be used to calculate the categorized sustainability improvement level using the formulas below:

$$\Delta \hat{E}_i(T_j) = \frac{\sum_{k=1}^{N_{E_i}} a_{i,k} \Delta E_{i,k}(T_j)}{\sum_{k=1}^{N_{E_i}} a_{i,k}}; \quad k = 1, 2, \dots, N_{E_i} \quad (3.5)$$

$$\Delta \hat{V}_i(T_j) = \frac{\sum_{l=1}^{N_{V_i}} b_{i,l} \Delta V_{i,l}(T_j)}{\sum_{l=1}^{N_{V_i}} b_{i,l}}; \quad l = 1, 2, \dots, N_{V_i} \quad (3.6)$$

$$\Delta \hat{L}_i(T_j) = \frac{\sum_{m=1}^{N_{L_i}} c_{i,m} \Delta L_{i,m}(T_j)}{\sum_{m=1}^{N_{L_i}} c_{i,m}}; \quad m = 1, 2, \dots, N_{L_i} \quad (3.7)$$

where a_j , b_j , and $c_j \in [1, 10]$ are the weighting factors that denote the relative importance of indicators among each category.

The above categorized sustainability improvement results can be used to evaluate the overall sustainability, $S_i(T_j)$, by firstly calculating the categorized sustainability that system can achieve after implementing a specific technology, which can be calculated as follows:

$$\hat{E}_i(T_j) = \Delta \hat{E}_i(T_j) + \hat{E}_i(0) \quad (3.8)$$

$$\hat{V}_i(T_j) = \Delta \hat{V}_i(T_j) + \hat{V}_i(0) \quad (3.9)$$

$$\hat{L}_i(T_j) = \Delta \hat{L}_i(T_j) + \hat{L}_i(0) \quad (3.10)$$

where $\hat{E}_i(0)$, $\hat{V}_i(0)$, and $\hat{L}_i(0)$ are the initial performance of economic, environmental, and social sustainability.

Then the overall sustainability after using a specific technology becomes:

$$S_i(T_j) = \frac{\|(\alpha \hat{E}_i(T_j), \beta \hat{V}_i(T_j), \gamma \hat{L}_i(T_j))\|}{\|(\alpha, \beta, \gamma)\|} \quad (3.11)$$

where α, β and γ are the weighting factors of categorized sustainability status; they follow the same rules as those used in Eq. (3.5)-(3.7).

In this case, technology integration must be taken into consideration as multiple technologies can be selected to contribute sustainability improvement simultaneously. It is assumed that the output of more than one technology being applied is equal to the summation of output of each individual technology. Given that a technology set (\hat{T}) including N_{Ti} technologies is selected, the change of system variables and categorized sustainability performance can be expressed as follows:

$$\Delta X_i(\hat{T}) = \sum_{j=1}^{N_{Ti}} \Delta X_i(T_j) \quad (3.12)$$

$$\Delta \hat{E}_i(\hat{T}) = \sum_{j=1}^{N_{Ti}} \Delta \hat{E}_i(T_j) \quad (3.13)$$

$$\Delta \hat{V}_i(\hat{T}) = \sum_{j=1}^{N_{Ti}} \Delta \hat{V}_i(T_j) \quad (3.14)$$

$$\Delta \hat{L}_i(\hat{T}) = \sum_{j=1}^{N_{Ti}} \Delta \hat{L}_i(T_j) \quad (3.15)$$

where $\hat{T} = \{T_1, T_2, \dots, T_{N_{Ti}}\}$; $X_i(\hat{T})$ is the performance of corresponding system parameters after the use of a set of sustainability improvement technologies.

Thus, the evaluation of categorized sustainability status and overall sustainability performance can be obtained by following Eqs. (3.8)-(3.11).

Capital investment on implementation of new technologies must be seriously taken into consideration as budget availability is one of the major constraints that influence the final decision toward sustainability improvement. In this chapter, it is assumed that there is no interaction among the selected technologies. Given that expense on adopting j -th technology can be denoted as $B_i(T_j)$, the total cost for using a set of technologies including N_{Ti} technologies can also be readily calculated as follows:

$$B_i(\hat{T}) = \sum_{j=1}^{N_{Ti}} B_i(T_j) \quad (3.16)$$

3.2.3 Identification of Optimal Decisions for First Phase Decision-making

The objective of first phase decision-making is to solve the most urgent requirements which is the mandatory constraints of system variables in must-be group with minimum budget spending. To identify the most cost effective sustainability improvement strategy for first phase decision-making, a simple solution searching methodology is used in this place. It is assumed that there are \hat{N}_{Ti} sustainability improvement strategies candidates for first phase decision-making.

In order to determine the best sustainability improvement strategy at this phase, a binary variable $y_{i,j}$ is assigned to each technology candidate. For j -th technology candidate in i -th life cycle stage:

$$y_{i,j} = \begin{cases} 1 & j\text{-th technology is selected} \\ 0 & j\text{-th technology is not selected} \end{cases} \quad j = 1, 2, \dots, M \quad (3.17)$$

Therefore, the total cost function can be expressed as:

$$B_i(\hat{T}) = \sum_{j=1}^{\hat{N}_{Ti}} y_{i,j} B_i(T_j) \quad (3.18)$$

The objective function for first phase decision making can be achieved as follows:

$$\min_{y_{i,1}, y_{i,2}, \dots, y_{i,\hat{N}_{Ti}}} B_i(\hat{T}) = \min \left(\sum_{j=1}^M y_j(s_i) B(T_j) \right) \quad (3.19)$$

There are a number of constraints that the optimization must achieve. First, system variables in must-be group must satisfy the defined limit, that is,

$$X_i(\hat{T}) \geq X_i^{MB} \quad (3.20)$$

where X_i^{MB} denotes the must-be constraint of system variables X_i .

Second, the impact brought by the change of system variables X_i must meet the minimum performance requirement of each selected sustainability indicator, categorized and overall sustainability status. The constraints can be expressed as:

$$I_i(\hat{T}) \geq I_i^{MB} \quad (3.21)$$

$$S_i(\hat{T}) \geq S_i^{MB} \quad (3.22)$$

where $I_i(\hat{T})$, and I_i^{MB} represent the performance of any indicators in i -th life cycle stage after applying technology set \hat{T} and its preset limit; $S_i(\hat{T})$, and S_i^{MB} denotes the sustainability status of i -th life cycle stage after applying technology set \hat{T} and its preset limit.

After executing the optimization shown in Eq. (3.19) with the consideration of multiple constraints (Eqs. (3.17), (3.20)-(3.22)) using Monte Carlo optimization, the most cost-effective technology or technology set should satisfy the preset goals. In the meanwhile, different categorized sustainability improvements will be achieved. It is of great important to reevaluate the sustainability performance for second phase decision making.

3.3 Second Phase Decision Making

The sustainability improvement from the life cycle perspective depends on a wide range of factors which involve both quantitative and qualitative. To increase the performance of life cycle based product sustainability, it is essential to prioritize the need of sustainability enhancement and provide appropriate effort to achieve the objective. It is essential to identify and implement the optimal improvement strategy to achieve stage based sustainability development goal with minimum amount of effort according to the developed priority order. The goal of second phase decision making is to prioritize the sustainability improvement efforts for all life cycle stages throughout the product life cycle and improve stage-based sustainability performance in a cost effective way accordingly. Therefore, an AHP based prioritization approach is use to prioritize the sustainability improvement efforts. A comprehensive optimization will be used to choose the right strategy to improve stage-based sustainability performance consecutively.

Prior to the strategy selection, an adjustment of the goal for sustainability improvement at each life cycle stage must be completed in order to achieve the best cost-effective solution. A general scheme of the goal adjustment is depicted in Figure 3.5. With the evaluation of stage-based sustainability performance S_i , stage-based sustainability

decision makers (SBDM) propose a temporary improvement goal S_i^{PS} and submit the information to decision makers at the life cycle level (LCDM). By taking into account of all information from the life cycle stages and outside regulations and uncertainties, an adjusted goal for i -th stage S_i^G is determined by LCDM. The adjustment process could be very objective and involves trade-offs from different perspectives. In the following evaluation, only S_i^G is used for second-phase decision-making. It must be pointed out that the adjusted goal may also include the guideline for each categorized sustainability performance.

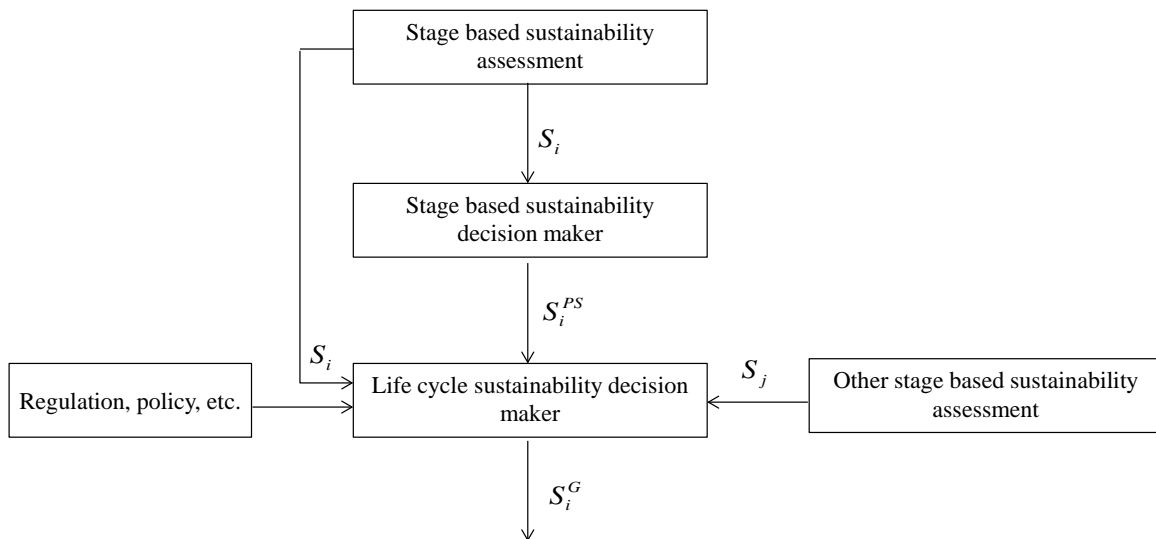


Figure 3.5. General scheme of goal adjustment.

3.3.1 Prioritization of Stage-based Improvement Effort

Analytic Hierarchy Process (AHP) is one of multi-criteria decision making method that was originally developed by Prof. Thomas L. Saaty. In short, it is a method to derive ratio scales from paired comparisons. The input can be obtained from actual measurement

such as price, weight etc., or from subjective opinion such as satisfaction feelings and preference. AHP allows some small inconsistency in judgment because human is not always consistent. The advantage of applying AHP based decision analysis approach to enhance life cycle based sustainability performance is that it allow decision makers to analyze complex decision-making problems using a systematic and comprehensive approach. AHP is capable of taking into consideration of criteria, stage-based sustainability status and goal, budget, and resources and inexorably creating an effective priority order based on reasonable judgements from decision makers in each life cycle stage and overall life cycle level.

The essence of AHP is to establish a pairwise comparison matrix illustrating the relative values of a set of attributes. To make tradeoffs among the many objectives and many criteria, the judgments that are usually made in qualitative terms are expressed numerically. To do this, rather than simply assigning a score out of a person's memory that appears reasonable, one must make reciprocal pairwise comparisons in a carefully designed scientific way. The fundamental scale used for the judgments is given in Table 3.1. Judgments are first given verbally as indicated in the scale and then a corresponding number is associated with that judgment. For instance, if attribute *A* is absolutely more important than attribute *B*, the judgement can be interpreted as *A* is 9 times more important than *B* and is rated at 9. In other words, *B* must be absolutely less important than *A* and is valued a 1/9.

Table 3.1. Scale of relative importance.

Intensity of importance	Definition
1	Equal important
2	Weak or slight
3	Moderate importance
4	Moderate plus
5	Strong importance
6	Strong plus
7	Very strong
8	Very, very strong
9	Extreme importance

In this chapter, the main steps to prioritize stage-based efforts for sustainability improvement using AHP are shown in Figure 3.6. The hierarchical decision-making process is divided into several levels. The top level of the hierarchy is the main goal of the second-phase decision-making. The lower level is to define key criteria for global priority. Then, all of the alternatives are evaluated to obtain local priorities with respect to specific criterion and the weight of all criteria are evaluated simultaneously. The bottom level is to integrate local priorities into one global priority and output final priority order for decision makers.

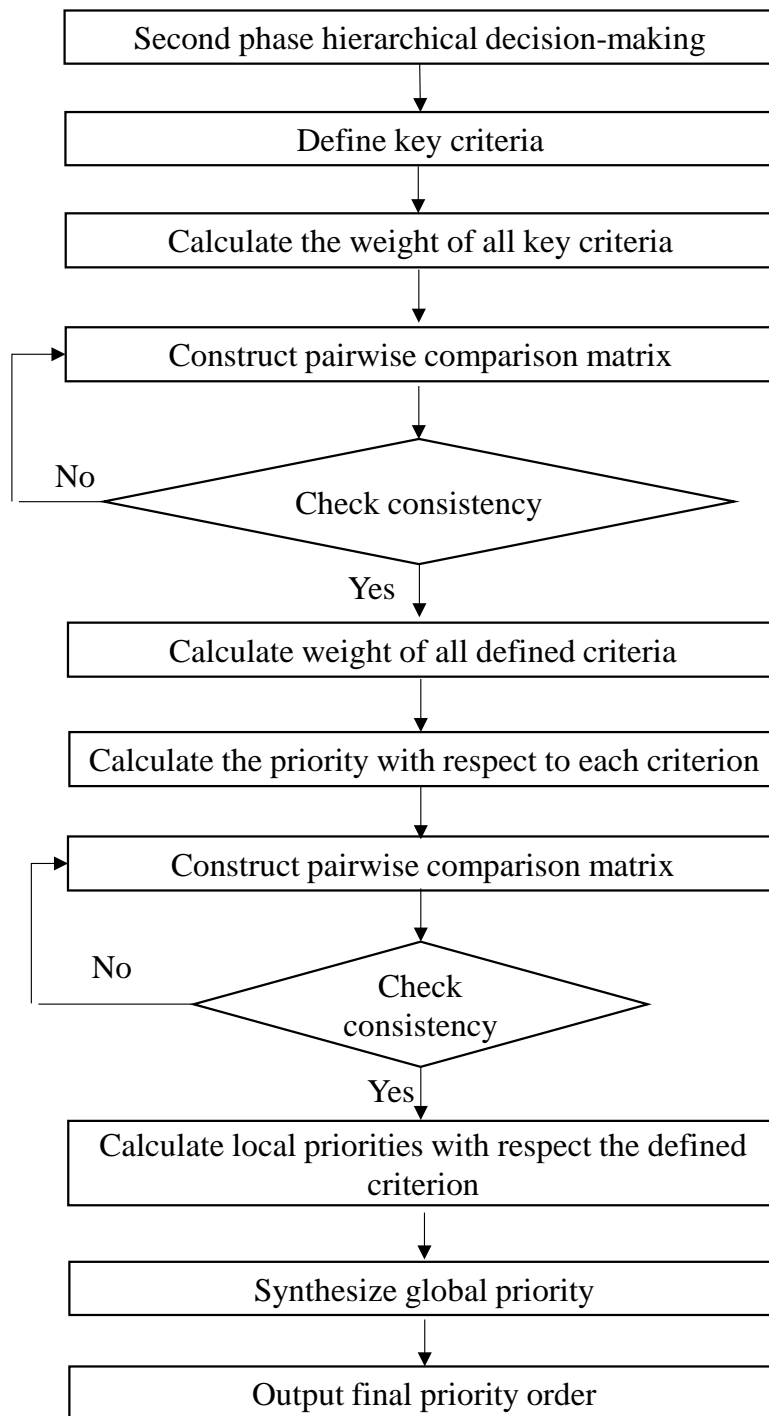


Figure 3.6. General scheme of AHP based prioritization process.

Given that the number of key criteria is m and the total number of options to compare is n , the pairwise comparison matrix A with respect to the selected criterion will be a $n \times n$ square matrix. For k -th criterion, the reciprocal matrix A for prioritizing n alternatives can be denoted as:

$$A_k = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix}_k ; k \in [1, m] \quad (3.23)$$

where

$$a_{ij} = W_i / W_j \quad i = 1, 2, \dots, n \quad (3.24)$$

$$a_{ij} = 1 / a_{ji} \quad i = 1, 2, \dots, n; \quad j = 1, 2, \dots, n \quad (3.25)$$

$$a_{ij} = 1 \text{ if } i = j \quad (3.26)$$

It is comprehensible that inconsistency might exist in matrix A due to the pairwise comparison among a large number n . Therefore, it is critical to quantify how consistent the judgements have been relative to large samples of purely random judgements in order to obtain a convincing result. In AHP method, Consistency Ratio (CR) is designed to measure the consistency level of the judgements.

$$CR = \frac{CI}{RI} \quad (3.27)$$

In Eq. (3.27), CI and RI are the Consistency Index and Random Index respectively.

CI can be expressed as:

$$CI = \frac{\lambda_{\max} - n}{n - 1} \quad (3.28)$$

where λ_{\max} is the maximal eigenvalue of matrix A .

The Random Index (RI) is an experimental value which depends on the total number of alternatives n . Table 3.2 shows the RI values with respect to different n values.

The pairwise comparison matrix A can be considered having an acceptable consistency if the value of CR obtained from Eq. (3.27) is less than a threshold value. Matrix A can then be used to derive meaningful priorities. If CR exceeds the threshold value, the judgments in matrix A are untrustworthy because they are too close for comfort to randomness and the exercise is valueless and reconstruction of matrix A will be required. In general, the value of threshold is defined as 0.1. However, it may vary with respect to n .

Table 3.2. Random Index.

M	2	3	4	5	6	7	8	9	10
RI	0	0.58	0.90	1.12	1.24	1.32	1.41	1.45	1.51

After the verification of consistency, priority order can then be calculated consequently. To obtain the local priority of the n options under k -th criterion, pairwise comparison matrix A must be normalized, that is:

$$\bar{A}_k = \begin{bmatrix} \bar{a}_{11} & \bar{a}_{12} & \cdots & \bar{a}_{1n} \\ \bar{a}_{21} & \bar{a}_{22} & \cdots & \bar{a}_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ \bar{a}_{n1} & \bar{a}_{n2} & \cdots & \bar{a}_{nn} \end{bmatrix}_k \quad (3.29)$$

where

$$\bar{a}_{ij} = \frac{a_{ij}}{\sum_{l=1}^n a_{lj}} ; i = 1, 2, \dots, n \quad (3.30)$$

The local priority order under k -th criterion can be calculated as:

$$P_k = \begin{bmatrix} p_1 \\ p_2 \\ \vdots \\ p_n \end{bmatrix}_k \quad (3.31)$$

where

$$p_i = \frac{\sum_{l=1}^n \bar{a}_{il}}{n} \quad i = 1, 2, \dots, n \quad (3.32)$$

Given that the total number of defined criteria is m , there are m local priority matrix obtained based on Eq. (3.31). These priorities represent the priorities of options in the same level of the hierarchy. The overall local priorities matrix $\hat{P} = [P_1, P_2, \dots, P_m]$ can be easily formed:

$$\hat{P} = \begin{bmatrix} p_{11} & p_{12} & \cdots & p_{1m} \\ p_{21} & p_{22} & \cdots & p_{2m} \\ \vdots & \vdots & \vdots & \vdots \\ p_{n1} & p_{n2} & \cdots & p_{nm} \end{bmatrix} \quad (3.33)$$

It is known that there are m criteria compared using Saaty's 1-to-9 scale. A pairwise comparison matrix of criteria C is obtained based on the decision maker's judgement. The formation of matrix C follows the rules in generating matrix A .

$$C = \begin{bmatrix} c_{11} & c_{12} & \cdots & c_{1m} \\ c_{21} & c_{22} & \cdots & c_{2m} \\ \vdots & \vdots & \vdots & \vdots \\ c_{m1} & c_{m2} & \cdots & c_{mm} \end{bmatrix} \quad (3.34)$$

where

$$c_{ij} = W_{c,i} / W_{c,j} \quad i = 1, 2, \dots, m; \quad j = 1, 2, \dots, m \quad (3.35)$$

$$c_{ij} = 1 / c_{ji} \quad i = 1, 2, \dots, m; \quad j = 1, 2, \dots, m \quad (3.36)$$

$$c_{ij} = 1 \text{ if } i = j \quad (3.37)$$

After the validation of the consistency of judgements using the procedure shown in Eqs. (3.27) and (3.28), the weighting factor matrix W for the m criteria can then be calculated by following the method in Eqs. (3.29)-(3.32):

$$W = [w_1 \quad w_2 \quad \cdots \quad w_m] \quad (3.38)$$

The local priorities are synthesized across all criteria determined at the top level of hierarchy in order to calculate the global priority of all options. The global priority order of n options can be obtained based on the following integration:

$$P_i = \hat{P} \times W \quad (3.39)$$

3.3.2 Identification of Second Phase Decision-making Strategy

The global priority order shown in matrix P_i provides a clear order of effort for the second phase of LCBDM. The second phase decision-making task is to consecutively examine and identify the most cost-effective sustainability improvement strategy based on the generated priority order. For the stage with highest order in the global priority matrix, the objective is to achieve the adjusted sustainability improvement setting with minimum

cost. Ideally, the strategy of sustainability improvement for the consequent stages can be achieve in the same manner. Note that the limited amount of total budget may not be sufficient to achieve the goal of sustainable development for all life cycle stage. The available amount of budget for next improvement action must be evaluated after the preceding improvement analysis. There are two distinct solution determining approaches in this section: (1) minimum cost solution; (2) maximum enhancement solution.

The first method is based on the fact that the available budget for sustainability improvement is sufficient for current stage. Therefore, the objective can be described as follows:

$$\min_{y_{i,1}, y_{i,2}, \dots, y_{i, \hat{N}_i}} B_i(\hat{T}) = \min \left(\sum_{j=1}^M y_j(s_i) B(T_j) \right) \quad (3.40)$$

The constraints for goal driven optimization are listed as follows:

$$y_{i,j} = \begin{cases} 1 & j\text{-th technology is selected} \\ 0 & j\text{-th technology is not selected} \end{cases} \quad j = 1, 2, \dots, M \quad (3.41)$$

$$\hat{E}_i(\hat{T}) \geq \hat{E}_i^G \quad (3.41)$$

$$\hat{V}_i(\hat{T}) \geq \hat{V}_i^G \quad (3.43)$$

$$\hat{L}_i(\hat{T}) \geq \hat{L}_i^G \quad (3.44)$$

$$S_i(\hat{T}) \geq S_i^G \quad (3.45)$$

$$\sum_{j=1}^{\hat{N}_i} y_{i,j} B_i(T_j) \leq B_{\text{lim}} \quad (3.46)$$

where $y_{i,j}$ is the decision variable; \hat{E}_i^G , \hat{V}_i^G , \hat{L}_i^G , and S_i^G are the pre-defined goals for economic, environmental, social, and overall sustainability respectively; $\hat{E}_i(\hat{T})$, $\hat{V}_i(\hat{T})$, $\hat{L}_i(\hat{T})$, and $S_i(\hat{T})$ are the performance of economic, environmental, social, and overall sustainability after implementing technology set \hat{T} respectively.

The second approach is applicable when the available budget cannot guarantee to use the most cost-effective solution to achieve the pre-defined goals which also means no solution can be found in minimum cost optimization. Therefore, the objective in this optimizing procedure is can be described as follows:

$$\max_{y_{i,1}, y_{i,2}, \dots, y_{i, \hat{N}_i}} S_i(\hat{T}) = \max \left(\frac{\|(\alpha \hat{E}_i(\hat{T}), \beta \hat{V}_i(\hat{T}), \gamma \hat{L}_i(\hat{T}))\|}{\|(\alpha, \beta, \gamma)\|} \right) \quad (3.47)$$

The constraints for budget driven optimization are listed as follows:

$$y_{i,j} = \begin{cases} 1 & j\text{-th technology is selected} \\ 0 & j\text{-th technology is not selected} \end{cases} \quad j = 1, 2, \dots, M \quad (3.48)$$

$$\sum_{j=1}^{\hat{N}_i} y_{i,j} B_i(T_j) \leq B_{\text{lim}} \quad (3.49)$$

$$\hat{E}_i(\hat{T}) \geq \hat{E}_i^{\min} \quad (3.50)$$

$$\hat{V}_i(\hat{T}) \geq \hat{V}_i^{\min} \quad (3.51)$$

$$\hat{L}_i(\hat{T}) \geq \hat{L}_i^{\min} \quad (3.52)$$

$$S_i(\hat{T}) \geq S_i^{\min} \quad (3.53)$$

where $y_{i,j}$ is the decision variable; B_{lim} is the budget limit; \hat{E}_i^{min} , \hat{V}_i^{min} , \hat{L}_i^{min} , and S_i^{min} are the minimum acceptable values of economic, environmental, social, and overall sustainability respectively; $\hat{E}_i(\hat{T})$, $\hat{V}_i(\hat{T})$, $\hat{L}_i(\hat{T})$, and $S_i(\hat{T})$ are the performance of economic, environmental, social, and overall sustainability after implementing technology set \hat{T} respectively.

In the second stage, the solution identification procedure is shown in Figure 3.7. The first step is to define the targeting life cycle stage according to the priority order. Secondly, cost-effective solution can be obtained based on first optimizing approach. The minimum budget to achieve the adjusted goal can then be compared to the available budget limit which is evaluated after every improvement action. This sustainability improvement strategy is valid only if the budget constraint is satisfied. Otherwise, the optimal strategy can only be calculated based on second optimizing approach. In the end, a complete strategy for second phase decision-making can be identified using Monte Carlo optimization.

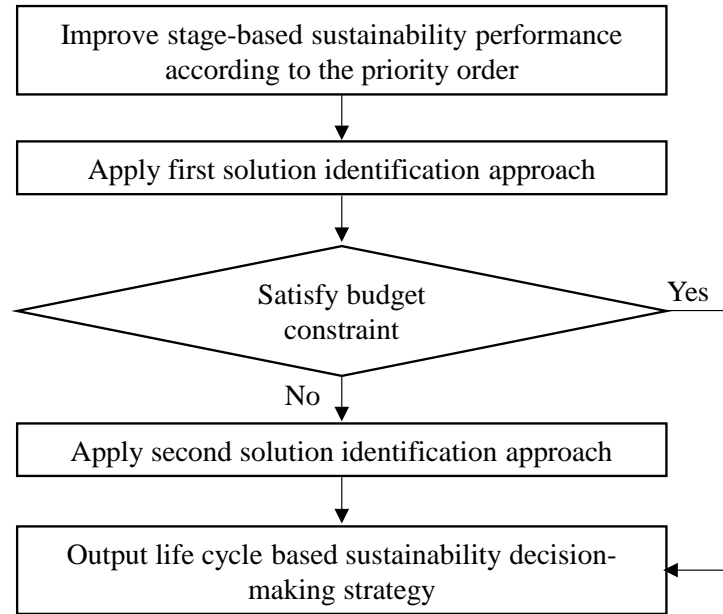


Figure 3.7. Solution identification procedure in second phase decision-making.

3.4 LCBDM Framework

To identify the superior strategy for life cycle based sustainability improvement, a consecutive procedure with two phases is introduced in Figure 3.8 which depicts the overall framework of LCBDM. The task of LCBDM can be addressed after executing the procedure for decision-making.

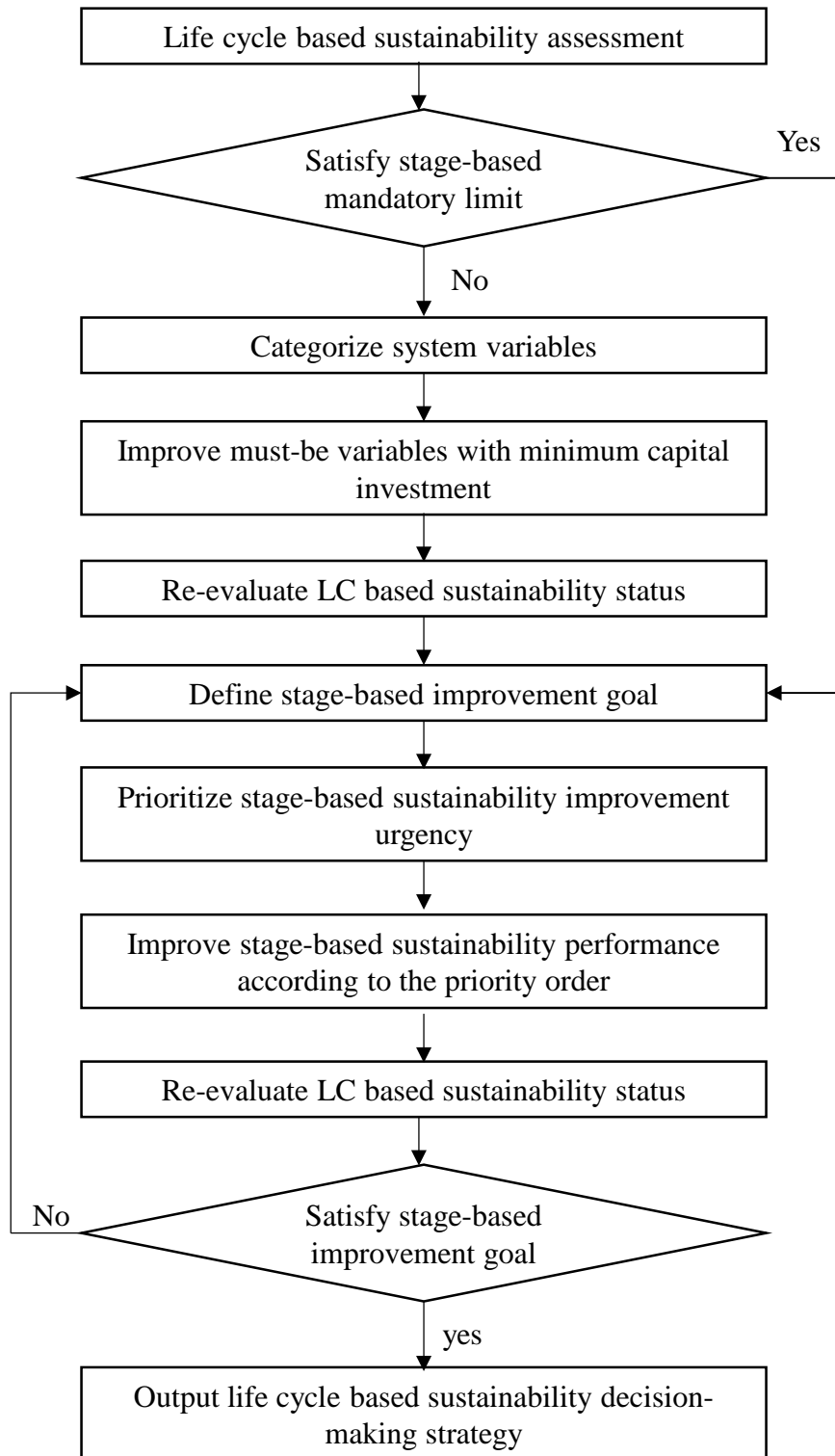


Figure 3.8. LCBDM framework.

3.5 Case Study

In this chapter, the case study of automotive nanopaint materials mentioned in Chapter 2 was selected to demonstrate the LCBDM framework. As shown in Figure 2.3, the life cycle of nanocoating technology is divided into five stages: (1) automotive nanocoating manufacturing process, (2) paint spray process, (3) coating curing process, (4) use and maintenance, and (5) end of use. This case study only considers the first three stages which are account for nanopaint film development and the available budget is set at $\$4.0 \times 10^6$.

3.5.1 Identification of Must-be Variables

In this section, the system variables in must-be group are determined based on the mandatory limits from all of the involved people, community, and organizations. In stage 1, it is required that no more than 3% of total amount of nanoparticles is being released to the manufacturing environment. In stage 2, annual VOC emission from the spraying process cannot exceed 2.46×10^4 kg which is equivalent to 0.8 kg/job. There is no must-be variable in stage 3. Table 3.3 illustrates the selected variables and their mandatory boundaries. The two must-be variables are also the direct indicators of V3 in the sustainability metrics system of stage 1 and V2 in the sustainability metrics system of stage 2. Thus, the goal of first phase decision making can be converted to the performance improvement of these two categories. Based on the normalization process shown in Chapter 2, the performance of indicator V3 for stage 1 must be improved from 0.17 to 0.42 while the performance of indicator V2 for stage 2 must achieve 0.66 from 0.6.

Table 3.3. Must-be variables in each individual life cycle stage.

Life cycle stage	Must-be variable	Current status	Mandatory boundary
Stage 1	The quantity of nanoparticles released to the environment	5%	$\leq 3.5\%$
Stage 2	VOC emission	0.9 kg/job	≤ 0.84 kg/job
Stage 3	None	---	---

3.5.2 Evaluation of Technology Candidates

It is comprehensible that applying effective technology or process modification could achieve the objective of sustainability improvement directly. In this work, a variety of technology candidates are identified as decision candidates for sustainability improvement at each stage and overall life cycle.

For stage 1, the selected technology candidates are:

$T_{1,1}$: Smart mixing agitator for mixing process. This technology could adjust the agitator operation to the desired paint quality including viscosity and nanoparticle dispersity with respect to the change in the batch production.

$T_{1,2}$: Advanced sealing system. The goal of this technology is to prevent excess volatile organic solvent, monomer, additives, and nanoparticle from being released to the working environment and preserve a certain amount of raw materials to improve material efficiency.

$T_{1,3}$: Air ventilation system. This technology aims at reducing any hazardous chemicals during the production through carrying them to the outside by high speed air flow.

$T_{1,4}$: Waste recycling unit. This technology intends to collect the wasted solid content during the batch production and reuse it.

Table 3.4, 3.5, and 3.6 shows the immediate effect on system variables and sustainability, the normalized improvement of categorized sustainability indices, and the capital cost of the technology candidates, respectively.

Table 3.4. The effect of technologies on indicator related system variables (stage 1).

Category	Indicator	Current value	T _{1,1}	T _{1,2}	T _{1,3}	T _{1,4}
Economic sustainability	E1 (\$/kg)	4.72	4.55	4.62	4.7	4.3
	E2 (\$/kg)	0.65	0.6	0.62	0.64	0.56
Environmental sustainability	V1 (kWh/kg)	5.9	5.45	5.63	5.81	4.66
	V2 (kg/kg)	0.5	0.48	0.47	0.48	0.46
	V3 (%)	5	4.2	3.5	4	3.8
	V4	0.7	0.66	0.4	0.45	0.55
Social sustainability	L1	0.75	0.81	0.78	0.8	0.8
	L2	0.35	0.42	0.55	0.59	0.38

Table 3.5. Normalized improvement of categorized sustainability indicators (stage 1).

Category	Indicator	T _{1,1}	T _{1,2}	T _{1,3}	T _{1,4}
Economic sustainability	E1	0.05	0.03	0.01	0.11
	E2	0.10	0.06	0.02	0.18
Environmental sustainability	V1	0.09	0.06	0.02	0.26
	V2	0.06	0.09	0.06	0.11
	V3	0.13	0.25	0.17	0.20
	V4	0.04	0.30	0.25	0.15
Social sustainability	L1	0.12	0.06	0.10	0.10
	L2	0.08	0.22	0.27	0.03

Table 3.6 Capital cost of technology candidates for stage 1.

Technology	T1,1	T1,2	T1,3	T1,4
Capital cost ($\times 10^5$ \$)	5.4	7.1	6.9	7.4

For stage 2, the selected technology candidates and their immediate effect on system variables are:

*T*_{2,1}: New air ventilation system. This technology could dramatically reduce the amount of undesirable VOC, nanoparticle and excess paint droplets in the spray booth by controlling the air flow speed.

*T*_{2,2}: Sludge treatment unit. The VOC content and nanoparticles aggregated in the sludge can be collected and treated by this unit. It could substantially reduce the quantity of hazardous materials emitted to the environment. In the meanwhile, the treatment of VOC content using RTO unit could provide additional energy to the manufacturing process.

*T*_{2,3}: Advanced robotic spray system. This new robotic spray system could control the flying path of paint droplets and generate an even spray pattern which forms a wet film with uniform thickness.

Table 3.7, 3.8, and 3.9 shows the immediate effect on system variables and sustainability, the normalized improvement of categorized sustainability indices, and the capital cost of the technology candidates, respectively.

Table 3.7. The effect of technologies on indicator related system variables (stage 2).

Category	Indicator	Current value	T _{2,1}	T _{2,2}	T _{2,3}
Economic sustainability	E1 (%)	75	76	76	80
	E2 (\$/vehicle)	5.4	5.3	5.26	5.25
Environmental sustainability	V1 (kWh/vehicle)	49.1	48.2	47.83	47.74
	V2 (kg/vehicle)	0.9	0.87	0.82	0.8
	V3 ($\times 10^{12}$ per m ³)	2.3	1.9	2.2	1.9
	V4 (%)	0.02	1.5	1.5	1.6
Social sustainability	L1	0.7	0.75	0.72	0.82
	L2	0.6	0.65	0.62	0.76

Table 3.8. Normalized improvement of categorized sustainability indicators (stage 2).

Category	Indicator	T _{2,1}	T _{2,2}	T _{2,3}
Economic sustainability	E1	0.03	0.03	0.14
	E2	0.08	0.11	0.12
Environmental sustainability	V1	0.08	0.11	0.11
	V2	0.03	0.08	0.10
	V3	0.11	0.03	0.11
	V4	0.10	0.10	0.08
Social sustainability	L1	0.06	0.03	0.15
	L2	0.06	0.02	0.18

Table 3.9. Capital cost of technology candidates for stage 2.

Technology	T _{2,1}	T _{2,2}	T _{2,3}
Capital cost ($\times 10^5$ \$)	6.7	5.5	7.4

For stage 3, 3 technology candidates and their immediate effect on system variables are:

*T*_{3,1}: Energy efficient heating material. This technology aims at replacing current ceramic heating strip inside of the radiation heating oven by energy efficient heating strips which could generate more heat comparing to the traditional baking oven.

*T*_{3,2}: Hot air recycling system. During coating curing, the majority of the hot air is being purged to the ambient environment. This technology could reuse a certain amount of hot air for the convection heating zone to save heating energy without affecting the solvent removal speed.

*T*_{3,3}: VOC RTO unit. One of the major tasks in coating curing process is the removal of VOC content in the coating film. The VOC content, if not being well managed, could lead to a serious environmental impact after being released to the natural environment. The addition of RTO unit could not only effectively control the VOC emission but also generate a certain amount of heating energy to compensate the energy loss.

Table 3.10, 3.11, and 3.12 shows the immediate effect on system variables and sustainability, the normalized improvement of categorized sustainability indices, and the capital cost of the technology candidates, respectively.

Table 3.10. The effect of technologies on indicator related system variables (stage 3).

Category	Indicator	Current value	T _{3,1}	T _{3,2}	T _{3,3}
Economic sustainability	E1 (\$/vehicle)	7.7	7.62	7.45	7.5
Environmental sustainability	V1 (kWh/vehicle)	70	69	67	68
	V2	0.01	0.01	0.01	0.01
Social sustainability	L1	1.4	1.42	1.43	1.45
	L2	0.9	0.91	0.92	0.92

Table 3.11. Normalized improvement of categorized sustainability indicators (stage 3).

Category	Indicator	T _{3,1}	T _{3,2}	T _{3,3}
Economic sustainability	E1	0.04	0.13	0.10
Environmental sustainability	V1	0.05	0.15	0.10
	V2	0.00	0.00	0.00
Social sustainability	L1	0.03	0.04	0.07
	L2	0.11	0.27	0.27

Table 3.12 Capital cost of technology candidates for stage 3.

Technology	T _{3,1}	T _{3,2}	T _{3,3}
Capital cost ($\times 10^5$ \$)	4.8	8.9	6.5

3.5.3 First Phase Decision Making

The analysis of LCBDM fundamentals elaborates that enhancement of must-be variables receives the highest improvement priority. Thus, the must-be variables and their mandatory boundaries shown Table 3.3 are the constraints for searching cost-effective

solution for sustainability improvement. For stage 1, the optimal decision must be able to reduce the quantity of nanoparticles released to the environment from 5% to no more than 3.5%. The best option for stage 2 could render a significant decrease of VOC emission from 0.9 kg/job to no more than 0.84 kg/job.

The optimal solution for stage 1 and 2 can be determined by the optimization process introduced in Eqs. (3.17)-(3.22), that is, implementation of technology $T_{1,2}$ for stage 1 and technology $T_{2,2}$ for stage 2. It is worth noting that the stage-based sustainability status must be re-evaluated for further analysis. Based on the defined sustainability metrics system shown in Chapter 2, the improved sustainability status for stage 1 and stage 2 are listed in Table 3.13. Consequently, the available budget for second phase decision making is reduced to \$ 2.74×10^6 .

Table 3.13. Sustainability performance of stage 1 and stage 2 after the application of first phase decisions.

Life cycle stage	Sustainability category	Current status
Stage 1	Economic	0.53
	Environmental	0.59
	Social	0.53
	Overall	0.55
Stage 2	Economic	0.62
	Environmental	0.61
	Social	0.61
	Overall	0.61

3.5.4 AHP Based Prioritization

The second phase decision making is to prioritize the sustainability improvement effort throughout the life cycle of the product. Given that decision makers at two levels (stage-based decision maker and life cycle decision maker) are involved in a complex decision making process in a hierarchical structure, the prioritization task must take into account all of the key factors. Based on pairwise comparison judgments, AHP based prioritization could integrate both the relative importance of criteria and stage-based sustainability preference measures into a single overall score for ranking decision order.

With the establishment of the prioritization goal, it is important to elicit pairwise comparison judgments of the evaluation criteria. In this work, three key criteria are selected to demonstrate the prioritization: improvement urgency (C1), enhancement easiness (C2), and resource availability (C3). After arranging the evaluation criteria into a matrix, judgments about their relative importance with respect to the overall goal are elicited by the brainstorm process of decision makers at two levels (Column 2-4 in Table 3.14). The pairwise comparison process is subjective and requires lots of consideration and trade-offs among many involved organizations. Therefore, the actual comparison process is not covered in this study.

Table 3.14. Pairwise comparisons of evaluation criteria.

	C1	C2	C3
C1	1	5	3
C2	1/5	1	1/3
C3	1/3	3	1

To make sure the consistency of the pairwise comparison, λ_{\max} , CI and RI are identified as 3.055, 0.028 and 0.58. Therefore, the consistency ratio (CR) can be obtained as 0.05 based on Eq. (3.27). Comparing to the preset limit 0.1, this consistency ratio indicates that the pairwise comparison of evaluation criteria is consistent. Based on the comparison data mentioned above, the weighting factor matrix that denotes the importance of the three criteria can be determined as:

$$W = [0.63 \quad 0.11 \quad 0.26]$$

Next pairwise comparisons of the sustainability improvement are determined. Each stage-based sustainability status is compared pairwise with respect to how much better one is than the other in satisfying each evaluation criteria. The comparison results with respect to three criteria are listed in Table 3.15, Table 3.16 and Table 3.17. The consistency assessment illustrates that the values of CR with respect to three different criteria are 0.04, 0.08 and 0.04 respectively. Therefore, the pairwise comparisons are valid and can be used toward further calculation. Based on the Eqs. (3.29)-(3.33), the overall local priority matrix can be calculated as:

$$\hat{P} = \begin{bmatrix} 0.67 & 0.28 & 0.27 \\ 0.27 & 0.07 & 0.67 \\ 0.06 & 0.64 & 0.06 \end{bmatrix}$$

Table 3.15. Pairwise comparisons of stage based sustainability performance based evaluation criterion C1.

	Stage 1	Stage 2	Stage 3
Stage 1	1	3	9
Stage 2	1/3	1	5
Stage 3	1/9	1/5	1

Table 3.16. Pairwise comparisons of stage based sustainability performance based evaluation criterion C2.

	Stage 1	Stage 2	Stage 3
Stage 1	1	5	1/3
Stage 2	1/5	1	1/7
Stage 3	3	7	1

Table 3.17. Pairwise comparisons of stage based sustainability performance based evaluation criterion C3.

	Stage 1	Stage 2	Stage 3
Stage 1	1	1/3	5
Stage 2	3	1	9
Stage 3	1/5	1/9	1

Based on the evaluation of key criteria and the corresponding local priority matrix, the global priority for the order of life cycle based decision making can be established by applying Eq. (3.39). The final priority order is:

$$P_i = [0.52 \quad 0.35 \quad 0.12]$$

3.5.5 Second Phase Decision-making

The priority analysis clearly describes the order of sustainability improvement effort. Stage 1 has the highest order, followed by stage 2 and then stage 3. Thus, the selection of sustainability improvement strategy can then be identified accordingly to fulfill the requirement of budget and improvement goal. Note that the stage-based sustainability improvement goal must be evaluated and approved by the life cycle level decision makers and stage-based decision makers to ensure the goal rationality. In this case, the sustainability improvement goals for three stages are described in Table 3.18. This study only focuses on the improvement of categorized sustainability status and overall sustainability performance of each stage rather than the more detailed sub-categorized indicators. It is worth noting that a more detailed improvement plan would be necessary for a practical project when sufficient data and accurate evaluation are available.

Table 3.18. The preset goal of sustainability improvement throughout the life cycle.

Life cycle stage	Sustainability category	Current status	Development goal
Stage 1	Economic	0.53	0.62
	Environmental	0.61	0.76
	Social	0.53	0.80
	Overall	0.56	0.73
Stage 2	Economic	0.62	0.68
	Environmental	0.61	0.67
	Social	0.61	0.66
	Overall	0.61	0.67
Stage 3	Economic	0.83	0.94
	Environmental	0.71	0.77
	Social	0.56	0.64
	Overall	0.70	0.79

The identification of improvement based minimum cost solution is applied to stage due to its highest priority order. Based on the predefined sustainability improvement goal for stage 1, Eqs. (3.40)-(3.45) are utilized to render the optimal solution to achieve the objective of sustainable development. By implementing technology set $T_{1,1}$ and $T_{1,3}$, the sustainability status of stage 1 can be increased from 0.56 to 0.75 with the capital cost of $\$1.23 \times 10^6$ which is below the total cost limit. Therefore, this sustainable development strategy is valid.

For stage 2, the available budget for sustainability improvement is $\$1.51 \times 10^6$. Based on the analysis of improvement based minimum cost solution, the effective approach is technology $T_{2,3}$ with the cost at $\$7.4 \times 10^5$. Comparing to the available budget, this approach could help stage reach the sustainability improvement goal within the budget limit.

Given that the accessible budget left for stage is only $\$7.7 \times 10^5$, the first analyzing approach, improvement based minimum cost solution, is applied to determine the effective path of sustainable development for stage 3. The optimal method of implementing technology $T_{3,2}$ requires the cost of $\$ 8.9 \times 10^5$ which is much higher than the available resources. Therefore, the second method to search for budget based maximum enhancement solution is applied to stage 3. Technology $T_{3,3}$ is the best option for stage 3 by taking into account of the budget limit.

Table 3.19 summarizes the detailed decisions for life cycle based sustainability improvement based on the comprehensive analysis. Stage 1 and stage 2 could achieve the pre-defined sustainability improvement goal while stage 3 could receive the best sustainability improvement effort within the budget limit. Figure 3.9 describes the effect before and after the selected life cycle based decisions.

Table 3.19. Decisions for life cycle based sustainability improvement.

Life cycle stage	Sustainability status		Optimal strategy for stage-based sustainability improvement
	Category	Performance	
Stage 1	Economic	0.62	First phase: $T_{1,2}$ Second phase: $T_{1,1}$ and $T_{1,3}$
	Environmental	0.80	
	Social	0.81	
	Overall	0.75	
Stage 2	Economic	0.68	First phase: $T_{2,2}$ Second phase: $T_{2,3}$
	Environmental	0.69	
	Social	0.67	
	Overall	0.68	
Stage 3	Economic	0.93	First phase: None Second phase: $T_{3,3}$
	Environmental	0.76	
	Social	0.73	
	Overall	0.81	

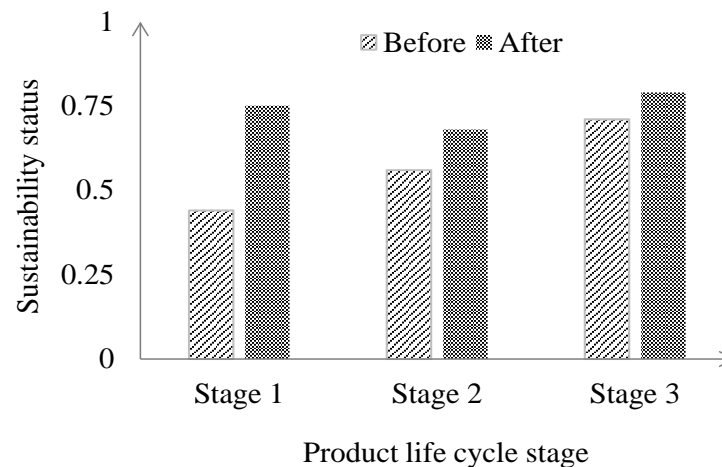


Figure 3.9. The sustainability status before and after the selected life cycle based decisions.

3.6 Conclusion

In response to the proposed framework of life cycle based sustainability assessment, the concept of life cycle based decision making for sustainable development is essential to promote the sustainability study to a much broader field. The significance of this study is to establish an effective methodology to assist the new decision-making need.

In investigating the need of decision-making at the life cycle level, we establish a two-phase decision-making procedures for identifying the most urgent sustainability improvement issues and proper manners for sustainable development. The first phase is to identify the must-be system variables in each individual life cycle stage and apply effective strategies to fulfill corresponding limits. The second phase is to prioritize the sustainability improvement for each life cycle stage and determine the best sustainability improvement effort with respect to the predefined sustainability goal consequently. Analytic Hierarchical Process plays the major role in the prioritization process with three distinct evaluating criteria.

With the introduced 10 technology candidates for the first three life cycle stages, the analyzing results show that implementation of technology $T_{1,2}$ for stage 1 and technology $T_{2,2}$ for stage 2 could satisfy the constraints of must-be variables. Technology set $T_{1,1}$ and $T_{1,3}$, and technology $T_{2,3}$ could help decision makers to achieve the predefined sustainability goals while technology $T_{3,3}$ is the best option for stage 3 by taking into account of the budget limit.

CHAPTER 4 MULTISCALE MODELING AND OPTIMIZATION OF NANOCLEARCOAT CURING FOR ENERGY EFFICIENT AND QUALITY ASSURED COATING MANUFACTURING

Clearcoat is a top layer of coating on vehicle surface. It protects the underlying coating layers from chemical corrosion, UV degradation, and mechanical damage (Seubert *et al.*, 2012). Owing to the increasing demand on high-performance coatings, nanopaint-based clearcoat has drawn great attention. Nanopaint is a type of nanocomposite material that incorporates organo-modified inorganic nanoparticles into a conventional thermoset polymeric resin. This type of coating material, if applied properly, can provide superior coating performance, such as anti-scratch, self-cleaning, self-healing, etc (Ajayan *et al.*, 2006; Nobel *et al.*, 2007; Pissis and Kotsilkova, 2007). A significant improvement of barrier properties compared to conventional polymeric coatings was also reported (Xiao *et al.*, 2010). Nanopaint could become a dominant automotive coating material in the near future.

Application of nanoclearcoat encounters a number of manufacturing challenges in spite of the promising coating features. Clearcoat curing is a critical manufacturing step in achieving expected high coating performance. This renders a need to investigate in depth nanoclearcoat curing fundamentals. A key technical concern is the curing environment that determines product quality. In curing, the presence of nanoparticles in paint could slow down solvent evaporation from the surface of a thin wet film, as the dissolved solvent in paint takes a tortuous path to reach the film surface. Cross-linking reactions taken place in the film is also affected by the nanoparticles both at the microscale and macroscale. Zhou *et al.* stated that inappropriate addition of nanoparticles could lead to an adverse impact on polymer network evolution (Zhou *et al.*, 2005). A natural question is whether a conventional

coating drying system can be used to cure nanoclearcoat to achieve its anticipated quality performance, and if so, how to adjust curing operational settings, especially when the size, shape, and volume fraction of nanoparticles in paint vary.

From the perspective of industrial manufacturing sustainability, the sustainability performance of nanoclearcoat curing process could substantially affect the overall industrial sustainability. Thus, it is essential to analyze the sustainability concerns of curing process by integrating process characterization and systematic sustainability assessment together. Due to the fact that there is a lack of data regarding the nanoclearcoat curing process, the investigation of process dynamics and product quality can be established by the multistage process modeling. Therefore, it is of great importance to investigate the process dynamics and product performance during material evolution.

A number of theoretical studies on the drying of polymer solution have been reported, which demand various types of physico-chemical property information for modeling (Alsoy and Duda, 1999; Price and Cairncross, 2000; Domnick *et al.*, 2011). Lou and Huang introduced an integrated macroscale modeling approach to investigate the dynamics of conventional clearcoat curing (Lou and Huang, 2000). Xiao *et al.* described a Monte Carlo simulation method to study polymer network formation at microscale (Xiao and Huang, 2009). Zhou *et al.* studied product formation processes, which improved the understanding of the correlation between material dynamics and product and process performance (Zhou *et al.*, 2013). It is known that coating defects could occur during curing if the operational setting is inappropriate. Price and Cairncross discovered that solvent residual in coating may lead to the generation of blisters if the coating temperature exceeds the bubble point (Price

and Cairncross, 2000). Domnick *et al.* introduced a statistical model to study the relationship between the pinhole density and the operational settings (such as oven temperature gradient and convection air velocity) (Domnick *et al.*, 2011). Integration of macroscopic process dynamics with product realization at the finer scales can deepen the understanding of nanocoating formation and thus help identify the most suitable strategy for nanocoating curing.

In this work, we introduce an integrated multiscale modeling and dynamic analysis method to study nanocoat curing. It aims at establishing quantitative correlation among coating material parameters, product quality, and process energy consumption. A general product quality and process efficiency analysis method will be also introduced. An optimization approach is then presented for deriving an optimal operational setting to minimize energy consumption while ensuring process and product quality. A comprehensive case study is presented to elaborate the process characterization and sustainability related study.

4.1 Objectives of Multiscale Product and Process Modeling

Clearcoat curing is a sophisticated, energy intensive operation in the automotive coating manufacturing industry. It becomes more challenging when the clearcoat is nanoparticles incorporated, as it is not fully understood how the nanoparticles and the polymer matrix interact in the coating layer during curing in a coating manufacturing. Curing oven is a usual manufacturing facility that is designed to have a number of operational zones, with the first one or two zones for radiation and convection based drying, and the rest four to five zones for convection based curing where polymeric reactions take

place. In production, vehicle bodies covered by a wet topcoat layer are moved by a conveyor one by one through a curing oven at a constant speed. In operation, four types of phenomena occur simultaneously, which are depicted in Figure 4.1. These include: (i) heat transfer within the coating film and with the drying environment, (ii) mass transfer of solvent within the film and its evaporation at the film surface, (iii) cross-linking reaction that leads to the formation of a nanoparticle-incorporated polymeric network, and (iv) film thickness change mainly due to solvent removal. In study, a macroscopic process model is needed to characterize the heating environment; at the meso-scale, solvent removal associated with film thickness change should be characterized; the cross-linking reaction and polymer network formation can be described by microscale models.

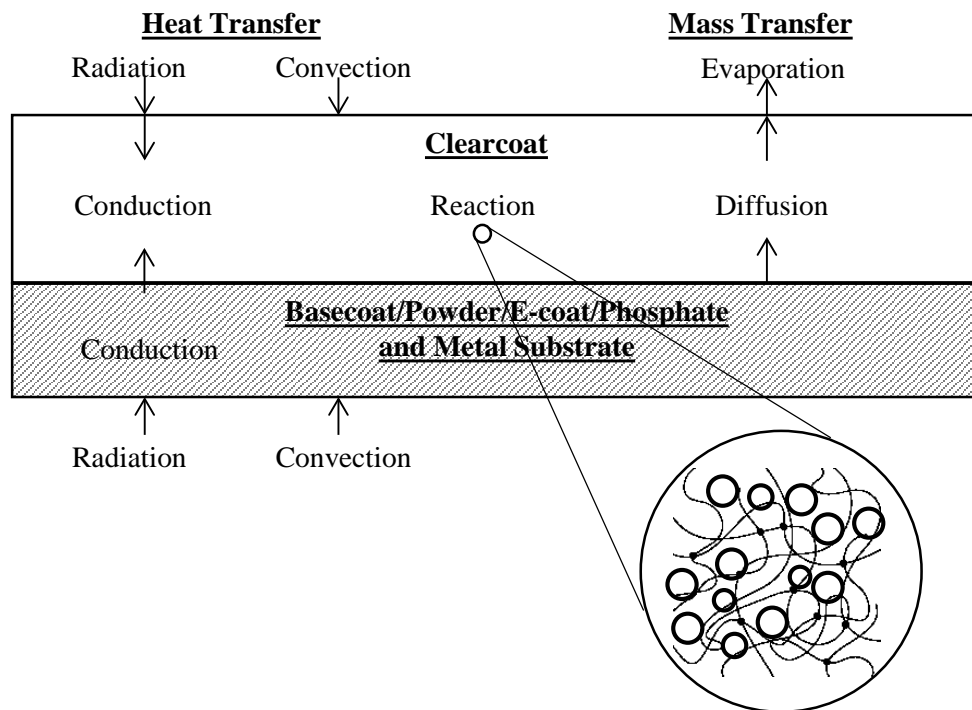


Figure 4.1. Transport phenomena and reaction occurred in the coating film during curing (Song and Huang, 2016).

4.2 Drying of Wet Coating Film

As stated, a curing oven usually is divided into a number of zones where heating mechanisms and operational settings are set differently. It is known that the amount of energy consumed for drying a nanoclearcoat on vehicle panels is significantly less than that for heating the substrate. It can be safely assumed that the temperature difference between the substrate and the coating layer is negligible throughout the curing process, as the Biot number in the heat transfer process is very small (Dickie *et al.*, 1997). Lou and Huang introduced a coating heating model for convention paint drying (Lou and Huang, 2000). It can be used to characterize nanocoating drying. The lumped parameter model is presented below.

$$\frac{dT(t)}{dt} = \begin{cases} \frac{\sigma \varepsilon}{\rho_m C_{pm} Z_m} (T_w^4 - T(t)^4) + \frac{h_v}{\rho_m C_{pm} Z_m} (T_a - T(t)), & \text{Radiation zone} \\ \frac{h_v}{\rho_m C_{pm} Z_m} (T_a - T(t)), & \text{Convection only zone} \end{cases} \quad (4.1)$$

where $T(t)$ is the temperature of the nanocoating film; T_w and T_a are the temperature of the oven wall and that of the convection air, respectively; ρ_m , C_p , and Z_m are the density, the heat capacity and the thickness of vehicle panels, respectively; σ and ε are the Stefan Boltzman constant and the emissivity, respectively; h_v is the heat transfer coefficient of the convection air, which is a function of the convection air velocity (v_a), i.e.,

$$h_v = \beta v_a^{0.7}, \quad (4.2)$$

The energy consumed during coating curing in the oven is the sum of the energy consumed in different zones of the oven from two different energy sources. The wall

radiation consumes electricity, while the hot convection air is provided by natural gas combustion. The energy consumption can be expressed as follows:

$$Q_t = \sum_{i=1}^{N_r} Q_{e,i} + \sum_{j=1}^{N_a} Q_{ng,j}, \quad (4.3)$$

where N_r and N_a are the number of radiation heating zones and that of the convection zones respectively; $Q_{e,i}$ and $Q_{ng,i}$ are the electricity and natural gas consumed in the i -th radiation zones and the j -th convection air zones, respectively.

Fundamental modeling of energy consumption in a curing process is challenging. However, empirical regression models that correlates the consumption of energy (electricity and natural gas) with curing over design (in terms of the length of each zone in the oven) and oven operating temperature of each zone can be readily derived (Papasavva *et al.*, 2002; Roelant *et al.*, 2004). In this work, the models for electricity consumption ($Q_{e,i}$) and natural gas consumption ($Q_{ng,i}$) during curing are as follows:

$$Q_{e,i} = 2.45L_i \exp\left(\frac{T_{w,i}}{688.2}\right) - 3.80L_i; \quad i = 1, 2, \dots, N_r \quad (4.4)$$

$$Q_{ng,j} = 0.0017(T_{a,j} - 294.11)L_j v_{a,j}; \quad j = 1, 2, \dots, N_a \quad (4.5)$$

where L is the length of a specific drying zone; $T_{w,i}$ and $T_{a,j}$ are the temperature of the oven wall and that of the convection air in each zone, respectively.

4.3 Solvent Removal from the Wet Film

Solvent is uniformly distributed within the wet coating layer on substrate. During drying, solvent in different locations within the film moves towards the coating surface and then evaporate. Along solvent removal, the thickness of the coating layer decreases. Typically, solvent removal rate is controlled by solvent evaporation from the coating surface

and solvent diffusion within the coating film. Known studies on drying coatings show that the rate of diffusion and evaporation are related with solvent concentration and temperature (Blandin *et al.*, 1987; Blandin *et al.*, 1987; Ion and Vergnaud, 1995; Henshaw *et al.*, 2006). Lou and Huang proposed a Fick's second law based solvent removal model for conventional clearcoat (Lou and Huang, 2000). Note that the presence of nanoparticles within a coating layer forces solvent to change diffusion pathways, which affects the solvent removal process to some extent. Therefore, the solvent removal model by Lou and Huang needs to be modified (Lou and Huang, 2000).

According to Falla *et al.* and Swannack *et al.* (Falla *et al.*, 1996; Swannack *et al.*, 2005), the solvent diffusivity for a nanocomposite ($D_n(t)$) is related to that for a conventional paint ($D_o(t)$) in the following way:

$$D_n(t) = \frac{1 - \varphi_n}{1 + 0.5\varphi_n} D_o(t), \quad (4.6)$$

where φ_n is the volume fraction of nanoparticles in a dry film (usually less than 10%). This equation is applicable to the case where the nanoparticles are spherical with no size limit. The solvent diffusivity in conventional paint $D_o(t)$ is expressed as (Blandin *et al.*, 1987; Blandin *et al.*, 1987; Lou and Huang, 2000):

$$D_o(t) = \eta \exp\left(-\frac{\gamma}{C} - \frac{E_d}{RT(t)}\right), \quad (4.7)$$

where η is a pre-exponential constant for diffusivity; γ is a constant; E_d is the activation energy for diffusion; R is the ideal gas constant.

By using the diffusivity for nano-film ($D_n(t)$), the solvent diffusion dynamics within the film can be expressed as:

$$\frac{\partial C(z,t)}{\partial t} = \frac{\partial}{\partial z} \left(D_n(t) \frac{\partial C(z,t)}{\partial z} \right), \quad (4.8)$$

where $C(z,t)$ is the mass concentration of solvent within the film; z is the thickness of the film.

The change of solvent content at the coating surface results from the solvent loss due to evaporation and solvent gain from the underlying film. Thus, the mass-transfer process at the coating surface and the solvent evaporation process can be modeled as (Cussler, 1997; King, 2013):

$$\frac{\partial C(z,t)}{\partial t} = \frac{D_n(t)}{Z_s} \frac{\partial C(z,t)}{\partial z} - \frac{K(P_{ls}(t) - P_{lb})}{\rho_s Z_s}, \quad (4.9)$$

where ρ_s is the density of irreducible components in the film; Z_s is the thickness of irreducible components in the film; K is the mass transfer coefficient; $P_{ls}(t)$ and P_{lb} are, respectively, the solvent partial pressure at the coating-air interface and its partial pressure in the bulk gas phase.

The solvent partial pressure at the coating-air interface ($P_{ls}(t)$) can be calculated as the vapor pressure of pure solvent at the current temperature multiplied by the activity of the solvent at the current polymer phase solvent concentration.⁹ We assume that the Flory–Huggins equation describes the solvent activity. Therefore,

$$P_{ls}(t) = P_l(t) \varphi_l \exp\left((1 - \varphi_l) + \chi(1 - \varphi_l)^2\right), \quad (4.10)$$

where χ is the Flory–Huggins interaction parameter; φ_l is the volume fraction of solvent; $P_l(t)$ is the vapor pressure of pure solvent at temperature $T(t)$. For the solvent contained in

the nanoclearcoat layer, the vapor pressure of pure solvent at the solid-air interface can be obtained based on the Antoine equation:

$$\ln P_l(t) = a - \frac{b}{c + T(t)}, \quad (4.11)$$

Note that solvent evaporation at a wet film surface is modeled as a moving boundary problem, as the thickness of the wet film decreases along the time. The initial and boundary conditions are expressed below:

$$C(z, 0) = C_0, \quad (4.12)$$

$$\frac{\partial C(0, t)}{\partial t} = 0, \quad (4.13)$$

In modeling, the coating film is vertically divided into N very thin slices, each of which has a same initial thickness (Δz_0). The solvent concentration in i -th slice $C(z_i, t)$ can be readily obtained through process dynamic simulation.

4.4 Film Thickness Modeling

The film thickness change occurs mainly due to solvent removal. Note that the average mass concentration of solvent, $\bar{C}(t)$, is defined as:

$$\bar{C}(t) = \frac{1}{N} \sum_{i=1}^N C(z_i, t), \quad (4.14)$$

Thus, the film thickness, $Z(t)$, can be estimated using the following formula:

$$Z(t) = \frac{\rho_l (V_s + V_n)(1 - \bar{C}(t)) + (\rho_s V_s + \rho_n V_n) \bar{C}(t)}{A \rho_l (1 - \bar{C}(t))}, \quad (4.15)$$

where A is the surface area of the substrate covered by the film; $V_l(t)$, V_s and V_n are the volumes of solvent, polymeric materials, and nanoparticles contained in the film, respectively.

Note that the final film thickness, $(Z(\infty))$, after the solvent is completely removed, is:

$$Z(\infty) = \frac{V_s + V_n}{A}, \quad (4.16)$$

This is the same as Eq. (4.15) when V_l reaches zero. In practice, however, the cured film will still contain a few percent of solvent residue. Thus, the average coating thickness is slightly greater than that evaluated using Eq. (4.15).

4.5 Monte Carlo Modeling for Cross-linking Reaction Characterization

Xiao *et al.* developed an off-lattice Monte Carlo (MC) modeling method to study the dynamic features of the nanocoating microstructure during curing (Xiao and Huang, 2009). That method can be used to predict coating quality, i.e., mechanical properties. It is known that in curing operation, polymer and nanoparticle interacts and cross-linking reactions occur. The polymer network formation is simulated in multiple stages including system creation, curing condition application, cross-linking chemical reaction, and multiple system relaxations. In this study, only spherical nanoparticles are incorporated in the polymer solution.

In simulation, the first step is to set up a simulation box in which the polymer beads representing monomers and cross-linkers, as well as a large number of nanoparticles, are randomly distributed to generate an initial system configuration. In the simulation system, the size and volume fraction of nanoparticles, the total number of effective monomers and

that of cross-linkers, and the number density of polymeric materials should be specified. Such information is used to identify the total number of nanoparticles as follows:

$$N_n = \text{int} \left(\frac{6 \varphi_n (N_b + N_c)}{\rho_p (1 - \varphi_n) \pi d_n^3} \right), \quad (4.17)$$

where ρ_p is the density of polymeric materials; N_b and N_c are the total number of effective monomers and that of cross-linkers, respectively; d_n and φ_n are the size and the volume fraction of nanoparticles, respectively.

The cubic simulation box can then be defined by calculating the initial edge length as:

$$l_0 = d_n \left(\frac{\pi N_n}{6\varphi_n} \right)^{1/3} \quad (4.18)$$

In simulation, there are three equilibrium states that the simulation system needs to reach during coating sample development. The first equilibration occurs after an initial configuration is generated; the second appears after the cross-linking reaction is accomplished; and the third is needed after the sample is cooled. The model takes into account the interaction among polymer beads and that between polymer beads and nanoparticles.

Cross-linking reaction takes place in the simulation system after the system reaches the first-stage equilibrium state. During the network formation, interrelated physical and chemical phenomena (i.e., polymer and nanoparticle movement and cross-linking reaction) occur simultaneously, which are influenced by the dynamically changed curing environment. The thermal profile is obtained from the macroscopic oven heating dynamic model in Eqs.

(4.1) and (4.2). The profile must be imposed in simulation to ensure a full realization of the required curing environment. Existing studies show that the reaction kinetics in a coating curing process can be characterized by an autocatalytic mechanism (Xiao *et al.*, 2010). Zhou *et al.* studied the curing process of thermosetting nanocoating materials, and showed that autocatalytic model could also be used to characterize the curing process (Cussler, 1997; Zhou *et al.*, 2005). However, nanoparticles added into the polymer matrix have a negative effect on polymer network formation (Yari *et al.*, 2014). Thus, the autocatalytic mechanism is used to model the reaction kinetics with the existence of nanoparticles in the polymer matrix. The chemical conversion rate can be calculated as

$$\frac{d\alpha(t)}{dt} = \zeta \exp\left(-\frac{E}{RT(t)}\right) \alpha(t)^m (1-\alpha(t))^n, \quad (4.19)$$

where $\alpha(t)$ is the conversion of cross-linking reaction; ζ is a polymerization reaction frequency factor; E is the activation energy; m and n are constants.

After the cross-linking reaction reaches its target conversion rate, the nanocoating sample will be cooled down to a normal temperature, which is followed by the second-stage equilibration. The cooling process is operated at a constant pressure.

4.6 Product Quality Analysis and Simulation Procedure

To ensure achievement of the anticipated functionalities in the final nanoclearcoat product, the curing process should meet the following standards: (i) the solvent residual is reduced to no more than 2% in the dried film; (ii) the conversion of cross-linking reaction reaches 95%; and (iii) the scratch resistance performance should be improved at least 45% over that offered by the conventional clearcoat.

4.6.1 Product Performance Evaluation

Before introducing a product quality analysis procedure, we describe a simulation method for product performance analysis. Note that the developed multiscale models can be used to generate a variety of valuable information about the macroscopic reactive drying operation and the meso- to micro-scale coating structural formation process. Correlating the structure with the product quality is a critical task. In this work, we focus on the coating scratch resistance performance which is qualitatively correlated with its elastic property quantified by Young's modulus. The change of Young's modulus is directly used to represent the change of coating scratch resistance performance. A deformation simulation that is a non-equilibrium deformation process is accomplished by an off-lattice mc-based method to establish a stress-strain relationship for modulus calculation.

In order to acquire a comprehensive and accurate simulation result, the deformation tensile tests are carried out in x, y, and z directions of the cubic simulation box. During a tensile test simulation, a series of strain increments are applied on the simulation system along a specific direction. The strain increment must be small enough in order to reveal practical deformation behavior. The corresponding normal stress of each strain increment is evaluated by adopting Virial theorem (Allen and Tildesley). It must be pointed out that a relaxation process must be included between two adjacent strain increments to approximate a real material deformation process. An averaged stress-strain curve obtained from three independent tensile tests in x, y, and z directions can be used to investigate the stress-strain behavior of the cured product. Through examining the contributions from different stresses,

the deformation behavior of the material can be clearly analyzed. Such behavior is capable of providing accurate evaluation of Young's modulus of the cured product.

Ideally, MC simulation and subsequent analysis of product performance should be conducted when the temperature profile of curing environment changes. However, the microscale simulation is time consuming, which makes design optimization extremely inefficient. Model to predict the mechanical properties of cured nanocomposite coating material has not been developed yet. Thus, it is of great importance to derive quantitative correlations between the overall coating mechanical performance and key material parameters based on the developed modeling and simulation method. The conversion rate of cross-linking reaction also plays a key role in evaluating coating mechanical property.²⁸ An empirical regression model that represents the relationship among the improvement of coating scratch resistance performance (SR) compared with cured conventional clearcoat, final reaction conversion ($\alpha(t^e)$), and the size (d_n) and volume fraction (φ_n) of nanoparticles can be generally expressed as:

$$SR = f\left(\alpha(t^e), d_n, \varphi_n\right), \quad (4.20)$$

In this work, the target clearcoat contains 5% of 20 nm nanoparticles. A series of tests based on the microscale MC simulation have been conducted to explore the relationship shown in Eq. (4.20). In simulation, a simplified temperature profile is used: the oven temperature which is initially set at 300K increases to 400K after 2000 Monte Carlo simulation cycles and then remains constant at 400 K until the cured coating material reaches the preset final conversion percentage ($\alpha(t^e)$) of polymer network, that is, 80%, 83%, 86%,

89%, 92%, 95%, and 98% respectively. Each simulation is repeated three times to obtain accurate results. The seven groups of simulation results lead to a specific form of Eq. (4.20):

$$SR = 8.27 \exp\left(1.01\alpha(t^e)^{33.44} - 3.06\right), \quad (4.21)$$

Note that this simplified relationship can only be applied to the cured coating material with final conversion percentage ($\alpha(t^e)$) greater than 80%. Having the above model, the mechanical improvement of a cured nanocoating with any proper combination of material parameter values can be readily calculated.

4.6.2 Energy Efficient Curing

Coating curing operation in a multi-zone oven is energy intensive. However, how to optimize oven operational settings to achieve most energy efficient curing has not been well studied, even for the curing of conventional clearcoat. In this work, we propose a curing optimization framework, where energy minimization is targeted and various produce and process constrains are imposed. The optimization model is presented below.

$$\min_{T_{w,1}, T_{w,2}, T_{a,1}, T_{a,2}, T_{a,3}, T_{a,4}, T_{a,5}, T_{a,6}} Q_t = \sum_{i=1}^{N_r} Q_{e,i} + \sum_{i=1}^{N_a} Q_{ng,i} \quad (4.22)$$

Subject to:

$$\frac{dT(t)}{dt} = \begin{cases} \frac{\sigma\varepsilon}{\rho_m C_{pm} Z_m} (T_w^4 - T(t)^4) + \frac{h_v}{\rho_m C_{pm} Z_m} (T_a - T(t)), & \text{Radiation zone} \\ \frac{h_v}{\rho_m C_{pm} Z_m} (T_a - T(t)), & \text{Convection only zone} \end{cases} \quad (4.1)$$

$$\frac{dT(t)}{dt} \leq 22.2 \quad (4.23)$$

$$\bar{C}(t^e) \leq 0.02 \quad (4.24)$$

$$\frac{d\alpha(t)}{dt} = \zeta \exp\left(-\frac{E}{RT(t)}\right) \alpha(t)^m (1-\alpha(t))^n \quad (4.19)$$

$$\alpha(t^e) \geq 0.95 \quad (4.25)$$

$$Q_{e,i} = 2.45L_i \exp\left(\frac{T_{w,i}}{688.2}\right) - 3.80L_i; \quad i = 1, 2, \dots, N_r \quad (4.4)$$

$$Q_{ng,j} = 0.0017(T_{a,j} - 294.11)L_j v_{a,j}; \quad j = 1, 2, \dots, N_a \quad (4.5)$$

$$SR = 8.27 \exp\left(1.01\alpha(t^e)^{33.44} - 3.06\right) \quad (4.21)$$

$$SR \geq 0.45 \quad (4.26)$$

$$T_{w,i} \in [400, 500] \quad (4.27)$$

$$T_{a,j} \in [400, 480] \quad (4.28)$$

where the decision variables in the objective function, $T_{w,i}$'s and $T_{a,j}$'s, are the wall temperatures and convection air temperatures in different operational zones of the oven; t^e denotes the ending time of curing process. Note that the achievement of reaction conversion constraint in Eq. (4.25) could lead to a SR value greater than 0.45 in Eq. (4.26). It will affect the optimization results only if Eq. (4.21) changes with respect to different coating composition.

4.6.3 System Simulation Procedure

The developed product, process, and optimization models are incorporated in a five-step simulation procedure that is described below.

Step 1. Input process design and operational parameters (e.g., the oven design with zone partition and heating types, operational restrictions, vehicle moving speed on conveyor, etc.), coating material parameters (i.e., solvent properties, paint properties including the size and volume fraction of nanoparticles), product quality specifications (i.e., solvent residual, cross-linking reaction conversion rate, and Young's modulus of cured product).

Step 2. Identify the optimal temperature settings for all the radiation and convection zones (i.e., $T_{w,i}$'s and $T_{a,j}$'s) through running the optimization model in Eq. (4.22) associated with the listed equality and inequality constraints.

Step 3. Use the identified temperature settings to calculate the following: (a) the coating temperature profile using Eqs. (4.1) – (4.2), (b) the solvent removal dynamics using Eqs. (4.6) – (4.13), (c) the coating thickness change using Eqs. (4.14) - (4.15), (d) the cross-linking conversion rate dynamics using Eq. (4.19), and (e) the coating scratch resistance performance using the method described in the above Product Performance Evaluation section.

Step 4. Plot the results obtained in Step 3. Although all of them have already met the process and product quality requirement, there could be some need for further exploration of opportunities of more significant improvement of product quality and process performance, after reviewing the plots. For instance, one may want to investigate how a further reduction of the solvent residue in the cured coating will impact the cross-linking conversion and/or scratch resistance performance, then the constraint, $\bar{C}(t^e) \leq 0.02$, in Eq. (4.24) can be adjust to a value smaller than 0.02. If any equality and/or inequality

expressions in the optimization model are changed, then go to Step 2; otherwise, proceed to the next step.

Step 5. Output a complete set of system input information, including the process specifications, nanomaterial data, and product quality requirement, as well as a complete set of optimization results, including the derived oven temperature settings, the achieved product quality data, and process energy consumption data.

4.7 Case Study

The developed modeling and optimization methodology has been used to study the optimal curing strategy for a given nanocoating material.

4.7.1 System Specification

The thermoset coating material is a hydroxyl-functional acrylic copolymer with a number average molecular weight of 2,880; the cross-linker is hexamethoxymethylmelamine, of which the molecular weight is 390. The nanoparticle component is nano-silica, which is of the size and the volume fraction at 20 nm and 5%, respectively. The initial solvent concentration of the wet clearcoat is 18% and the film thickness is 60 μm . The densities of the solvent, the polymeric material, and the nanoparticle are 0.81 g/cm^3 , 1.2 g/cm^3 , and 2.4 g/cm^3 , respectively. The curing oven is 124.2 m long, which is divided into seven zones of different lengths (see Column 3 in Table 4.1). The line speed of vehicle moving through the oven is 0.069 m/s. The convection air velocity from the nozzles in the radiation heating zones is 0.18 m/s and that in the convection heating zones is 1.8 m/s. In simulation, parameters β , η , r , K , χ , a , b , c , and E_d are 22, 9.38×10^{-6} cm^2/s , 0.19, 9.49×10^{-11} $\text{g}/\text{cm}^2 \cdot \text{atm} \cdot \text{s}$, 0.93, 2.60, 472.92, -94.43, and 32.7×10^3 J/mol, respectively. To simplify the

simulation process, the solvent vapor partial pressure at the bulk air is assumed to be 0. The reaction kinetics data for simulating the cross-linking reaction, ζ , E , m , and n , are 9.72×10^6 , 72.66×10^3 J/mol, 0.71, and 1.23, respectively.

Table 4.1. Oven temperature setting for a conventional clearcoat system

Zone No.	Heating mechanism	Zone length (m)	Radiation wall temperature (K)		Convection air temperature (K)	
			Optimal	Industrial	Optimal	Industrial
1	Radiation/ Convection	20.73	474	473	434	403
2		13.41	483	478	459	468
3	Convection	23.67	N/A		436	428
4		23.67			424	418
5		23.67			418	418
6		10.54			418	418
7	Air cooling	9.14			300	300

4.7.2 Solution Identification and Coating Dynamics

The optimization model was used to identify an optimal oven operational strategy, i.e., the optimal setting of the radiation and convection air temperatures in the seven operational zones. The derived temperature settings in different zones are shown in Table 4.1 (see the two columns under the heading, “Optimal”). The energy consumption data in each operational zone of the oven is listed in Table 4.2 (see the two columns also under the heading, “Optimal”). As shown, the total amount of energy consumed is 63.25 kWh per vehicle.

Table 4.2. Energy consumption of different oven temperature settings in curing process

Zone number	Energy consumption (kWh/vehicle)			
	Optimal		Industrial	
	Electricity	Natural gas	Electricity	Natural gas
1	22.36	0.89	22.21	0.69
2	15.32	0.68	14.84	0.71
3	N/A	10.28	N/A	9.70
4		9.41		8.97
5		8.97		8.97
6		4.00		4.00
Total	71.89		70.00	

Using the oven temperature settings, the coating layer heating profile, the solvent residue dynamics, the coating thickness change, and the cross-linking reaction rate dynamics can be obtained, which are plotted in Figure 4.2 (see the solid curves). It is shown in Figure 4.2(a) that the curing operation takes 1,800 sec. In drying, the coating temperature increases quickly due to the strong radiation in zones ① and ②. As the drying proceeds, the coating temperature increment becomes slower in zones ③ and ④, and stable at around 417 K in zones ⑤ and ⑥. Figure 4.2(b) shows that the solvent in the film is mostly removed in the first two zones. But in the end of zone ⑦, there is still 2% of solvent remained in the dry film; at that time the coating thickness is reduced to 48.29 μm (see Figure 4.2(c)). The cross-linking reaction rate dynamics in Figure 4.2(d) indicates that the reaction takes place quickly in zones ③ and ④, and reaches 95.0% in the end of zone ⑦. Figure 4.3 demonstrates the micro-structure of the nanocoating after curing. The tensile property of the nanocoating is

quantified using Young's modulus. It shows that the cured nanocoating layer can achieve 46.50% of improvement of scratch resistance (S) over the conventional coating layer.

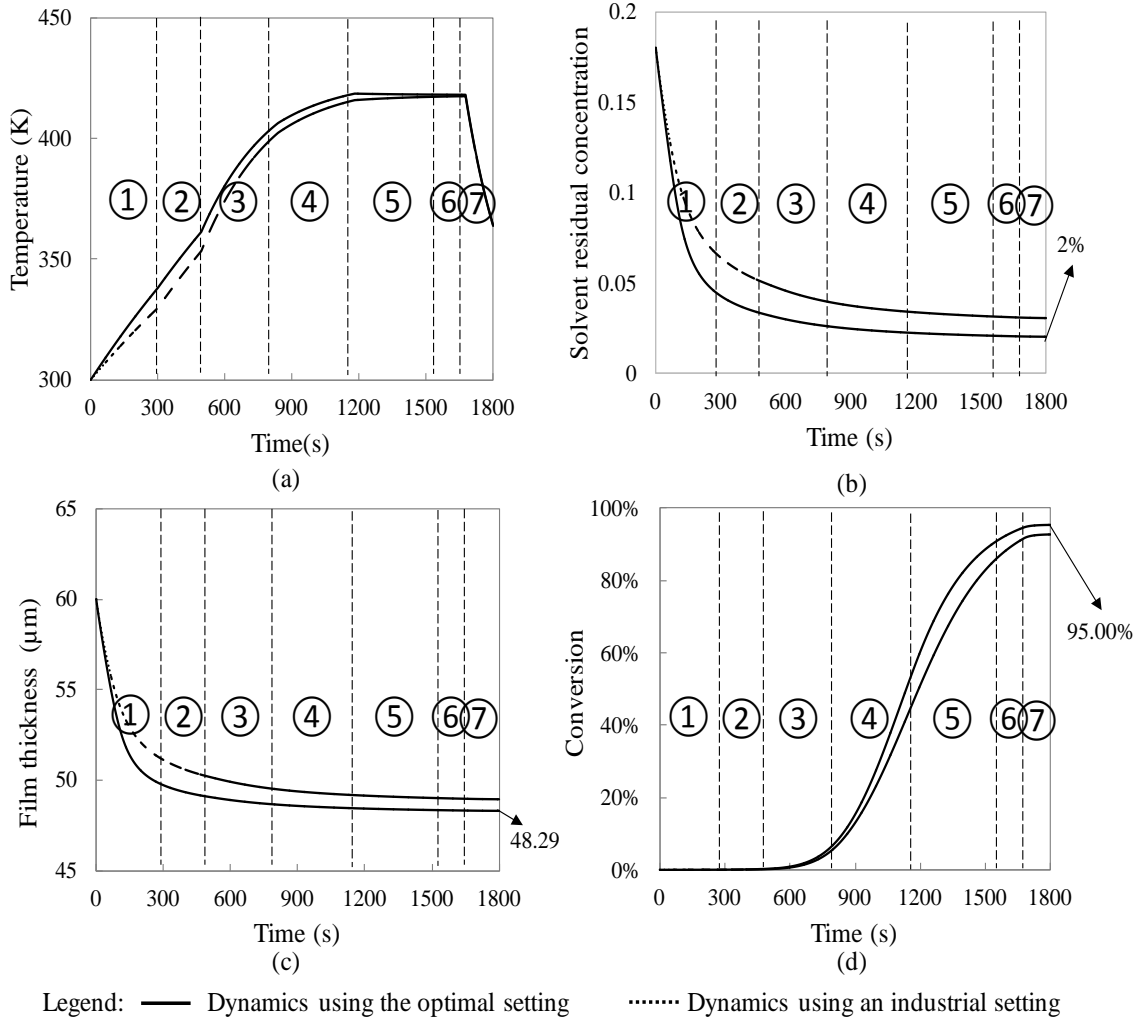


Figure 4.2. Coating performance under new oven operational setting: (a) coating temperature profile; (b) concentration of solvent residual in nanocoating; (c) thickness of nanocoating; (d) conversion rate of cross-linking reaction in nanocoating.

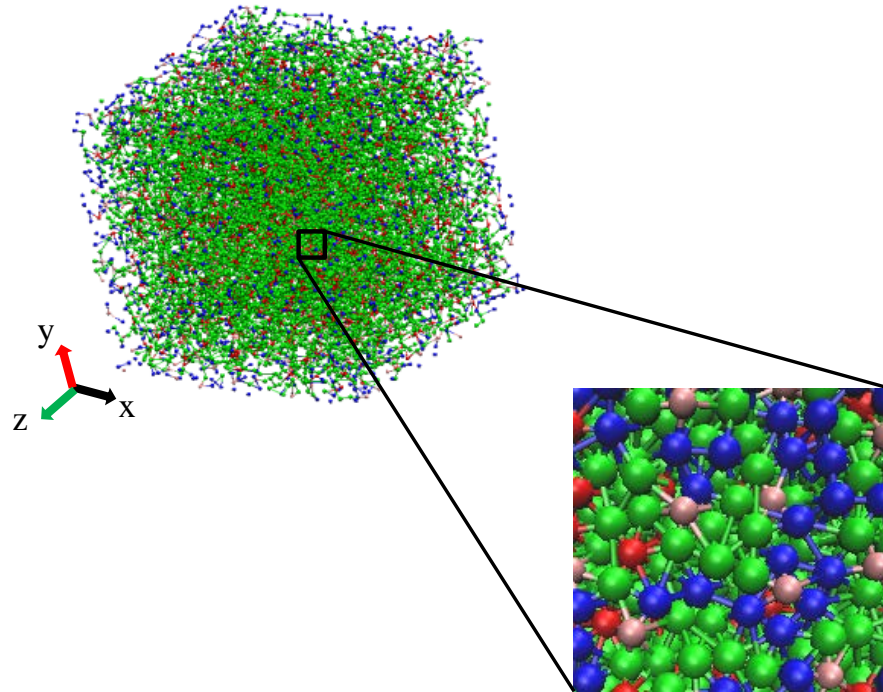


Figure 4.3. Micro-structure of the cross-linked nanocoating layer.

4.7.3 Performance Comparison Using an Industrial Setting

One task of this work is to study if the known industrial oven design and operational setting used for curing the conventional paint based clearcoat is appropriate for curing nanoclearcoat. The industrial setting (i.e., the wall and convection air temperatures in the seven zones of the same oven) is listed in Table 4.1 (see the columns under the heading, “Industrial”). Using this setting, which is lower than the optimal except for one convection air temperature, the coating temperature dynamics is obtained, which plotted in Figure 4.2(a) (see the dotted line). It is shown that the coating temperature is always lower than that using the optimal setting, with the maximum difference of about 8K in zone ②. This means the nanocoating layer does not receive enough energy for drying and curing.

Consequently, the solvent removal becomes slower; in the end of the process, the solvent residue in the coating is 3.1% (see the dotted line in Figure 4.2(b)). This is understandable because in the nanoclearcoat, the presence of nanoparticles makes the solvent diffusion within the film more difficult, and the energy provided for solvent evaporation using the industrial setting is not that sufficient. Because of this slower solvent diffusion and removal, the film thickness reduction process becomes slower accordingly, giving the final thickness of 48.94 μm (see the dotted line Figure 4.2(c)), which is slightly thicker than the one drying using the optimal setting (48.29 μm). Note that Figure 4.3(d) shows that the cross-linking reaction conversion can reach only 92.26%, which is below the minimum requirement of 95%. Using the industrial setting, the estimated scratch resistance improvement can reach only 42.57%; this is below the minimum requirement of 45%. Energy consumption, however, is 2.70% lower than the one using the optimal operational setting, which is shown in Table 4.2 (under the heading of “Industrial”). Apparently, the nanocoating using the known industrial setting cannot achieve the anticipated product quality performance.

4.7.4 Product Quality Satisfactory Region Using Different Nanopaint

Note that the nanopaint used in the case study has the nanoparticle size and volume fraction of 20 nm and 5%, respectively. It is known that the nanoparticle size and volume fraction of commercial nanopaint are in the range of 10 to 40 nm and 2 to 10%, respectively. Thus, it is worthwhile to investigate whether the identified optimal oven operational setting can ensure the nanoclearcoat quality through the curing operation when the coating material composition changes.

By applying the identified optimal oven operational setting, a series of modeling and simulation are conducted on the nanoclearcoat material with the nanoparticle size and volume fraction of commercial nanopaint from 10 to 40 nm and from 2 to 10%, respectively. Figure 4.4(a) depicts the correlation between the cross-linking conversion rate versus the nanoparticle size and the volume fraction of the nanoparticles in the nanopaint, while Figure 4.4(b) demonstrates how the scratch resistance performance changes along the change of nanoparticle size and the volume fraction of nanoparticles in nanopaint; both are derived using the previously optimized settings for the oven wall temperatures and the convection air temperatures. For the minimum requirement of the cross-linking conversion rate set to 95%, Figure 4.4(a) marks a quality satisfactory region in the plane of nanoparticle size versus volume fraction. For the minimum requirement of the scratch resistance improvement of 45%, Figure 4.4(b) shows a quality satisfactory region also in the plane of nanoparticle size versus volume fraction. Figure 4.5 combines the quality satisfactory regions in Figure 4.4(a) and (b). As shown, the darker area, which is the overlap of the two regions, provides a guideline for choosing nanoparticle size and volume fraction in order to meet the quality requirement of both the cross-linking conversion rate and the improvement of scratch resistance.

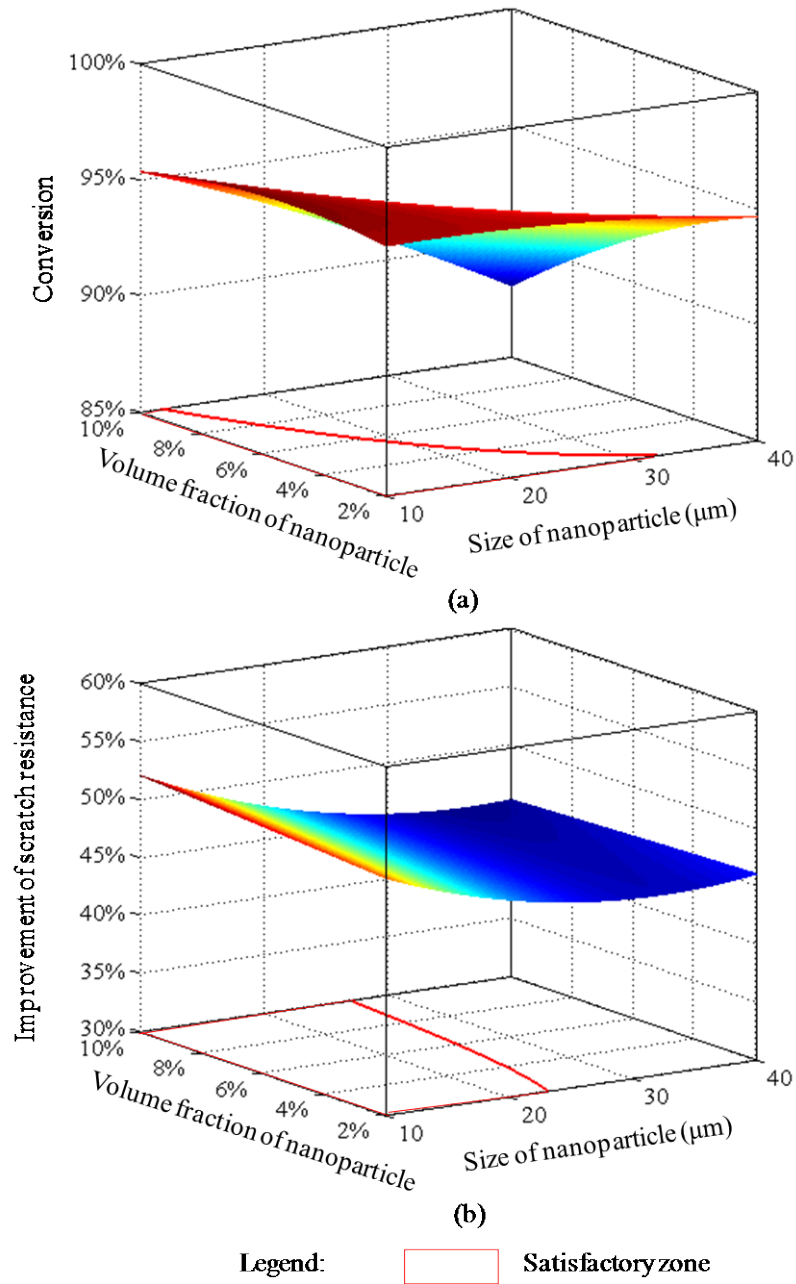


Figure 4.4. Coating quality performance using different nanopaint compositions: (a) conversion rate of cross-linking reaction, and (b) improvement of scratch resistance.

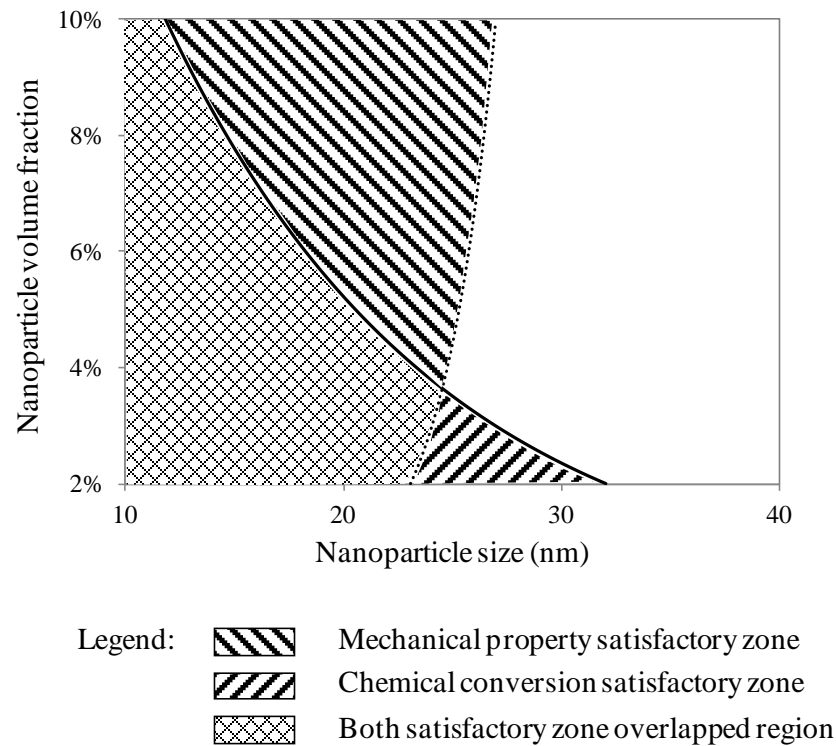


Figure 4.5. Quality satisfactory zones with respect to different nanopaint compositions.

4.8 Concluding Remarks

Nanopaint becomes a very promising coating material in manufacturing industries. Nanopaint based clearcoat is an excellent example in automotive coating. However, there is a lack of fundamental study on cost-effective and quality assured nanoclearcoat curing. It is of great importance to dynamically characterize nanocoating curing under industrial oven operational settings. In this work, a multiscale modeling and simulation methodology is introduced, which can be used to characterize various chemical and physical phenomena in curing operation, which is a critical stage in coating manufacturing. The developed integrated models allow the formulation of an optimization model, targeting minimum energy cost, while all process performance and product quality specifications are considered.

The comprehensive case study demonstrates the methodological efficacy. The methodology is general; it can be applied to the study on nanocoating curing using different nanopaint materials in various coating manufacturing operations.

CHAPTER 5 SUSTAINABILITY ASSESSMENT AND PERFORMANCE IMPROVEMENT OF ELECTROPLATING PROCESS SYSTEMS

The electroplating industry is extremely critical in end-product manufacturing in many industries, such as the aerospace, appliances, automotive, electronics, and heavy equipment industries. The industry transforms raw parts received from suppliers to the finished components coated with specific metals to enhance the aesthetic appearance, corrosion prevention, as well as other engineering functionalities. For example, plated chrome grilles are widely used in automotive bodies for protection and aesthetics (Chase, 1996). Parts used in aerospace industry are often coated with special materials to obtain various functionalities (Jingshuang *et al.*, 1996). A typical electroplating process can be composed of a number of processes for cleaning, rinsing, and plating operations (Gong *et al.*, 1997). In production, workpieces are cleaned, etched, electroplated, and finished by dipping into a series of operating units that contain a combination of corrosive, metal, and/or chemical solutions. Various chemicals are used in the cleaning units, where the chemicals make workpiece surface ready for plating. Electrolytic plating, electroless plating, and chemical and electrochemical conversion processes are typically used in the industry (Schlesinger and Paunovic, 2011).

The electroplating industry is considered one of the most polluting industries in the U.S. largely due to the emission of hazardous chemicals and toxic waste in different forms. Toxic chemicals, such as cyanide, acid, and alkaline are widely used for cleaning and plating processes while heavy metals, such as zinc, copper, silver, chrome, and nickel, are plated on the work piece surface (Gong *et al.*, 1997). More than 100 different toxic chemicals, metals, and other regulated pollutants are generated during operation (Luo and Huang, 1997).

Manufacturing quality products consume a huge amount of fresh water in multiple rinsing processes, which are installed after parts cleaning and plating. Energy is mainly used to facilitate cleaning operations and direct deposition of metal ions to the surface of products. In addition, process, product, and material replacement or modification for waste reduction could affect product quality and other aspects in manufacturing; this could be sensitive to economic and social sustainability performance.

Deep understanding of electroplating systems is essential to address the challenges brought by excessive water and energy consumption and severe toxic chemical emission. A variety of systematic process models have been developed to characterize electroplating systems. Huang and associates conducted a thorough investigation on parts cleaning and rinsing in different operating models (Schlesinger and Paunovic, 2011). The fundamental models were developed to describe the dynamic behavior associated with dirt removal, chemical and water consumption and waste generation mechanisms. Luo and Huang applied an intelligent decision support approach to reduce wastewater through drag-out minimization (Luo and Huang, 1997). Luo and coworkers proposed a set of sludge models to characterize the generation of sludge during parts cleaning and rinsing (Luo *et al.*, 1998). Yang *et al.* designed a water reuse system to maximize the reuse of rinsing water in rinsing steps that are described by the first principles based process models (Yang *et al.*, 1999; Yang *et al.*, 2000). Girgis and Huang conducted methodological study on technology integration for sustainable manufacturing in the surface finishing industry (Girgis, 2011). Liu and West studied galvanostatic pulse and pulsed reverse electroplating of gold on a rotating disk electrode and presented an on–off pulse-plating model for an accurate prediction of current

efficiency during plating operations (Liu and West, 2011). Bhadbhade and Huang also developed effective tools for sustainable electroplating operations (Bhadbhade, 2015)

Considering the importance of the electroplating sector in the supply chain of manufacturing, it is important to gain a deep understanding of the status of electroplating systems from the economic, environmental, and societal point of view and apply proven methods and technologies to enhance sustainability performance. Nevertheless, sustainability study of electroplating system has not been fully explored yet other than well-tested electroplating process models.

As one of the top priorities of the metal finishing industry, pollution prevention (P2) has gained tremendous attention due to the increasing stringent environmental regulations regarding discharges (Cushnie Jr, 1994; Theodore, 1994). P2 is the use of source reduction techniques to achieve the maximum feasible reduction of all wastes (wastewater, solid waste, and air emissions) generated at production sites in order to mitigate risks to human health and the environment. All types of waste released to the air, water and land are addressed through P2. Extensive effort for improving operations in the industry has been made over past decade to design more efficient manufacturing processes without compromising product quality. A variety of P2 technologies have been developed for the electroplating industry. They mainly focused on source reduction, recycling/reuse, pretreatment, technology change, use of alternative materials, in-plant recovery/reuse and treatment (Lou and Huang, 2000). Typically the effectiveness of P2 technologies is always limited as most of them are technically quite basic. For instance, a longer drainage time is preferred for drag-out minimization, but undesirable for maintaining production rate. The reduction of water and

chemical usage, sludge and hazardous waste generation can lead to limited economic benefits of adopting P2 technologies. The implementation of these technologies, however, always requires a significant capital investment for change of processes and the use of alternative. Therefore, P2 technologies could pose some economic burden for the metal finishing industry.

The Profitable Pollution Prevention (P3) concept was first introduced to encourage the electroplating industry to achieve growth of economic benefit and simultaneously mitigate environmental impact at the lowest cost (Lou and Huang, 2000). A series of P3 technologies have been developed to minimize chemical, water and energy consumption as well as hazardous waste emission based on comprehensive modeling and analysis of electroplating system. The target of P3 is to maximize economic benefits while minimizing adverse environmental impact. Production rate could be optimized to gain maximum economic profit. Nevertheless, the lack of social sustainability evaluation leads to the approach being impracticability from the point of view of sustainable development. Piluso and Huang introduced a new concept called collaborative profitable pollution prevention to address the sustainability concern for large industrial zones (Piluso and Huang, 2009). There was still a lack of comprehensive evaluation of social aspects although they discussed basic social considerations.

In order to guide the sustainable development of industrial system, the effective approach must be able to accomplish both comprehensive sustainability assessment and accurate evaluation of available development options to make appropriate suggestion for sustainable development. Comprehensive sustainability assessment requires quantitative

measurement of how sustainability performs at economic, environmental, and social fields. Accurate and effective evaluation of system sustainability status using carefully selected sustainability metrics can facilitate decision making and action taking to achieve an anticipated sustainability goal. As of today, a number of sustainability metrics systems have already been created and used for performing sustainability assessment. For instance, the IChemE and AIChE sustainability metrics are widely adopted in the chemical and allied industries; both contain three sets of metrics for assessing economic, environmental, and social sustainability (Sikdar, 2003; Clift, 2006; Da Costa and Pagan, 2006). The assessment utilizes the system information provided by sustainability models or other means (e.g., direct and/or indirect measurements). Many other types of sustainability metrics are also available. The Dow Jones Sustainability Indices assess corporate business sustainability, which creates global indexes tracking the financial performance of leading sustainability-driven companies (López *et al.*, 2007). BASF has created and implemented eco-efficiency sustainability metrics which mainly focuses on economic and environmental performances (Landsiedel and Saling, 2002; Saling *et al.*, 2002; Shonnard *et al.*, 2003). However, most of existing sustainability metrics systems can be only references for the sustainability assessment of electroplating systems. Therefore, it is of great importance to generate a specific metrics system particularly for evaluating sustainability performance of the electroplating industry. Note that the result of sustainability assessment can be largely affected by particular process variables and subjective judgements such as weighting factors. These process variables should be accurately defined, and appropriate weight factors for the selected sustainability indicators must be carefully selected prior to sustainability assessment.

This chapter presents a framework, namely sustainable electroplating processes (SEP) which investigates electroplating systems by addressing economic, environmental, and social issues systematically. This is the first sustainability framework designed for the electroplating industry. It clearly elaborates the key aspects for evaluating sustainability status of electroplating processes and decision-making efforts. A complete sustainability metrics system can then be generated with respect to the interest of electroplating industry from sustainability point of view. A methodology for evaluating sustainability performance and selecting effective technologies is also introduced. Case studies are provided to demonstrate the framework.

5.1 Fundamentals for Process Sustainability

The fundamental of SEP is to enhance the performance of the electroplating industry from both economic and social aspects while addressing the pollution issue. More specifically, the merit of SEP is to simultaneously achieve waste reduction, production improvement, as well as social satisfaction enhancement (Figure 5.1).

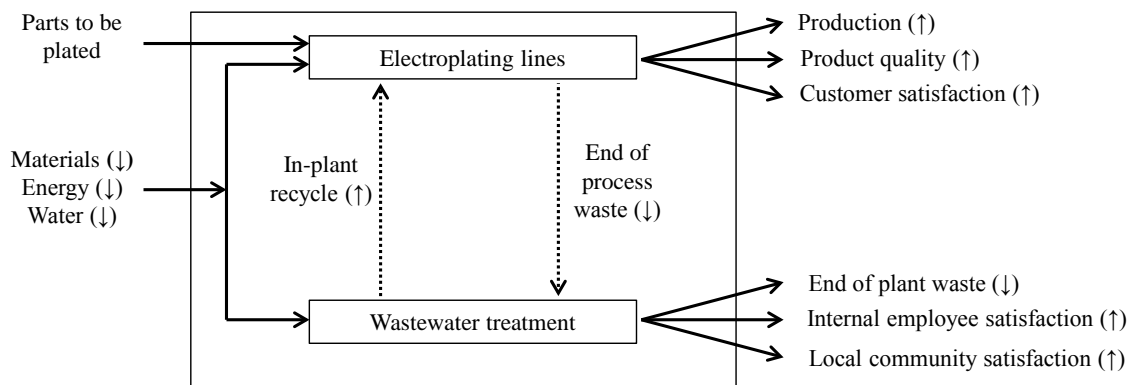


Figure 5.1. Sketch of an electroplating plant with sustainability concerns.

The concept of SEP can be expressed as:

$$\text{SEP} = \text{Waste}\downarrow + \text{Production}\uparrow + \text{Satisfaction}\uparrow \quad (5.1)$$

Waste reduction is the best approach to mitigate the impact on natural environment and therefore improve environmental sustainability. The reduction of waste emission and hazardous chemical consumption can also significantly alleviate the health burden on human beings. In the meantime, minimization of water and energy consumption can directly contribute to environmental sustainability. The waste reduction in Eq. (5.1) can be elaborated as:

$$\text{Waste}\downarrow = \text{Sludge}\downarrow + \text{Chemicals}\downarrow + \text{Water}\downarrow + \text{Energy}\downarrow \quad (5.2)$$

According to the P3 concept, it is possible to make profits through reducing waste from electroplating processes. In addition, the assurance of product quality requires lowering the product defect rate, which can boost the revenue in return. The production rise in Eq. (5.1) can be expressed as:

$$\begin{aligned} \text{Production}\uparrow = & \text{Product quality}\uparrow + \text{Production rate}\uparrow + \text{Operating cost}\downarrow \\ & + \text{Capital cost}\downarrow + \text{Chemical cost}\downarrow \end{aligned} \quad (5.3)$$

Note that the reduction of hazardous chemical consumption and safer electroplating process can lead to the increase of employee satisfaction. External satisfaction takes into consideration of both local community and customers. The reduction of hazardous waste can lead to a rise of the satisfaction of local community while the increase of product quality can gain higher satisfaction from customers. Therefore, the social aspects can include the followings:

$$\text{Social sustainability}\uparrow = \text{Customer satisfaction}\uparrow + \text{Employee satisfaction}\uparrow$$

+ Local community satisfaction↑ (5.4)

5.2 Sustainability Metrics System

An effective sustainability metrics system should be capable of providing deep understanding of sustainability performance of electroplating systems. The desired sustainability metrics system should establish an appropriate measurement that can address the stakeholder's economic interest, severe environmental concerns as well as social impact simultaneously. Selection of sustainability indicators is challenging. In this study, an investigation of electroplating systems from the perspective of supply chain is used to generate proper sustainability evaluating indicators. Figure 5.2 depicts the position of the electroplating industry in the supply chain of product manufacturing. The electroplating industry mainly plays the role of an intermediate service process which receives the unfinished parts from suppliers and transforms them into components with exceptional functionalities and appearance for downstream industries. In production, waste streams generated in process are pretreated in plants. In this section, we introduce a sustainability metrics system to evaluate the sustainability performance of electroplating systems.

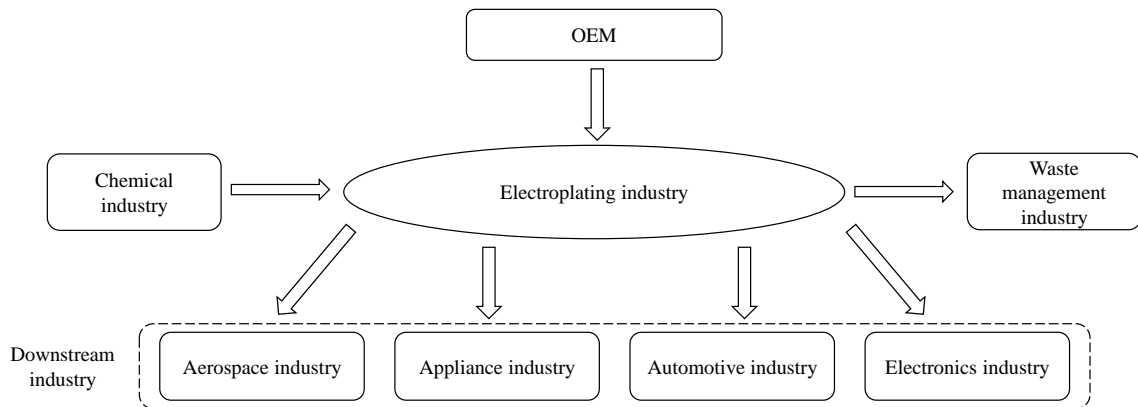


Figure 5.2. Electroplating-industry-centered supply chain.

5.2.1 Economic Sustainability Indicators

The main economic interest of the electroplating industry involves profit, cost, and investment. More specifically, the revenue comes from the sales of finished product. The cost consists of the expense that is needed to maintain normal operation of the company and the cost of materials, energy, and water. Investment focuses on technology innovation and application, employee's training and education. Note that the product quality in the electroplating industry is also a significantly important factor that influences economic performance, product defect rate during production and product return rate after shipment should also be seriously considered. Therefore, economic sustainability indicators should illustrate the impact of gross sales, net margin, investment due to system upgrade and new technology application, and product quality. A complete package of economic sustainability indicators is listed in Table 5.1.

Table 5.1. Economic sustainability indicators.

Economic Sustainability Indicator		Unit
Profit, value and tax	Value added	\$/y
	Value added per unit value of sales	\$/y
	Value added per direct employee	\$/y
	Net income	\$/y
	Net income per direct employee	\$
	Return on average capital employed	%/y
Investments	Percentage increase in capital employed	%/y
	Employees with post-school qualification	%
	New appointments/number of direct employees	%/y
	Training expense as percentage of payroll expense	%
	Ratio of indirect jobs / number of direct employees	%
	Investment in education/employee training expense	\$/y
	Investment in technologies to improve product quantity and process safety	\$
Product quality	Product return rate after shipment	%
	Product defect rate during production	%
	Percentage of finished product delivered on time	%

5.2.2 Environmental Sustainability Indicators

As pollution prevention is the top priority of the electroplating industry, environmental sustainability indicators must elaborate the impact of water, raw material, and energy consumption, human health burden as well as toxic and non-toxic waste emission. A good fraction of the chemicals used for cleaning and plating is carried out by workpieces and enter the rinsing systems or evaporate in the working environment. Energy is consumed

in cleaning and plating processes. Fresh water is used mainly to clean the remaining dirt and toxic chemicals on workpiece surface. Possible water recycle may come from the water reuse within manufacturing processes or recycling from wastewater treatment facility. Due to the difference of toxicity and human health impact, the impact from cleaning chemicals and plating chemicals should be considered separately. A complete package of environmental sustainability indicators is listed in Table 5.2.

Table 5.2. Environmental sustainability indicators.

Environmental Sustainability Indicator		Unit
Energy	Total net primary energy usage rate	kJ/y
	Percentage total net primary energy sourced from renewable	%
	Total net primary energy usage per kg product	kJ/Kg
	Total net primary energy usage per finishing line	kJ
	Total net primary energy usage per unit value added	kJ/\$
Material (excluding fuel and water)	Total cleaning chemical usage	kg/kg
	Total cleaning chemical usage per kg product	kg/kg
	Total cleaning chemical usage per unit value added	kg/\$
	Total plating chemical usage	kg/y
	Total plating chemical usage per kg product	kg/kg
	Total plating chemical usage per unit value added	kg/\$
	Percentage of chemical recycled from wastewater treatment facility	%
Water	Total water consumption	kg/y
	Net water consumed per unit mass of product	kg/kg
	New water consumed per unit value added	kg/\$
	Fraction of water recycled within the company	%
Emission	Hazardous liquid waste per unit value added	kg/\$
	Hazardous liquid waste per kg product	kg/kg
	Percentage of wastewater treated within the company	%
	Total other hazardous waste per unit value added	kg/\$
	Total other hazardous waste per kg product	kg/kg
	Human health burden per unit value added	kg/\$
	Non-hazardous waste generated	kg/y

5.2.3 Social Sustainability Indicators

Social sustainability is designed to evaluate the internal and external environment around the company. It is vital to identify quantifiable indicators to evaluate the performance of sustainability, although the social aspect in sustainability assessment is difficult to evaluate as most analyses are subjective and hard to quantify. The analysis of internal environment ought to provide adequate analysis on process safety and human resources while evaluation of external environment concentrates on the feedback from customer and local community. The overall social sustainability indicators for the electroplating industry are listed in Table 5.3.

Table 5.3. Social sustainability indicators.

Social Sustainability Indicator		Unit
Workplace	Benefits as percentage of payroll expense	%
	Employee turnover	%
	Promotion rate (number of promotions/number employed)	%
	Working hours lost as percent of total hours worked	%
Safety	Process safety index	
	Number of process safety analysis	/y
	Number of process maintenance	/y
Society	Number of stakeholder meetings per unit value added	/\$
	Indirect community benefit per unit value added	\$/
	Number of complaints from local community per unit value added	/\$
	Number of complaints from downstream customers	/y
	Percentage of finished product delivered on time	%
	Number of legal actions per unit value added	/\$

The proposed sustainability metrics system, if applied appropriately, can lead to an accurate and comprehensive sustainability evaluation which investigates the important factors as follows: number of production lines, production capacity, parts defect rate, water consumption, water recycle rate, energy consumption, cleaning chemical consumption, plating chemical consumption, chemical recycle rate, and waste emission. Note that sustainability assessment is heavily dependent on data availability and accuracy, it is comprehensible that a simplified version of this metric system can be applied to some specific cases.

5.3 Systematic Sustainability Assessment

This work adopts a systematic sustainability assessment approach developed by Liu and Huang (Liu and Huang, 2012; Liu and Huang, 2013). For a process system of interest, a selected sustainability metrics set for the sustainability assessment is denoted as:

$$S = \{E, V, L\}, \quad (5.5)$$

where $E = \{E_i \mid i = 1, 2, \dots, F\}$ is the set of economic sustainability indicators;

$V = \{V_i \mid i = 1, 2, \dots, G\}$ is the set of environmental sustainability indicators; and

$L = \{L_i \mid i = 1, 2, \dots, H\}$ is the set of social sustainability indicators.

To combine a number of sustainability aspects to a composite number can not only significantly enhance the evaluation process but also present the result in a holistic way. Therefore, it is required that all the data used should be normalized first by comparing them with company targets or industry best practice in application. The sustainability performance of the selected electroplating system can be easily evaluated by adopting the well-defined indicators. These data can be used to estimate the categorized sustainability of the system, i.e., E , V , and L , which are called the composite sustainability indices, and estimated using the following formulas:

$$E = \frac{\sum_{i=1}^F a_i E_i}{\sum_{i=1}^F a_i} \quad (5.6)$$

$$V = \frac{\sum_{i=1}^G b_i V_i}{\sum_{i=1}^G b_i} \quad (5.7)$$

$$L = \frac{\sum_{i=1}^H c_i L_i}{\sum_{i=1}^H c_i} \quad (5.8)$$

where a_i , b_i , and $c_i \in [1, 10]$ are the weighting factors associated with the corresponding indices, reflecting the relative importance of the individual indices in overall assessment. The weighting factors should be determined by users based on their organizations' strategic plans and business development objectives. All of the weighting factor can be assigned to 1 if all the factors are considered equally important.

The overall sustainability performance of the system, S , can be evaluated using the composite indices, E , V , and L , with the weighting factors assigned again by the industrial organization, i.e.,

$$S = \frac{\|(\alpha E, \beta V, \gamma L)\|}{\|(\alpha, \beta, \gamma)\|} \quad (5.9)$$

where α , β , and γ are the weighting factors for evaluating overall sustainability performance following the same rules as mentioned previously. In general, the overall sustainability status of electroplating system has a value between 0 and 1 as S is still normalized.

5.4 Sustainability Assessment of Technology Candidates

It is comprehensible that the electroplating industry has to implement effective technologies to modify or optimize process, product and materials to improve its

sustainability performance and thus achieve long-term sustainable development. A thorough investigation of the sustainability improvement potential by implementing candidate technologies is essential to sustainable decision-making.

Identification of candidate technologies requires process characterization, experts' knowledge, etc. The selected sustainability metrics system for assessing system sustainability performance should also be used to evaluate the sustainability improvement potential of candidate technologies. It is very challenging to effectively quantify the categorized sustainability improvement under complicated scenario, especially when multiple technology candidates are involved in decision-making. Multiple technologies, if used simultaneously, may technically interact each other. The improvement may not be equal to the simple summation of the individual improvement benefits in most cases. An accurate evaluation of sustainability improvement potential requires a significant amount of expert's knowledge from suppliers, engineers, and other involved professionals. Appropriate process simulation is also extremely critical during the evaluation. Therefore, this chapter aims at presenting a general discussion for sustainability improvement rather than providing a comprehensively arithmetic methodology to evaluate technology integration.

Given that a technology set (T) including m technologies is selected from N technology candidates, the categorized sustainability improvement results, economic sustainability performance ($E(T)$), environmental sustainability performance, ($V(T)$), and social sustainability performance ($L(T)$) can be used to evaluate the overall sustainability

status ($S(T)$) after implementing the technology set based on the evaluation of all indicators with the application of multiple technologies, that is:

$$S(T) = \frac{\|(\alpha E(T), \beta V(T), \gamma L(T))\|}{\|(\alpha, \beta, \gamma)\|} \quad (5.10)$$

5.5 Capital Investment Evaluation

Capital investment on implementation of new technologies must be seriously taken into consideration as budget availability is one of the major constraints that influence the final decision towards sustainability improvement (Liu and Huang, 2012). It is easy to evaluate the capital cost when only one technology is to be applied. However, installation of multiple technologies can either increase the application difficulty which may lead to a rise of individual cost or result in some benefit which could reduce the individual cost. The actual total cost for purchasing multiple technologies may not be equal to the summation of the price of acquiring each individual technology. Let the cost on adopting each technology be denoted as B_i . Then the total cost for using a technology set including m technologies can be readily calculated as follows:

$$B_t = p \sum_{i=1}^m B(T_i); \quad m \in [1, N]; \quad (5.11)$$

where p is the coefficient that denotes the cost change due to the simultaneous application of all m technologies. p is equal to 1 if there is no interaction among m technologies.

In order to compare the development options for decision-making, the investment efficiency (I_{eff}) of sustainability improvement with respect to the capital cost can be calculated as:

$$I_{eff} = \frac{\Delta S(T)}{B} \quad (5.12)$$

where $\Delta S(T)$ denotes the improvement of sustainability performance after implementing technology set (T). The larger value I_{eff} is, the more efficient the capital investment is.

5.6 Goal Setting and Need for Sustainability Performance Improvement

In this work, we focus on one-stage sustainability improvement. The goal of the improvement can be determined based on the organization's strategic plan, where specific economic, environmental, and social development goals are denoted as:

E^{sp} = the economic sustainability goal,

V^{sp} = the environmental sustainability goal,

L^{sp} = the social sustainability goal.

By following the same approach used in Eq. (5.9), the overall sustainable development goal can be expressed as:

$$S^{sp} = \frac{\|(\alpha E^{sp}, \beta V^{sp}, \gamma L^{sp})\|}{\|(\alpha, \beta, \gamma)\|}, \quad (5.13)$$

where α , β , and γ take the same values as those used in Eq. (5.9) for consistency.

Given the overall budget limit (B_{limit}) for capital investment, an idea technology or technology set has to fulfill the following requirement:

$$S(T) \geq S^{SP} \quad (5.14)$$

$$E(T) \geq E^{SP} \quad (5.15)$$

$$V(T) \geq V^{SP} \quad (5.16)$$

$$L(T) \geq L^{SP} \quad (5.17)$$

$$B_t \leq B_{\text{limit}} \quad (5.18)$$

5.7 Identification of Superior Technologies

A simple, yet effective approach is introduced here to suggest appropriate technology or technology set which can help decision-makers to promote sustainability improvement. Sustainability assessment of electroplating systems and potential technologies as well as the analysis of capital investment mentioned earlier can then be used to systematically fulfill the technology identification task. The ideal solution which can be one or multiple technologies has to achieve the requirement of sustainability improvement and not exceed the investment budget limit at the same time.

To help the industrial organization select a solution most suitable for the system, the methodology should generate the following types of information:

- a) Evaluate current sustainability status with Eqs. (5.5)-(5.9) using selected sustainability indicators.
- b) Set sustainability improvement goal. If the sustainability status is unsatisfactory, then continue.
- c) Generate the improvement options based on the availability of technologies. For instance, $2^N - 1$ technology sets can be obtained, if N technologies are identified.
- d) Investigate the capabilities of the technologies for the improvement of economic, environmental, social, and overall sustainability.
- e) The total cost for the selected set of technologies can also be calculated using Eq. (5.11). The investment efficiency I_{eff} can be calculated based on Eq. (5.12) accordingly.
- f) Eliminate the technology set of which either the capital cost exceeds the budget limit or the improvement does not meet the expectation.

g) Prioritize the remaining technology set according to the improvement percentage within budget limit, capital investment with the satisfaction of sustainable development goal, as well as the investment efficiency.

With these, the industrial organization should be able to select the most preferred technology or technology set for application.

5.8 Case Study

An electroplating company with a number of zinc plating lines is selected to study the applicability of the introduced sustainability metrics system and performance improvement method. A representative zinc plating line is selected, which has a production capacity of six barrels of parts per hour, 110 kg/barrel, and the plant operates 300 days/yr. Figure 3 shows a flowsheet of the plating process. The purchase price of unfinished parts and the sale price of plated products are \$4/kg and \$4.8/kg, respectively. Electricity is the only the energy source for the line and the annual energy consumption is 4.02×10^6 kWh/yr. Fresh water consumption is at 1.33×10^5 m³/yr. The alkaline solvent used for part cleaning is consumed at the rate of 0.0062kg/kg-part; the plating chemical (Zinc Chloride) is consumed at the rate of 0.025kg/kg-part. The total hazardous waste emission is 0.04 kg/kg-part. The parts return rate is 8%, based on the company's record. The company receives about 20 complains per year from the local community and end-use companies. The process safety is rated on a scale of 0 to 100 with 0 being no safety and 100 the safest. Based on the feedback from a group of process and environmental experts, the current process safety is rated at 65. The process safety analysis is conducted once a month. It is assumed that 30 employees are hired for production of a three-shift per day. The average annual salary of employees is in the range of \$45,000.

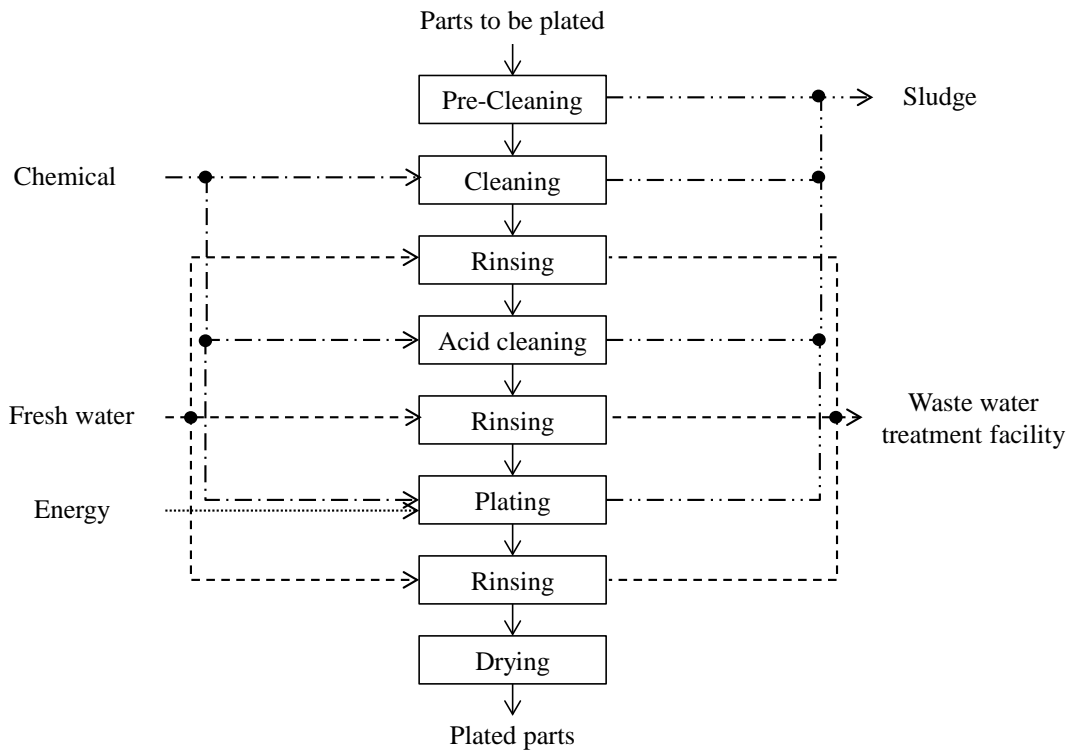


Figure 5.3. Typical electroplating process.

5.8.1 Selection of Sustainability Indicators

A small set of sustainability indicators metrics system listed Table 5.4 is used for evaluate process performance. The assessment result is shown in Table 5.5. The evaluation result of each indicator under best and worst scenarios are also provided in order to process the data normalization of which the calculated results are shown in the last column of Table 5.5. A project team of company management personnel, engineers, suppliers, customers, and some local community representatives is formed to determine the weighting factors for sustainability assessment. The agreed weighting factors for the five economic indicators, six environmental indicators, and three social indicators are (1, 2, 1, 1, 3), (1, 1, 2, 2, 2, 5),

and (1, 1, 1), respectively. The categorized performance of economic, environmental, and social sustainability is 0.34, 0.46, and 0.38, respectively, while the overall sustainability performance can be obtained as 0.40 with respect to equally important triple bottom line.

Table 5.4. Selected sustainability metrics.

Metrics	Indicators		Value
Economic sustainability	E1	Value added	\$
	E2	Value added per direct employee	\$
	E3	Net income	\$
	E4	Capital investment on new technology	\$
	E5	Product defect rate	%
Environmental sustainability	V1	Total net energy usage per unit value added	kWh/\$
	V2	Total net energy usage per kg product	kWh/kg
	V3	Hazardous cleaning chemical usage per kg product	kg/kg
	V4	Hazardous plating chemical usage per kg product	kg/kg
	V5	Net water consumed per kg product	kg/kg
	V6	Hazardous liquid waste per unit value added	kg/\$
Social sustainability	S1	Number of complaints	/y
	S2	Number of process safety analysis	/y
	S3	Process safety index	

Table 5.5. Result of system sustainability assessment.

Metrics		Current	Worst	Best	Normalized
Economic sustainability	E1	3.8×10^5	1.0×10^5	5.0×10^5	0.70
	E2	1.27×10^4	7.0×10^3	3.0×10^4	0.25
	E3	8.89×10^4	0	2.0×10^5	0.44
	E4	0	0	3.50×10^5	0.00
	E5	8%	15%	2%	0.54
Environmental sustainability	V1	1.06	1.6	0.5	0.49
	V2	0.85	1.6	0.4	0.63
	V3	0.0062	0.0085	0.0004	0.28
	V4	0.025	0.05	0.008	0.60
	V5	0.028	0.1	0.0025	0.74
	V6	0.06	0.1	0.005	0.63
Social sustainability	S1	20	100	0	0.80
	S2	12	0	52	0.23
	S3	65	0	100	0.65

5.8.2 Technology Candidate Selection

The increasing interest on sustainable development requires industrial systems to make appropriate technology realization decisions to enhance sustainability performance. A number of electroplating specific P3 technologies have been developed by integrated process design and operational optimization (Lou and Huang, 2000; Xiao and Huang, 2012). Four different technologies that could potentially improve the sustainability performance to the next level will be investigated in this study. A comprehensive sustainability evaluation on these technologies is essential for sustainability performance improvement.

Technology 1: Cleaning and rinse operation optimization technology. In any plating line, each step of cleaning (e.g., presoaking, soaking, electro-cleaning, and acid cleaning) is always followed by one or two steps of rinse. Chemical conservation and wastewater reduction are largely dependent on chemical concentration setting, chemical feeding policy, rinsing water flow rate, as well as cleaning and rinse time. Most unfinished parts are equally treated in the cleaning and rinsing tanks without taking into consideration of dynamic chemical concentration in the tanks due to chemical reactions between cleaning chemicals and dirt on treated work pieces. In operation, the concentration of cleaning chemicals left in the tank can only be adjusted periodically rather than dynamically. Thus, constant treatment time often leads to over-cleaned parts which result in a higher chemical and water consumption and under-cleaned parts which may cause some product defects. Based on a two-layered hierarchical dynamic optimization technique, the optimal settings for chemical concentration and rinsing water flow rate are identified for unit-based consumption minimization in the lower layer of this technology. In the upper layer, the processing time distributions for all the cleaning and rinse operations are adjusted so as to explore the global opportunities of minimizing the overall operating cost and waste generation. The developed technology is capable of generating a dynamically adjustable cleaning and rinsing operation, based on the evaluation of job order change, waste generation in different process units, chemical and energy consumption, etc. This technology can contribute significantly to the minimization of the quantity and toxicity of wastewater while maintaining the production rate (Gong *et al.*, 1997).

Figure 5.4 depicts the change of dirt residue on the work pieces before and after implementing this technology. An electroplating process with conventional operating approach is shown in Figure 5.4(a). Due to the consumption of cleaning chemical along the time, the work pieces entered the clean tank at the beginning would have over-cleaning issue while the ones cleaned in the end would not get sufficient cleaning if constant treatment time is applied. Both scenarios may lead to serious product quality issues consequently. With the application of this technology, parts are equally cleaned while the reduction of chemical and water usage as well as a rise of production rate are achieved simultaneously (Figure 5.4(b)).

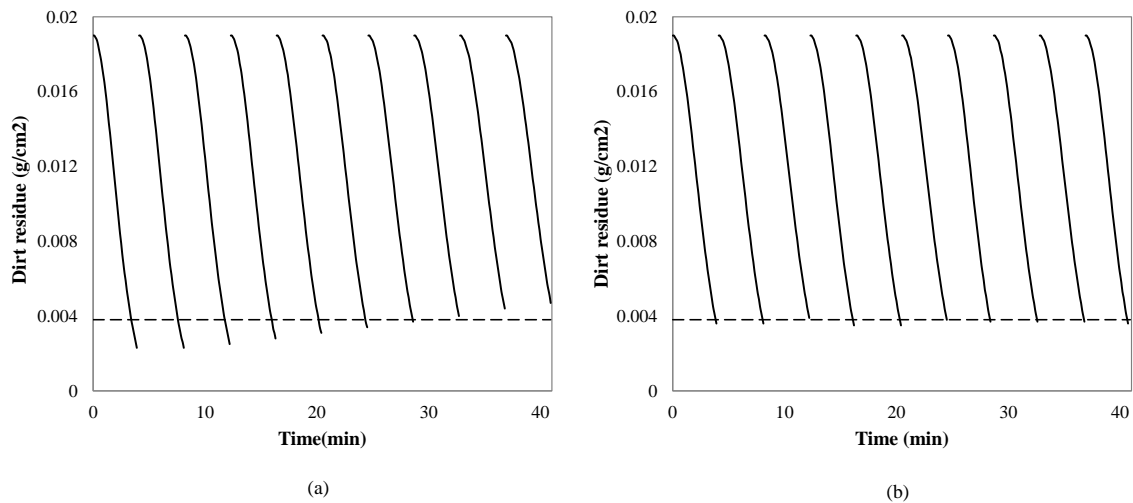


Figure 5.4. Dynamics of the dirt residue on the surface of parts through a cleaning process: (a) using a conventional cleaning technique, and (b) using an optimized cleaning technique (Bhadbhade, 2015).

The adoption of technology 1 will lead to a substantial reduction of the usage of cleaning chemicals and fresh water which also results in a significant reduction of hazardous waste emissions. The production rate will have a small rise while energy consumption

slightly decreases. However, the process becomes more complicated and slightly more dangerous. Therefore, process safety check and analysis need to be accomplished more frequently in order to avoid any accident.

Technology 2: Optimal water use and reuse network design technology. In an electroplating line, freshwater is fed to different rinse units for rinsing off the dirt and solution residues on the surface of parts. Water that is used from a specific rinsing unit can either partially or entirely be reused by some rinsing steps. By this technology, an optimal water allocation network can be designed for a plating line of any capacity, and the optimal operation strategy for the network can also be developed based on rinsing water flow dynamics (Yang *et al.*, 1999; Zhou *et al.*, 2001). Figure 5.5(b) describes a modified water use and reuse network based on this technology. Comparing to the traditional electroplating process (Figure 5.5(a)), this technology maximizes the use and reuse of water which leads to the substantial sustainable development.

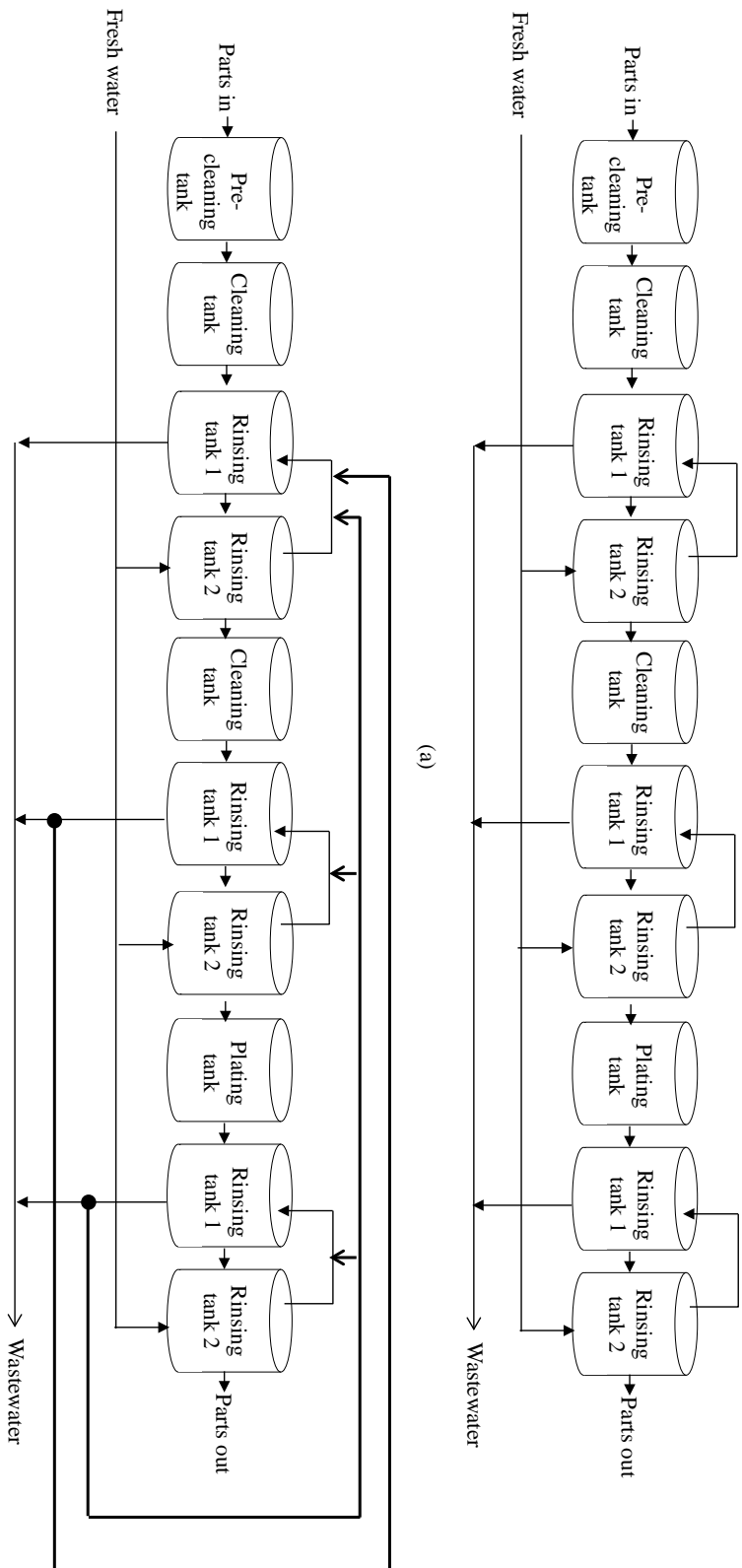


Figure 5.5. Water use and reuse in a plating line: (a) the original process flow sheet, and (b) the new process flow sheet with an embedded optimal water use and reuse network design technology.

The biggest advantage of applying technology 2 is the reduction of water consumption as well as corresponding waste emission. The consumption of cleaning and plating chemicals do not have significant change. On the contrary, it can also result in a slight decrease in production rate due to additional processes and a rise of energy consumption due to additional equipment. In the meanwhile, water reuse leads to a slight increase of process complexity and product defect rate. More frequent process check is also needed to ensure the process safety.

Technology 3: Near-zero chemical and metal discharge technology. In electroplating operations, huge amounts of chemical solvents and plating solutions are consumed not only because of the chemical reaction but also due to the loss from drag-out which is washed off as waste emission. The developed technology can be used to design an effective direct recovery system based on a reverse drag-out concept that can minimize drag-out related chemical/metal loss safely (Zhou *et al.*, 2001). Figure 5.6(a) depicts a traditional plating process of which the plated parts are treated in a series of rinsing tanks with flow rinsing water to wash off the remaining plating solution. A new modified process based on this technology is presented in Figure 5.6(b). A series of static rinsing method based rinsing units form a solution recovery system in which freshwater is periodically fed into rinse unit R_N first, and the solution-containing rinse water in R_N then flows to R_{N-1} , ..., and R_1 periodically. Finally, the solution containing rinse water in R_1 is periodically pumped into plating unit E to maximize the use of plating solution by recovering the unnecessary loss of plating solution. This process modification can also be applied to the cleaning process to maximize the use of cleaning chemicals and avoid unnecessary drag-out.

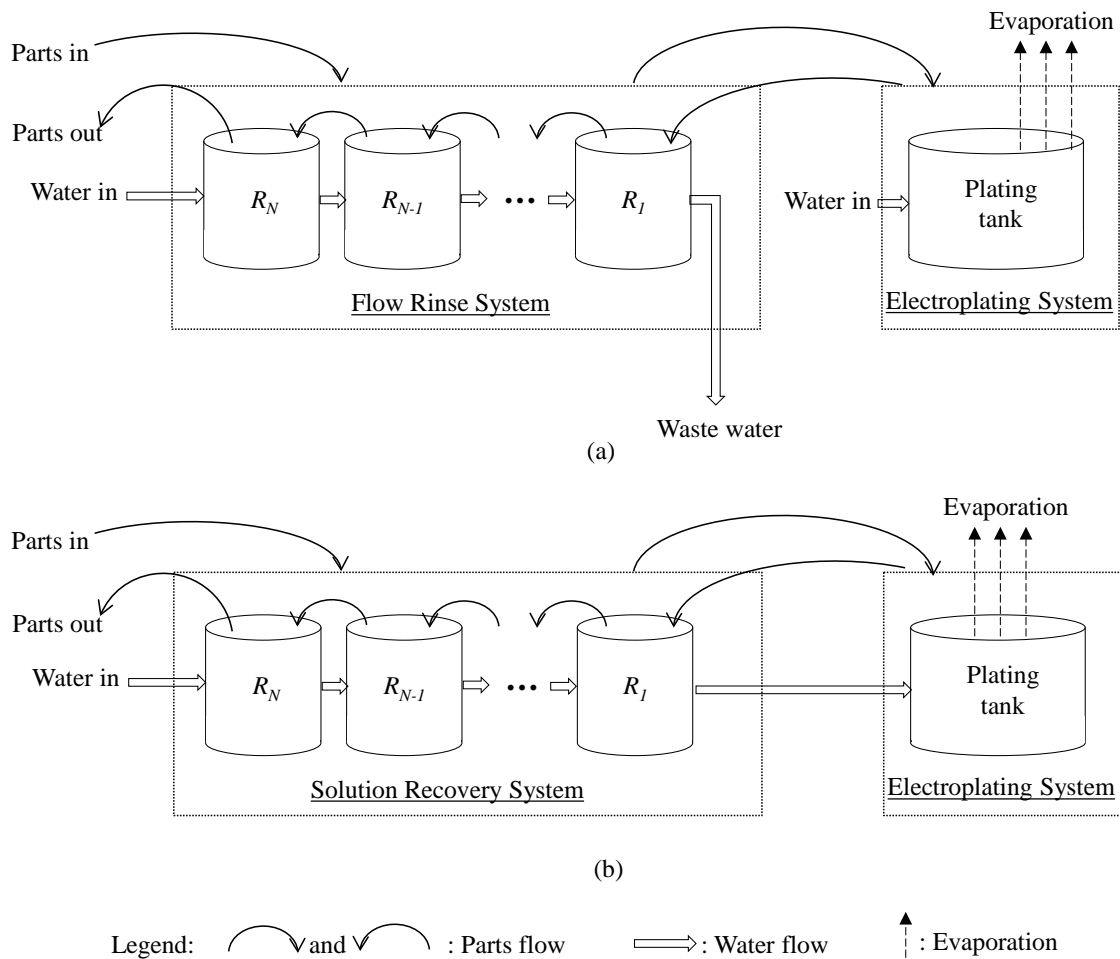


Figure 5.6. Design schemes for electroplating and rinsing: (a) The original electroplating process with a flow rinse system, and (b) the modified electroplating process with a solution recover system using a static rinse system (Zhou *et al.*, 2001).

The most improvement with the application of technology 3 is the reduction of waste emission through minimizing chemical consumption as well as waste emission. Water consumption can be reduced dramatically due to the static rinsing method and the reduction of chemicals left on electroplating parts. The usage of cleaning and plating chemicals can also be reduced accordingly. However, the drag-out minimization process leads to a decrease of production rate and increase of energy consumption due to additional processing

time. In the meanwhile, more frequent process check is also needed to ensure the process safety.

Technology 4: Environmentally conscious dynamic hoist scheduling technology (Kuntay *et al.*, 2006). Source reduction can be achieved through dynamic hoist scheduling during production. With the unit-based minimization of chemical and water consumption, while meeting product quality requirement, the amount of waste generated in each units can then be calculated. An optimal hoist schedule with maximum production rate and minimum waste generation can be identified consequently using various techniques such as graph-assisted search algorithm (Xu and Huang, 2004).

With the application of dynamic scheduling technology, a dynamically adjustable production schedule can be obtained based on the evaluation of job order change, waste generation in different process units, chemical and energy consumption. In the meanwhile, parts are cleaned and plated with the reduction of chemical and water usage simultaneously. The dynamic control of electroplating process from the application of Technology 4 results in significant reduction of the non-value added time and increase of production rate thereafter. The usage of cleaning and plating chemicals as well as energy consumption can also be minimized to some extent. However, it requires substantial investment in dynamic process control and product quality analysis. More frequent process check is also needed to ensure the process safety.

5.8.3 Sustainability Assessment of Technologies

The four selected technologies can improve system performance in different ways, which can be demonstrated through sustainability assessment using appropriate

sustainability indicators. For the four technologies, there are a total of 15 different technology sets, including four sets with one technology each, six sets with two different technologies each, four sets with three different technologies each, and one set of all four technologies.

Sustainability assessment of the four individual technologies and sustainability improvement potential are conducted first. Tables 6 through 9 show the evaluation of the sustainability performance after application each technology in the process. Note that the application of technologies may result in a decrease of production rate or an increase of energy consumption and process safety index, and thus the improvement of certain categories of sustainability can be negative. The investments for the use of the four technologies are $\$9.45 \times 10^4$, $\$6.55 \times 10^4$, $\$7.75 \times 10^4$, and $\$1.26 \times 10^5$, for Technology 1, 2, 3, and 4, respectively. As one of the key indicators in economic sustainability, the investment on technology is also included in the evaluation (E4). The sustainability assessment is shown in Table 10. The efficiency of capital investment is listed in the last column of Table 10.

Table 5.6. Sustainability assessment of technology 1.

Metrics		T1	Normalized result	Improvement
Economic sustainability	E1	3.86×10^5	0.72	0.02
	E2	1.29×10^4	0.26	0.01
	E3	9.60×10^4	0.48	0.04
	E4	9.45×10^4	0.24	0.24
	E5	4%	0.85	0.31
Environmental sustainability	V1	1.05	0.50	0.00
	V2	0.84	0.63	0.00
	V3	0.003	0.68	0.40
	V4	0.02	0.71	0.12
	V5	0.0264	0.75	0.02
	V6	0.035	0.68	0.05
Social sustainability	S1	20	0.80	0.00
	S2	24	0.46	0.23
	S3	50	0.50	-0.15

Table 5.7. Sustainability assessment of technology 2.

Metrics		T2	Normalized result	Improvement
Economic sustainability	E1	3.75×10^5	0.69	-0.01
	E2	1.25×10^4	0.24	-0.01
	E3	8.71×10^4	0.44	-0.01
	E4	6.55×10^4	0.16	0.16
	E5	7%	0.62	0.08
Environmental sustainability	V1	1.10	0.45	-0.04
	V2	0.88	0.60	-0.03
	V3	0.005	0.43	0.15
	V4	0.025	0.60	0.00
	V5	0.0211	0.81	0.07
	V6	0.042	0.61	-0.02
Social sustainability	S1	40	0.60	-0.20
	S2	24	0.46	0.23
	S3	45	0.45	-0.20

Table 5.8. Sustainability assessment of technology 3.

Metrics		T3	Normalized result	Improvement
Economic sustainability	E1	3.70×10^5	0.68	-0.02
	E2	1.23×10^4	0.23	-0.01
	E3	8.70×10^4	0.43	-0.01
	E4	7.75×10^4	0.19	0.19
	E5	6%	0.69	0.15
Environmental sustainability	V1	1.11	0.44	-0.05
	V2	0.89	0.59	-0.04
	V3	0.004	0.56	0.27
	V4	0.022	0.67	0.07
	V5	0.0254	0.77	0.03
	V6	0.01	0.95	0.32
Social sustainability	S1	15	0.85	0.05
	S2	24	0.46	0.23
	S3	57	0.57	-0.08

Table 5.9. Sustainability assessment of technology 4.

Metrics		T4	Normalized result	Improvement
Economic sustainability	E1	4.07×10^5	0.77	0.07
	E2	1.36×10^4	0.29	0.04
	E3	1.08×10^4	0.54	0.09
	E4	1.26×10^4	0.31	0.31
	E5	3%	0.92	0.38
Environmental sustainability	V1	1.01	0.54	0.04
	V2	0.81	0.66	0.03
	V3	0.002	0.80	0.52
	V4	0.017	0.79	0.19
	V5	0.026	0.76	0.02
	V6	0.035	0.68	0.05
Social sustainability	S1	20	0.80	0.00
	S2	24	0.46	0.23
	S3	60	0.60	-0.05

Table 5.10. Results of sustainability improvement with respect to different technology options.

No.	Selected Technology	E	V	L	S	B ($\times 10^4$ \$)	Ieff ($\times 10^{-6}$)
1	T(1)	0.56	0.68	0.59	0.61	9.45	6.46
2	T(2)	0.45	0.60	0.50	0.52	6.55	7.94
3	T(3)	0.48	0.75	0.63	0.63	7.75	8.13
4	T(4)	0.62	0.72	0.62	0.65	12.55	5.18
5	T(1,2)	0.49	0.71	0.55	0.59	15.2	3.88
6	T(1,3)	0.51	0.80	0.61	0.65	16.34	3.98
7	T(1,4)	0.60	0.73	0.60	0.65	20.9	3.11
8	T(2,3)	0.47	0.76	0.56	0.61	13.59	4.49
9	T(2,4)	0.51	0.71	0.58	0.61	18.15	3.36
10	T(3,4)	0.53	0.82	0.63	0.67	19.29	3.47
11	T(1,2,3)	0.50	0.80	0.59	0.64	21.38	2.99
12	T(1,2,4)	0.53	0.73	0.58	0.62	25.69	2.41
13	T(1,3,4)	0.56	0.82	0.63	0.68	26.78	2.54
14	T(2,3,4)	0.52	0.81	0.59	0.65	24.17	2.69
15	T(1,2,3,4)	0.55	0.85	0.63	0.69	30.86	2.24

5.8.4 Technology Recommendation

It is assumed that this plating company sets its economic, environmental, and social sustainability goals, E^{sp} , V^{sp} , and L^{sp} , are 0.51, 0.72, and 0.61, respectively. The overall sustainable development goal is thus 0.62, according to Eq. (13). The overall limit of investment is defined as $\$2.2 \times 10^5$ at the same time.

According to Step (e) of the technology identification procedure, Technology set No. 12, 13, 14, and 15 are eliminated at the first place because of excess capital investment compared to the budget limit. The overall sustainability improvement brought by the application of technology set No. 1, 2, 5, 8, and 9 does not meet the requirement (i.e., 0.62). Technology set No. 3 can only enhance the economic sustainability to 0.48. The performance of social sustainability with the application of technology set No. 11 is 0.59, which is under the limit of 0.61. Therefore, only technology set No. 4, 6, 7, and 10 meet all the requirements for sustainability improvement. Table 11 shows the analysis result (the technology sets use the same index number for consistency). The final results are then prioritized under three different orders. If the company wants to achieve the maximum improvement of sustainability, then the technology set No. 10 is the top choice while set No. 4, 6, and 7 can reach same sustainability performance. If the company prefers the lowest investment, then the order changes to No. 4, 6, 10, and then 7. If the investment efficiency is the priority, then the recommended technology sets are in the order of No. 4, 6, 10, and then 7.

Table 5.11. Results of sustainability decision-making analysis.

No.	Selected Technology	E	V	L	S	B ($\times 10^4$ \$)	Ieff ($\times 10^{-6}$)
4	T(4)	0.62	0.72	0.62	0.65	12.55	5.18
6	T(1,3)	0.51	0.80	0.61	0.65	16.34	3.98
7	T(1,4)	0.60	0.73	0.60	0.65	20.9	3.11
10	T(3,4)	0.53	0.82	0.63	0.67	19.29	3.47

5.9 Concluding Remarks

As one of the most polluting industries, electroplating must make a great effort on pollution prevention. In the meanwhile, the economic and social interest of the industry must also be taken into consideration. The sustainable development of electroplating industry (SEP) framework provides clear guidance for the electroplating industry to evaluate performance and enhance development from sustainability point of view, not only maintaining the significance of traditional P2 but also taking economic and social aspects into account. A comprehensive sustainability metrics system is developed based on the analysis of SEP framework. Effective sustainability assessment is then conducted to provide deep insight on system sustainability performance. A number of P3 technologies are also examined with the proposed sustainability metrics system. Based on the systematic decision-making approach introduced, the industry can then select the most practical technology or technology set to enhance its sustainability performance for short-term and long-term sustainable development.

CHAPTER 6 FUZZY DYNAMIC PROGRAMMING BASED MULTISTAGE DECISION-MAKING APPROACH FOR LONG-TERM SUSTAINABILITY IMPROVEMENT

Sustainability which is highly associated with people, planet, and profit is widely considered a continuous terminology—sustainable development (SD). Sustainable development is essentially the improvement of the three pillars of sustainability, that is, economics, environment and society. There are two key concepts associated with sustainable development: the concept of ‘essential needs’ for the living of human beings and the idea of limitations imposed by the stage of technology and social organization on the environment’s ability to meet present and future needs (WCED, 1987). According to The World Bank (Bank, 2016), sustainable development is to achieve the growth that must be both socially acceptable and environmentally benign to build shared prosperity for meeting the needs of today’s population and continuing to meet the needs of future generations.

Nowadays, sustainability and sustainable development are gaining more and more attention from a variety of fields including industry, academia, government, and so on. The challenge of meeting human development needs while protecting the earth's life support systems confronts scientists, technologists, policy makers, and communities from local to global levels. Numerous scientists also introduced many approaches to enhance the sustainability performance. Many of them are very effective and easy to follow. For instance, Liu and Huang created a Monte Carlo-based sustainability enhancement method for sustainability improvement at single stage (Liu and Huang, 2015). Song and coworkers proposed a sustainability assessment and improvement framework for the short-term sustainable development of electroplating systems (Song *et al.*, 2016). A practical

sustainability based technology evaluation and selection approached was introduced to achieve short term sustainability improvement goal (Liu and Huang, 2012).

Nevertheless, to deliver the benefit for people, planet, and prosperity requires not only short term sustainability effort to solving the immediate sustainability needs but also long-term sustainability roadmap that could guide current and future developing path of the activities of human beings. According to the “2030 Agenda for Sustainable Development” published by United Nations’ Sustainable Development Knowledge Platform (Platform, 2015), the goals and targets of sustainable development in the next fifteen years are: (i) end poverty and hunger and ensure that all human beings can fulfill their potential in dignity and equality and in a health environment; (ii) protect the planet from degradation through sustainable consumption and production; (iii) ensure that all human beings can enjoy prosperous and fulfilling lives and that economic, social and technological progress occurs in harmony with nature. The view of sustainability from the United Nations highlights the significance of long-term sustainable development. However, most of existing studies only focus on a one-stage development effort although sustainable development requires efforts on both short-term and long-term actions. Piluso *et al.* studied a fuzzy logic based approach to short-term to midterm prediction for sustainability improvement of industrial systems under uncertainty (Piluso *et al.*, 2010). It is of great importance to extend current studies concentrating one-stage or short-term sustainability improvement effort to the longer view.

Long-term sustainable development involves a series of development actions taken in consecutive improvement stages. It is comprehensible that effective science and technology are critical to achieve the goal of sustainable development. Development plan

must be carefully determined at each stage in order to reach the ultimate development goal. Therefore, long-term sustainable development can be transformed to sequential multistage decision-making (MDM). Figure 6.1 depicts the multistage decision-making to achieve sustainable development. However, there are two major challenges that must be tackled clearly.

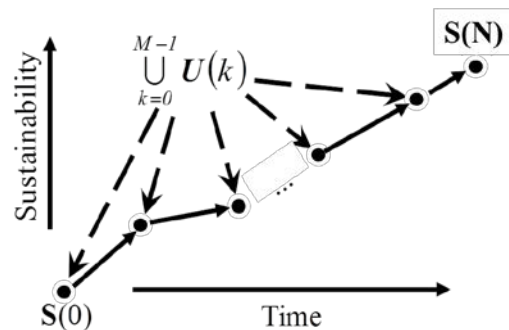


Figure 6.1. General scheme of long-term sustainable development (Liu *et al.*, 2009).

The first challenge in sustainability improvement is the uncertainty issues involved in the sustainability assessment and decision-making. Piluso and coworker pointed out that the existence of various types of uncertainties that are associated with the available data poses a great challenge to the analyzing accuracy of sustainability assessment (Piluso *et al.*, 2010). Sustainability assessment and decision-making for sustainable development are always accompanied by the intrinsic nature of uncertainty and subjective. In sustainability study, data and information uncertainty arises from the complex nature of industrial systems (Dovers *et al.*, 1992; Howarth, 1995). For example, the multifaceted makeup of the inter-entity dynamics, dependencies, and relationships, the prospect of forthcoming environmental policies, and the interrelationship among the triple-bottom-line aspects of

sustainability are always uncertain. Sometimes, the data about material or energy consumption, toxic/hazardous waste generation, and market fluctuation, etc., of an industrial system are often incomplete and imprecise. What's more, the constraints and objective of sustainable development might have some degree of freedom rather than being crisply defined. Uncertainties also appear in the activities for future planning, such as regulation changes, supply chain structures, etc.

In addition, it is also arguable that sustainability assessment and sustainable development are considered subjective concepts in which human factors are heavily involved in the whole process. Sustainability assessment involves many subjective judgments including the use of weighting factors. Although economic sustainability involves mostly the objective evaluation of deterministic variables through economic ways, environmental sustainability typically consists of both objective and subjective aspects that cannot be obtained accurately. In addition, evaluating social sustainability also contains analysis of many subjective objects. Therefore, the multistage decision-making task will incontrovertibly aggregate the uncertainty issues in each stage and leads to the result of long-term multistage sustainable development less trustable.

The other major challenge in the long-term sustainable development is the lack of effective methodology to identify the optimal development strategy. There is an urgent need for the development of predictive multistage models for decision making (Hersh, 1999). To solve the multistage decision-making problems, a number of approaches have been developed for this purpose including multi-criteria decision-making (MCDM) approach (Greening and Bernow, 2004), decision support systems (DSS) (Hersh, 1999), Scenario Tree

(Høyland and Wallace, 2001), and so on. Among a number of well-known multistage optimization methods, dynamic programming (DP) is a powerful optimization technique that is particularly applicable to many complex problems requiring a sequence of interrelated decisions (Denardo, 2012). The DP as a theory for dealing with a wide range of problems encountered in design, pattern recognition, control theory, and resource allocation problems has been around for almost four decades (Sakoe and Chiba, 1978; Bertsekas *et al.*, 1995; Bellman and Dreyfus, 2015).

Given that the conventional DP approach commonly addresses only deterministic values, it cannot be applied to the sustainability study where uncertainty issue exists (Bellman and Dreyfus, 2015). Recently, fuzzy dynamic programming (FDP), which rely heavily on the integration of conventional DP and fuzzy set theory, is developed as a technique for solving problems that involve subjective and uncertain objectives (Bellman and Zadeh, 1970; Kacprzyk and Esogbue, 1996; Slowiński, 2012). With a modified approach to evaluate sustainability performance, FDP could be used to establish an optimal development path for long-term sustainable development by relying on fuzzy set theory addressing uncertainty and subjective issue and DP identifying multistage optimal decisions (Huang, 2008; Piluso and Huang, 2008; Liu *et al*, 2009).

In this chapter, a fuzzy dynamic programming based multistage decision-making approach is introduced to provide optimal decisions for long-term sustainability improvement of industrial systems. A general framework of multistage optimization task and the fundamental knowledge of fuzzy set theory are mentioned at the beginning. Fuzzy set theory is then applied to evaluate the sustainability performance and satisfaction of goal

achievement. The development actions taken at each stage are also evaluated based on fuzzy set theory. Then FDP approach is used to find the best development path with the established state transition function. A simplified case study is used to demonstrate the efficacy of this methodology.

6.1 Framework of Multistage Decision-Making

In 2008, Huang developed a framework for multistage hierarchical decision making methodology for sustainable development of industrial systems by resorting to the fuzzy set theory and a dynamic programming technique (Huang, 2008). The effectiveness of the methodology was tested by solving a simple two-stage sustainable development program. Piluso and Huang then presented the basic approach of the methodology (Piluso and Huang, 2008). Based on this methodology, Liu *et al.* (2009) studied a system design modification problem for sustainability performance.

In this work, a general framework of the MDM is introduced to better describe the task of long-term sustainability improvement. The multistage decision-making task denoted as Figure 6.1 will be studied as a stage-wised sustainability improvement problem. As shown in Figure 6.2, the overall sustainable development consists of N different consecutive improvement stages. If the status quo of system sustainability is $X(0)$, and a strategic plan provided by industrial decision makers is to improve the level of sustainability to $X(N)$ in N stages (e.g., N years), then the task should be to identify N sets of strategies, $U(k)$, $k = 0, 1, \dots, N-1$. In practice, various mathematical approaches may identify multiple development plans which can satisfy all of the requirements. The optimal plan can then be selected with different optimization approaches. From the systems science point of view, this type of

sustainability development task is a multistage optimization problem. This study applies a fuzzy dynamic programming based approach to identify the best solution for planning long-term sustainable development.

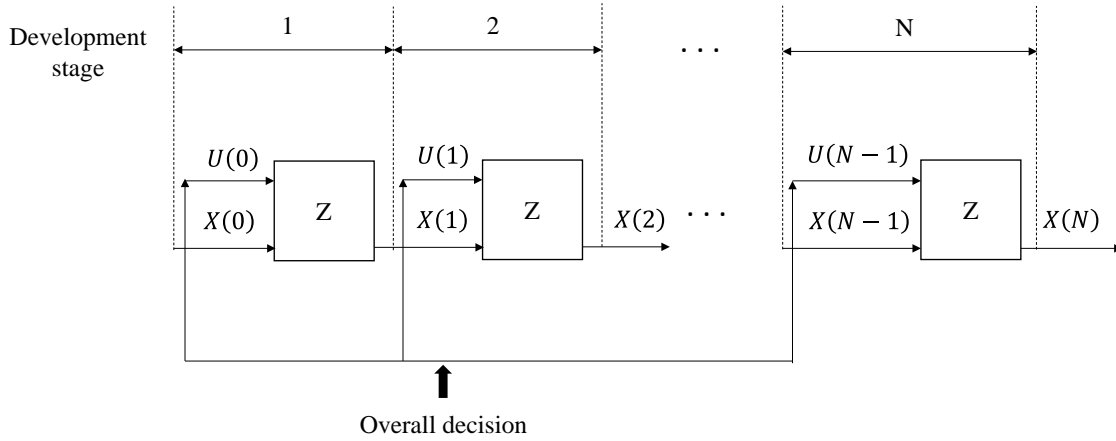


Figure 6.2. Multistage decision-making framework.

The sustainability status $X(k-1)$ can be obtained from the development result of stage $(k-1)$. In order to make the right decision at stage k , an appropriate development goal $X_G(k)$ must be defined by experts to motivate the development. A final decision for stage k , $U(k-1)$ can be made by integrating the current and targeting sustainability status, and constraints of decision actions:

$$U(k-1) = f(X(k-1), X_G(k), C(k)) \quad (6.1)$$

where $C(k)$ represents the constraints that are confronted at stage k .

Based on the stage-based analysis of sustainability enhancement, the overall development path is highly associated to the N development actions implemented consecutively in N stages and the sustainability status at the initial and final development path. Thus, the selected long-term development decision D can be expressed as

$$D = F(U(0), U(1), \dots, U(k-1), X(0), X(N)) \quad (6.2)$$

where the actual sustainability status at the end of development $X(N)$ and defined sustainability improvement goal $X_G(N)$ should be the same.

A number of major tasks need to be completed based on the proposed framework. The first task is to evaluate sustainability status $X(k)$ at each stage, from the beginning of developing period to the end. The evaluation must provide an effective way to overcome the challenge posed by the existence of various uncertainties which appear in the data and information either available or to be acquired. The second one is to identify appropriate development action $U(k)$ which leads to the change of sustainability status from $X(k)$ to $X(k+1)$. The state transition function associated with the decision action must be accurately established based on the comprehensive evaluation of development action $U(k)$. The third one is to select the optimal development plan based on the evaluation of system status, development actions, and given constraints.

6.2 Fuzzy Set Theory

In order facilitate the introduction of FDP methodology, general definitions of fuzzy sets are described in this section (Bellman and Zadeh, 1970).

Definition 1: Fuzzy set

Let $X = \{x\}$ be a collection of objects, then a fuzzy set A in X is defined to be a set of ordered pairs:

$$A = \{(x, \mu_A(x))\}, \quad x \in X \quad (6.3)$$

where $\mu_A(x)$ is called the grade of membership of x in A , and $\mu_A : X \rightarrow M$ is a function from X to a space M called the membership space. Note that the membership function $\mu_A(x)$ typically has the upper and lower boundaries of 1 and 0 which represent the highest and lowest grades of membership. A high value of membership function implies that it is very likely for x to be in A . An example of fuzzy membership function $\mu_A(x)$ is depicted in Figure 6.3.

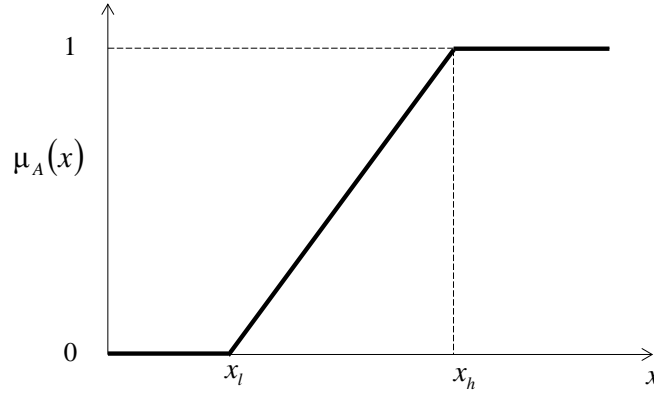


Figure 6.3. Example of fuzzy membership function.

Definition 2: The union of two fuzzy sets

Let A and B be two fuzzy sets with membership functions $\mu_A(x)$ and $\mu_B(x)$ respectively. The membership function of the union $C = A \cup B$ is obtained as:

$$\mu_C(x) = \mu_A(x) \vee \mu_B(x), \quad x \in X \quad (6.4)$$

The operation shown in Eq. (6.4) can be calculated as:

$$\mu_A(x) \vee \mu_B(x) = \max(\mu_A(x), \mu_B(x)) \quad (6.5)$$

Definition 3: The intersection of two fuzzy sets

Similar to the Definition 2, the membership function of the intersection $D = A \cap B$ is defined as:

$$\mu_D(x) = \mu_A(x) \wedge \mu_B(x) = \min(\mu_A(x), \mu_B(x)), \quad x \in X \quad (6.6)$$

Similar to Eq. (6.5), Eq. (6.6) can be expressed as:

$$\mu_A(x) \wedge \mu_B(x) = \min(\mu_A(x), \mu_B(x)) \quad (6.7)$$

6.3 Fuzzy Set Theory Based Sustainability Assessment with Uncertainty

Accurate sustainability assessment of industrial systems is the foundation towards industrial sustainable development. The sustainability evaluating tool, sustainability metrics system, must be carefully selected. Note that sustainable development requires the evaluation of system sustainability status at each stage, it is assumed that the selected sustainability metrics system consists of the best indicators to characterize the system sustainability performance and remains the same in the whole development period.

Typically, sustainability assessment involves the evaluation of both objective and subjective information. The analysis of economic sustainability is generally objective; environmental sustainability assessment involves objective and subjective analysis; social sustainability assessment contains mostly subjective judgement which may not have deterministic values. In addition, to handle the uncertain data and information involved in the evaluation may increase the complexity of system analysis. In this work, fuzzy set theory is applied to characterize the sustainability status as well as the improvement potential for the decision candidates.

6.3.1 Fuzzy Set Theory Based Sustainability Performance Assessment

For a process system of interest, a selected sustainability metrics set for the sustainability assessment is denoted as:

$$S = \{E, V, L\}, \quad (6.8)$$

where $E = \{E_i | i = 1, 2, \dots, N_E\}$ is the set of economic sustainability indicators; $V = \{V_i | i = 1, 2, \dots, N_V\}$ is the set of environmental sustainability indicators; $L = \{L_i | i = 1, 2, \dots, N_L\}$ is the set of social sustainability indicators. N_E , N_V , and N_L are the number of indicators that can be used to quantify economic, environmental, and social sustainability, respectively.

The sustainability status at stage k , $X(k)$, can be expressed as

$$X(k) = \{X^E(k), X^V(k), X^L(k)\} \quad (6.9)$$

where: Economic sustainability	$X^E(k) = \{X_i^E(k) i = 1, 2, \dots, N_E\}$
Environmental sustainability	$X^V(k) = \{X_i^V(k) i = 1, 2, \dots, N_V\}$
Social sustainability	$X^L(k) = \{X_i^L(k) i = 1, 2, \dots, N_L\}$

Given that the analysis involves data with certainty and subjective judgement, all of the indices associated with uncertainty data are evaluated based on fuzzy set theory while the rest indices are evaluated through conventional normalization. By using selected sustainability indices, the status of the sustainability of system can be assessed using the data collected from the system. For i -th economic sustainability indicator where uncertainty issues exists, the evaluation can be obtained as:

$$X_i^E(k) = \mu_p^{E,i}(X(k)), \quad i = 1, 2, \dots, N_E \quad (6.10)$$

where $\mu_p^{E,i}(X(k))$ which has a value between 0 and 1 is the performance fuzzy membership function to characterize the system status $X(k)$ using i -th economic sustainability indicator. An example of the fuzzy membership function which defines as the performance of system status under i -th economic sustainability indicator can be calculated as:

$$\mu_P^{E,i}(X(k)) = \begin{cases} 0 & 0 \leq X(k) \leq X_{i,low}^E \\ \frac{X(k) - X_{i,low}^E}{X_{i,high}^E - X_{i,low}^E} & X_{i,low}^E < X(k) < X_{i,high}^E \\ 1 & X(k) \geq X_{i,high}^E \end{cases} \quad (6.11)$$

where $X_{i,low}^E$ and $X_{i,high}^E$ are the constants that define the boundaries of fuzzy membership functions.

With the application of fuzzy set theory, the evaluation of system status using j -th environmental sustainability indicator and l -th social sustainability indicator can be expressed as:

$$X_j^V(k) = \mu_P^{V,j}(X(k)), \quad j = 1, 2, \dots, N_V \quad (6.12)$$

$$X_l^L(k) = \mu_P^{L,l}(X(k)), \quad l = 1, 2, \dots, N_L \quad (6.13)$$

where the example fuzzy membership function, $\mu_P^{V,j}(X(k))$ and $\mu_P^{L,l}(X(k))$ can be defined as:

$$\mu_P(X_j^V(k)) = \begin{cases} 0 & 0 \leq X(k) \leq X_{j,low}^V \\ g(X(k), X_{j,low}^V, X_{j,high}^V) & X_{j,low}^V < X(k) < X_{j,high}^V \\ 1 & X(k) \geq X_{j,high}^V \end{cases} \quad (6.14)$$

$$\mu_P(X_l^L(k)) = \begin{cases} 0 & 0 \leq X(k) \leq X_{j,low}^L \\ h(X(k), X_{j,low}^L, X_{j,high}^L) & X_{j,low}^L < X(k) < X_{j,high}^L \\ 1 & X(k) \geq X_{j,high}^L \end{cases} \quad (6.15)$$

where $X_{i,low}^V$, $X_{i,high}^V$, $X_{i,low}^L$ and $X_{i,high}^L$ are the constants that define the boundaries of fuzzy membership functions; functions $g(X(k), X_{j,low}^V, X_{j,high}^V)$ and $h(X(k), X_{j,low}^L, X_{j,high}^L)$ are determined by experts and stake holders.

Note that the evaluation process shown in Eq. (6.11) can be easily transformed to normalization when crisp and deterministic data are available. These data can be used to estimate categorized sustainability for the system, i.e. $X^E(k)$, $X^V(k)$, and $X^L(k)$, which are called the composite sustainability indices. In practice, all of the data has the range between 0 and 1 evaluated by either conventional normalization or fuzzy membership function. The results calculated through fuzzy membership function can be treated as conventional normalized values which makes it possible to integrate fuzzy grades and normalized values together. Therefore, evaluation of $X^E(k)$, $X^V(k)$, and $X^L(k)$ can be achieved by acquiring the weighted summation through applying a set of weighting factors which are generally defined by experts.

$$X^E(k) = \sum_{i=1}^{N_E} a_i X_i^E(k) \quad (6.16)$$

$$X^V(k) = \sum_{j=1}^{N_V} b_j X_j^V(k) \quad (6.17)$$

$$X^L(k) = \sum_{l=1}^{N_L} c_l X_l^L(k) \quad (6.18)$$

where a_i , b_i , and c_i are the weighting factors associated with indices, reflecting the relative importance of an individual index against others in overall assessment. In this work, $\sum_{i=1}^{N_E} a_i$,

$\sum_{j=1}^{N_V} b_j$, and $\sum_{l=1}^{N_L} c_l$ are all equal to 1.

The overall sustainability performance at stage k ($X^S(k)$) can be obtained based on the integration of $X^E(k)$, $X^V(k)$, and $X^L(k)$. In this study, a conventional weighted summation based sustainability integration approach is used, that is:

$$X^S(k) = \left\| \left(\alpha X^E(k), \beta X^V(k), \gamma X^L(k) \right) \right\| \quad (6.19)$$

where α , β , and γ are the assigned weighting factors for economic, environmental, and social sustainability respectively and $\alpha + \beta + \gamma = 1$.

Note that the value of $X^E(k)$, $X^V(k)$, and $X^L(k)$ obtained based on corresponding fuzzy membership function are between 0 and 1, the final sustainability status $X^S(k)$ is also between 0 and 1.

6.3.2 Fuzzy Set Theory based Evaluation of Sustainability Improvement Actions

Given that a decision set is selected for sustainability improvement within the defined period, a comprehensive evaluation of the impact of each action is essential for the optimization. It is assumed that there is no interaction among the decision candidates and the adoption of any specific decision is independent with the starting sustainability status. In other words, the selected decision candidates can be applied to any developing stage.

Due to the fact that the fundamental sustainability assessment is subjective and involves many uncertainty issues, the evaluation of sustainability improvement potential with respect to the decision candidates will also consist of uncertainty which can be characterized by the proposed fuzzy set theory. For a specific decision candidate c_i being using at stage k , the impact to each sustainability indicators when applying this decision to the system can be expressed as:

$$\Delta X_i^E(k)_{c_i} = X_i^E(k)_{c_i} - X_i^E(k) \quad (6.20)$$

$$\Delta X_j^V(k)_{c_i} = X_j^V(k)_{c_i} - X_j^V(k) \quad (6.21)$$

$$\Delta X_l^L(k)_{c_i} = X_l^L(k)_{c_i} - X_l^L(k) \quad (6.22)$$

where $\Delta X_i^E(k)_{c_i}$, $\Delta X_j^V(k)_{c_i}$, and $\Delta X_l^L(k)_{c_i}$ are the net change of i -th economic sustainability indicator, j -th environmental sustainability indicator, and l -th social sustainability indicator when applying decision c_i , respectively; $X_i^E(k)_{c_i}$, $X_j^V(k)_{c_i}$, and $X_l^L(k)_{c_i}$ are the performance of i -th economic sustainability indicator, j -th environmental sustainability indicator, and l -th social sustainability indicator when applying decision c_i , respectively;

The change of categorized sustainability status after implementing decision c_i can be calculated as

$$\Delta X^E(k)_{c_i} = \sum_{i=1}^{N_E} a_i \Delta X_i^E(k)_{c_i} \quad (6.23)$$

$$\Delta X^V(k)_{c_i} = \sum_{j=1}^{N_V} b_j \Delta X_j^V(k)_{c_i} \quad (6.24)$$

$$\Delta X^L(k)_{c_i} = \sum_{l=1}^{N_L} c_l \Delta X_l^L(k)_{c_i} \quad (6.25)$$

where $\Delta X^E(k)_{c_i}$, $\Delta X^V(k)_{c_i}$, and $\Delta X^L(k)_{c_i}$ are the net change of economic, environmental, and social sustainability performance when applying decision c_i , respectively.

$$\Delta X^S(k)_{c_i} = X^S(k)_{c_i} - X^S(k) \quad (6.26)$$

where the overall sustainability performance after adopting decision c_i , $X^S(k)_{c_i}$ can be obtained by following Eqs. (5.10)-(5.19).

As mentioned earlier, the improvement potential for any decision candidates is independent to the sustainable development stages. Therefore, the improvement potential for the three categorized sustainability and overall sustainability can also be expressed as:

$$\Delta X^E(k)_{c_i} = \Delta X_{c_i}^E \quad (6.27)$$

$$\Delta X^V(k)_{c_i} = \Delta X_{c_i}^V \quad (6.28)$$

$$\Delta X^L(k)_{c_i} = \Delta X_{c_i}^L \quad (6.29)$$

$$\Delta X^S(k)_{c_i} = \Delta X_{c_i}^S \quad (6.30)$$

6.4 Fuzzy Set Theory based Goal and Constraints Evaluation

There are two key parameters in the fuzzy dynamic programming optimization, fuzzy membership of goal satisfaction and decision constraints. The evaluation of these two aspects are presented in the following content.

6.4.1 Satisfaction Evaluation of Sustainability Goal Attainment

With the results of sustainability assessment under uncertainty, it is required to analyze the relative satisfaction of the sustainability achievement. Such achievement involves the assessment of overall achievement and categorized sustainability achievement. The fuzzy membership function which evaluates the satisfaction of categorized sustainability goal achievement based on the calculated categorized sustainability status is expressed as:

$$\mu_S^E(X^E(k)) = \begin{cases} 0 & 0 \leq X^E(k) \leq X_{low}^E \\ \frac{X^E(k) - X_{low}^E}{X_{up}^E - X_{low}^E} & X_{low}^E < X^E(k) < X_{up}^E \\ 1 & X^E(k) \geq X_{up}^E \end{cases} \quad (6.31)$$

$$\mu_S^V(X^V(k)) = \begin{cases} 0 & 0 \leq X^V(k) \leq X_{low}^V \\ \frac{X^V(k) - X_{low}^V}{X_{up}^V - X_{low}^V} & X_{low}^V < X^V(k) < X_{up}^V \\ 1 & X^V(k) \geq X_{up}^V \end{cases} \quad (6.32)$$

$$\mu_S^L(X^L(k)) = \begin{cases} 0 & 0 \leq X^L(k) \leq X_{low}^L \\ \frac{X^L(k) - X_{low}^L}{X_{up}^L - X_{low}^L} & X_{low}^L < X^L(k) < X_{up}^L \\ 1 & X^L(k) \geq X_{up}^L \end{cases} \quad (6.33)$$

There are three different approaches to obtain the satisfaction of overall sustainability achievement. The first approach is to directly define the membership function to assess such satisfaction. This method can be applied to the scenarios that only focus the overall sustainability status. An example of the membership function is shown as:

$$\mu_S(X^S(k)) = \begin{cases} 0 & 0 \leq X^S(k) \leq X_{up}^S \\ \frac{X^S(k) - X_{low}^S}{X_{up}^S - X_{low}^S} & X_{low}^S < X^S(k) < X_{up}^S \\ 1 & X^S(k) \geq X_{up}^S \end{cases} \quad (6.34)$$

The second method is the weighted summation method which can be expressed as:

$$\mu_S(X^S(k)) = \alpha \mu_S^E(X^E(k)) + \beta \mu_S^V(X^V(k)) + \gamma \mu_S^L(X^L(k)) \quad (6.35)$$

where α, β and γ are the same weighting factors used in Eq. (6.19).

The final method to acquire the satisfaction of overall sustainability performance is through fuzzy operation, that is:

$$\mu_S(X^S(k)) = \mu_S^E(X^E(k)) * \mu_S^V(X^V(k)) * \mu_S^L(X^L(k)) \quad (6.36)$$

where operation “*” stands for the fuzzy operation which includes “ \vee ” and “ \wedge ”. In this work, operation “ \wedge ” is chosen to calculate the categorized sustainability performance.

6.4.2 Analysis of Constraints with Respect to Decision Candidates

Three different aspects associated with the decision candidates, cost, implementing time, and improvement potential can pose various constraints to the selection of improvement actions. In this section, such constraints are evaluated through corresponding fuzzy membership functions.

Budget availability is the main constraint toward selection of stage-based decisions. Adequate budget could substantially boost the sustainability improvement as most effective technologies are accompanied by higher cost. To adapt the practical budget issue, the boundaries of the cost of developing actions have some freedom rather than being strictly defined. Assume that the total available budget is B_{tot} and the budget for stage k is B_k^{set} , for each development stage,

$$B_k^{set} \leq B_{tot} \quad (6.37)$$

$$B_{tot} = \sum_{k=1}^N B_k^{set} \quad (6.38)$$

For k -th stage, the fuzzy membership function of the satisfaction of budget constraint is:

$$\mu_C^B(B^U(k)_{c_i}) = \begin{cases} 1 & 0 \leq B^U(k)_{c_i} \leq B_k^{(I)} \\ \frac{B_k^{(II)} - B^U(k)_{c_i}}{B_k^{(II)} - B_k^{(I)}} & B_k^{(I)} < B^U(k)_{c_i} < B_k^{(II)} \\ 0 & B^U(k)_{c_i} \geq B_k^{(II)} \end{cases} \quad (6.39)$$

where $B^U(k)_{c_i}$ is the cost of i -th decision being applied in k -th stage; $B_k^{(I)}$ and $B_k^{(II)}$ are constants being used to evaluate the budget constraint.

Figure 6.4 elaborates the fuzzy membership function of $\mu_C^B(B^U(k)_{c_i})$. The budget constraint is fully satisfied when the cost of improvement action is less than $B_k^{(I)}$, partially satisfied when it is between $B_k^{(I)}$ and $B_k^{(II)}$, and not allowed when it exceeds $B_k^{(II)}$. If all development stages could have equal amount budget for sustainability improvement, then Eq. (6.38) can be expressed as:

$$B_k^{set} = \frac{1}{N} B_{tot} \quad (6.40)$$

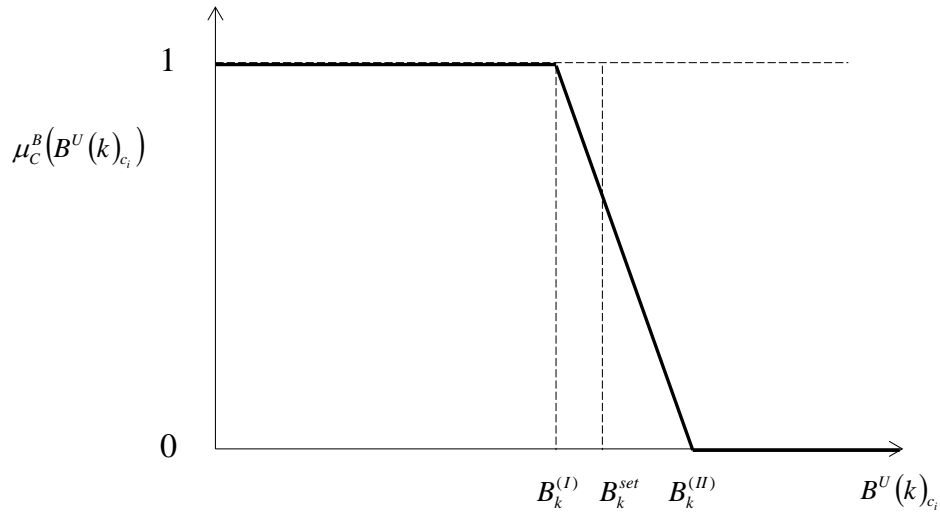


Figure 6.4. Fuzzy membership function of the satisfaction of budget constraint.

The second constraint being considered during the planning of long-term sustainable development is the implementing time required by the decision actions. Typically, the total project can be divided into N periods which have same time span. Assume that the time period for each stage is t_{set} , the total development span is expressed as:

$$t_{tot} = N t_{set} \quad (6.41)$$

Similar to the budget constraint, the time constraint is also given a certain degree of freedom comparing to the rigorous boundaries used in most conventional studies. For k -th stage, the fuzzy membership function of the satisfaction of time constraint is:

$$\mu_C^t(t^U(k)_{c_i}) = \begin{cases} 1 & 0 \leq t^U(k)_{c_i} \leq t_k^{(I)} \\ \frac{t_k^{(II)} - t^U(k)_{c_i}}{t_k^{(II)} - t_k^{(I)}} & t_k^{(I)} < t^U(k)_{c_i} < t_k^{(II)} \\ 0 & t^U(k)_{c_i} \geq t_k^{(II)} \end{cases} \quad (6.42)$$

where $t^U(k)_{c_i}$ is the cost of i -th decision being applied in k -th stage; $t_k^{(I)}$ and $t_k^{(II)}$ are constants being used to define the fuzzy membership function.

Figure 6.5 shows the satisfactory fuzzy membership function of time constraint. It is expected the implementing time of each decision action should follow the time schedule. The decision action is also acceptable to some extent if the time usage is between $t_k^{(I)}$ and $t_k^{(II)}$. The decision action has little use when the implementing time is more than $t_k^{(II)}$ which might delay the whole project.

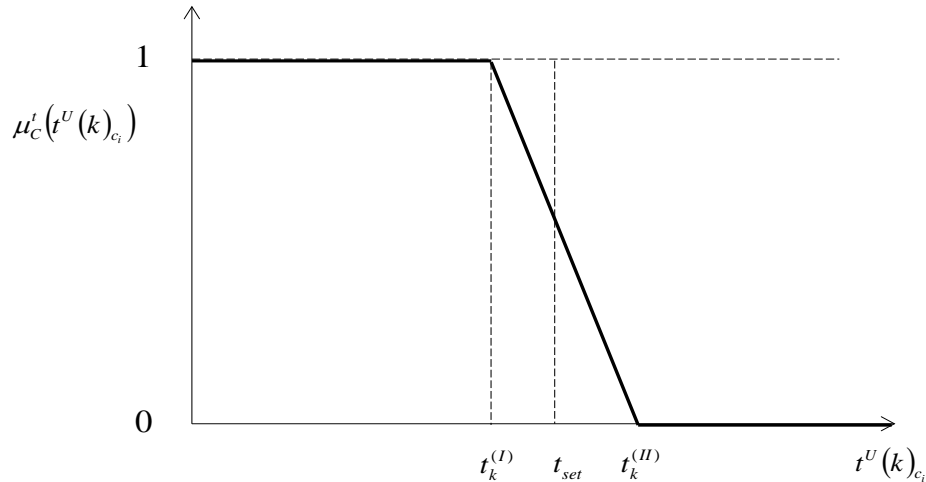


Figure 6.5. Fuzzy membership function of the satisfaction of time constraint.

The last constraint being considered during the planning of long-term sustainable development is the sustainability improvement potential by the decision actions. A well-planned long-term sustainability improvement should contain multiple consecutive stages with steadily and positively improving performance which does not yield undesirable enhancement patterns that significantly fluctuate at certain stages. Figure 6.6 illustrates two different plans of MDM for long-term sustainability improvement. For the developing plan shown in Figure 6.6 (a), the improvement of system status changes significantly with respect to certain stages and some stages might not have positive improvement at all (Figure 6.6 (b)). On the contrary, the improvement decision shown in Figure 6.6 (c) could lead to a desirable change of system status among the development stages (Figure 6.6 (d)). Therefore, the satisfaction of the sustainability improvement potential by the decision actions at each stage must be evaluated.

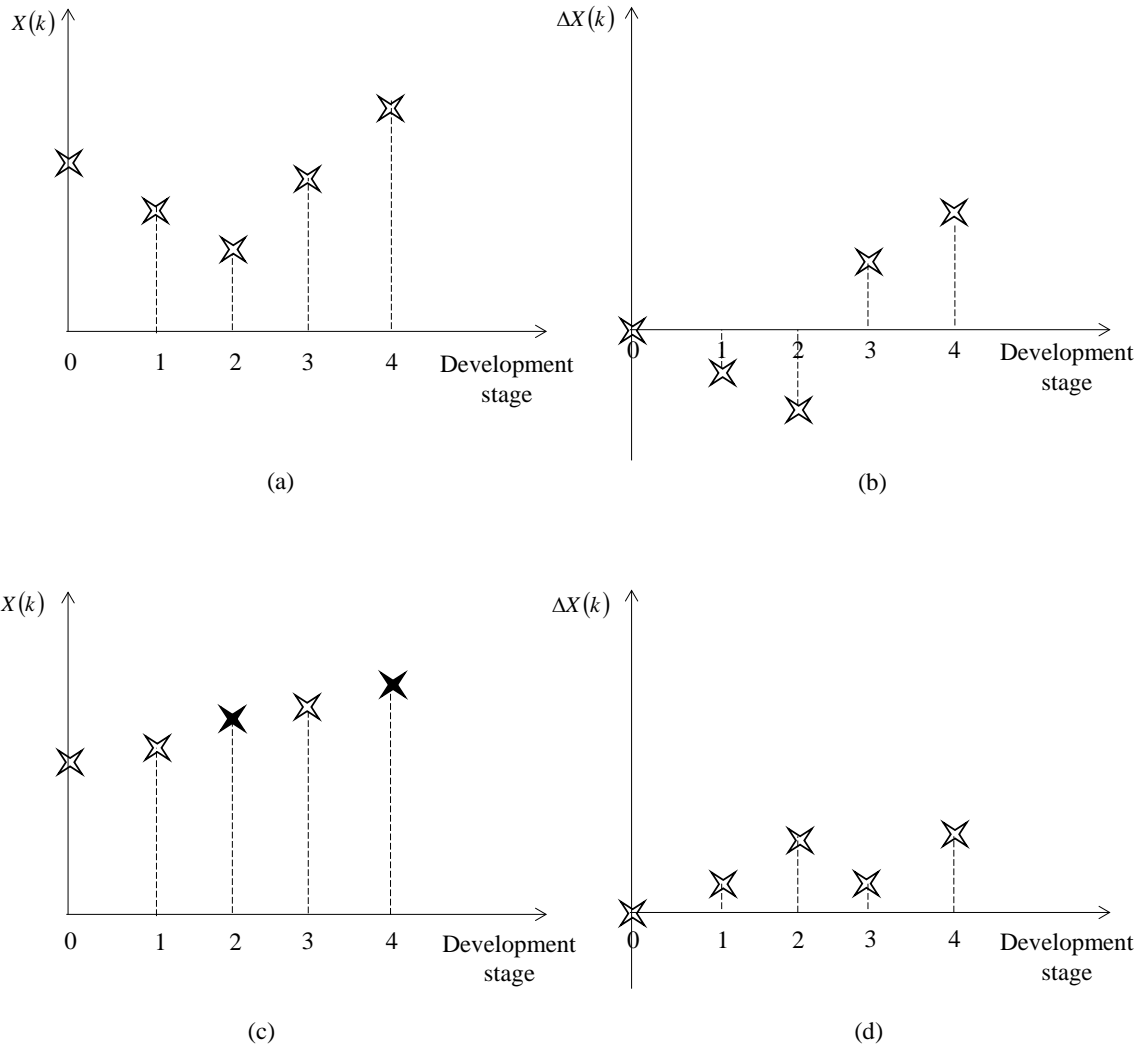


Figure 6.6. Different paths of sustainability improvement plans and corresponding trend of stage-based improvement (Huang, 2008).

The improvement potential can be analyzed as the improvement potential of three categorized sustainability performance, and that of the overall sustainability performance. Decision makers' knowledge can be used to build similar fuzzy membership function to characterize the satisfaction of improvement potential of economic sustainability aspect, $\mu_C^I(\Delta X^E(k)_{c_i})$, environmental sustainability aspect $\mu_C^I(\Delta X^V(k)_{c_i})$, and social sustainability

aspect $\mu_C^I(\Delta X^L(k)_{c_i})$. The fuzzy membership grade for overall sustainability status $\mu_C^I(\Delta X^S(k)_{c_i})$ can be obtained by either constructing an actual fuzzy membership function or calculating as follows:

$$\mu_C^I(\Delta X^S(k)_{c_i}) = \mu_C^I(\Delta X^E(k)_{c_i}) \wedge \mu_C^I(\Delta X^V(k)_{c_i}) \wedge \mu_C^I(\Delta X^L(k)_{c_i}) \quad (6.43)$$

Based on the evaluation of three decision constraints, the overall fuzzy grade for implementing i -th decision action at stage k can be expressed as:

$$\mu_C(U(k)_{c_i}) = \mu_C^B(B^U(k)_{c_i}) \wedge \mu_C^I(t^U(k)_{c_i}) \wedge \mu_C^I(\Delta X^S(k)_{c_i}) \quad (6.44)$$

6.5 Optimization Based Fuzzy Dynamic Programming Approach

The traditional (crisp) dynamic programming method is concerned with the objective function that maximizes or minimizes subject to some clearly defined constraints such as cost, time, and number of crew. On the contrary to the conventional dynamic programming approach, the objective and restricting constraints for long-term sustainable development are generally not clearly defined. In order to apply fuzzy dynamic programming approach to long-term sustainable development problems, the decision is defined as the confluence of goals and constraints.

The basic form of FDP involves the time-invariant finite-state deterministic system under control. The temporal evolution is described by the state transition function:

$$f : X \times U \rightarrow X \quad (6.45)$$

$$X(k+1) = f(X(k), U(k)) \quad (6.46)$$

where $X(k)$ and $X(k+1)$ are the sustainability status at the developing stage k and $k+1$, respectively; $U(k)$ is the selected decision action at k ; f is a given function from $X \times U$ to X . It is assumed that X and U are finite.

For the development at stage k , decision action $U(k)$ is subjected to a fuzzy constraint $\mu_c(U(k))$ and a fuzzy satisfaction of the expected sustainability status (development goal of stage k) $\mu_s(X_G(k+1))$. According to the definition of fuzzy decision, final decision incorporates the fuzzy constraints of the decision action and the fuzzy goals, that is:

$$\begin{aligned} \mu_D(U(0), U(1), \dots, U(N-1) | X(0)) \\ = \mu_c(U(0)) \wedge \mu_c(U(1)) \wedge \dots \wedge \mu_c(U(N-1)) \wedge \mu_s(X_G(N)) \end{aligned} \quad (6.47)$$

where $X(0)$ is the initial state, and action $U(0)$ is the decision for first state.

Note that the MDM process consists of N consecutive stages in which the starting sustainability status of a specific stage is the developing goal of preceding stage. For the N -th stage, the fuzzy satisfaction of its starting sustainability status is also equal to that of the sustainability improvement goal in $(N-1)$ stage. The following operation can be obtained according to the state transfer function in Eq. (6.46):

$$\mu_s(X_G(N-1)) = \mu_c(U(N-1)) \wedge \mu_s(X_G(N)) \quad (6.48)$$

Therefore, a general expression of the fuzzy decision shown in Eq. (6.47) is expressed as:

$$\mu_D(U(0), U(1), \dots, U(N-1) | X(0)) = \bigwedge_{k=1}^{N-1} (\mu_c(U(k)) \wedge \mu_s(X_G(k+1))) \quad (6.49)$$

The optimal sequence of controls $U(0)^*, U(1)^*, \dots, U(N-1)^*$ can then be identified as:

$$\begin{aligned}
& \mu_D(U(0)^*, U(1)^*, \dots, U(N-1)^* | X(0)) \\
&= \max_{U(0), U(1), \dots, U(N-1)} (\mu_D(U(0), U(1), \dots, U(N-1) | X(0))) \\
&= \max_{U(0), U(1), \dots, U(N-1)} \left(\bigwedge_{k=1}^{N-1} (\mu_C(U(k)) \wedge \mu_S(X_G(k+1))) \right)
\end{aligned} \tag{6.50}$$

Due to the fact that FDP approach is a backward solution searching method, the ultimate goal of sustainability improvement is defined at the first place while the initial sustainability status can also be assessment at the same time. It must be pointed out that the optimal decision set identified through FDP may not be able to connect these two sustainability status together at certain circumstance. In such case, the ultimate goal of sustainable development must be adjusted according to the gap obtained during the initial round of FDP optimization.

6.6 Optimization Procedure based Fuzzy Dynamic Programming Approach

To identify the optimal plan for multistage sustainable development, a seven-step procedure is introduced below. The identified technology sets can meet the economic, environmental, and social sustainability goals to the level that the industrial organization satisfies.

Step 1. Create an evaluating system to analyze the sustainability status. All of the key fuzzy membership functions and normalization standards are defined in the system based on the sustainability evaluating metrics system that could over the whole development period.

Step 2. Use defined sustainability evaluating system to assess the improvement potential of all decision action candidates which are typically scientific technologies.

Step 3. Generate the fuzzy membership function of the satisfaction of goal attainment and the fuzzy membership function of the constraint satisfaction.

Step 4. Define the ultimate sustainability improvement goal and transform the sustainability status into the fuzzy satisfaction of goal attainment.

Step 5. Apply the FDP approach to calculate the fuzzy grade of all possible development paths and calculate the fuzzy satisfaction grade of the decision actions in the defined stages.

Step 6. Check if the development path can link the initial sustainability status and ultimate development goal together. If not, go back to Step 4 and adjust the improvement goal.

Step 7. Select the development path with highest fuzzy grade of decisions.

After executing the procedure above, the decision set has the highest fuzzy grade is the optimal developing plan for the long-term multistage sustainability improvement task

6.7 Case Study

In this section, a simplified four-stage eight-year sustainability improvement task is investigated in this work to demonstrate the FDP based long-term sustainability improvement methodology. The duration of each stage is 2 years. The budget for the first stage is \$500,000 with an increasing rate of 10% in each of the following stages. Therefore, the total budget is expected at \$2,684,000 and stage-based budget is set at \$50,000, \$55,000, \$60,500, and \$66,500, respectively. Based on the sustainability assessment, current sustainability status is 0.4 while the ultimate improvement goal is temporarily set at 0.8.

To facilitate the analysis, this study only investigates the overall sustainability status and corresponding improvement rather than considering the categorized sustainability performance. The fuzzy membership function of the satisfaction of goal attainment is established as:

$$\mu_s(X_G(k)) = \begin{cases} 0 & 0 \leq X_G(k) \leq 0.15 \\ 1.67X_G(k) - 0.17 & 0.15 < X_G(k) < 0.75 \\ 1 & X_G(k) \geq 0.75 \end{cases} \quad (6.51)$$

This fuzzy membership function can be interpreted as: sustainability status below 0.15 is not acceptable; sustainability status between 0.15 and 0.75 is partially acceptable; sustainability performance beyond 0.75 is absolutely acceptable although the ultimate goal is set at 0.8. Therefore, the fuzzy satisfactory grade for final sustainability goal is 1.

10 technology candidates are selected as the decision actions for the sustainability development in four consecutive stages. The detailed information associated with the technology candidates is listed in Table 6.1.

Table 6.1 Information of the selected technology candidates.

Technology candidate	Improvement potential	Cost (\$)	Implementing time (year)
T1	0.04	50,000	1.65
T2	0.06	52,000	1.80
T3	0.08	57,000	1.70
T4	0.09	54,000	2.00
T5	0.11	59,000	1.80
T6	0.12	61,000	1.95
T7	0.15	65,000	2.15
T8	0.18	64,000	2.20
T9	0.19	69,000	2.20
T10	0.21	67,000	2.30

To evaluate the satisfaction grade of budget constraint, a fuzzy membership function of the satisfaction of budget constraint is introduced based on Eq. (6.39):

$$\mu_C^B(B^U(k)_{c_i}) = \begin{cases} 1 & 0 \leq B^U(k)_{c_i} \leq 0.9B_k^{set} \\ 2.57 - \frac{B^U(k)_{c_i}}{0.35B_k^{set}} & 0.9B_k^{set} < B^U(k)_{c_i} < 1.25B_k^{set} \\ 0 & B^U(k)_{c_i} \geq 1.25B_k^{set} \end{cases} \quad (6.52)$$

where B_k^{set} denotes the preset budget boundary in k -th stage; $B^U(k)_{c_i}$ is the actual cost of technology C_i which is independent on developing stages.

Correspondingly, the fuzzy membership to characterize the satisfaction of time constraint for decision actions is expressed as:

$$\mu_C^t(t^U(k)_{c_i}) = \begin{cases} 1 & 0 \leq t^U(k)_{c_i} \leq 1.6 \\ 2 - 1.25t^U(k)_{c_i} & 1.6 < t^U(k)_{c_i} < 2.4 \\ 0 & t^U(k)_{c_i} \geq 2.4 \end{cases} \quad (6.53)$$

The fuzzy membership to characterize the satisfaction of stage-based improvement constraint for decision actions is expressed as:

$$\mu_C^I(\Delta X^S(k)_{c_i}) = \begin{cases} 0 & 0 \leq \Delta X^S(k)_{c_i} \leq 0.04 \\ 25\Delta X^S(k)_{c_i} - 1 & 0.04 < \Delta X^S(k)_{c_i} < 0.08 \\ 1 & \Delta X^S(k)_{c_i} \geq 0.08 \end{cases} \quad (6.54)$$

In order to identify the long-term development plan, the state transition function used in this study is defined as:

$$X(k+1) = X(k) + \Delta X(k)_{c_i} \quad (6.55)$$

Applying the backward recurrence based FDP method, the optimal path to achieve the sustainability improvement by 0.4 can be determined and shown in Figure 6.7:

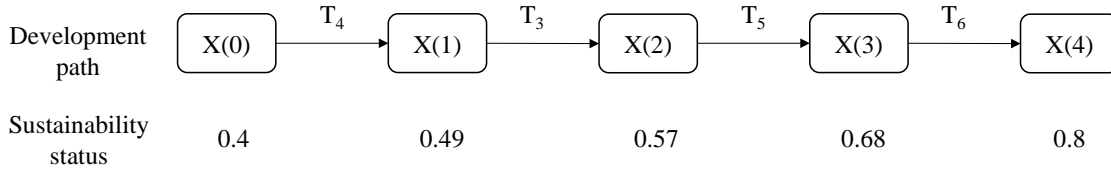


Figure 6.7. Optimal sustainable development strategy.

Table 6.2 illustrates the categorized fuzzy grade of constraint satisfaction. The fuzzy satisfactory grade of the four development action are 0.49, 0.61, 0.75, and 0.56 respectively. The cost of technology 4 poses the biggest limit to the development plan. By implementing such a development plan, the fuzzy grade of optimal sequence is 0.49.

Table 6.2 Fuzzy grade of constraint satisfaction of the selected development plan.

Technology	Budget constraint	Improvement constraint	Time constraint	Total
T4	0.49	1	0.50	0.49
T3	0.61	1	0.88	0.61
T5	0.79	1	0.75	0.75
T6	0.95	1	0.56	0.56

Although the sequence (T4, T3, T5, and T6) leads to the achievement of preset ultimate goal at 0.8, the fuzzy grade of this sequence is only at 0.49. There are also two more options that must be pointed out here and worth for decision makers taking into consideration. The first sequence (T2, T3, T5, and T6) could result in a much higher fuzzy grade of decision sequence at 0.56 (Table 6.3) and the final sustainability status can reach 0.77 which is also in the absolutely acceptable range. The control constraint is the implementing time of technology 6 used in stage 4. The adoption of this development plan would need decision-makers to adjust the original goal of long-term sustainability improvement.

Table 6.3 Fuzzy grade of constraint satisfaction of the second development plan.

Technology	Budget constraint	Improvement constraint	Time constraint	Total
T2	0.60	1	0.75	0.60
T3	0.61	1	0.88	0.61
T5	0.79	1	0.75	0.75
T6	0.95	1	0.56	0.56

The primary limit for this development plan is the implementing time of technology 6. The second sustainability improvement plan (T3, T6, T4, and T7) is capable of achieving

the sustainability improvement goal at 0.84 while the fuzzy grade of this sequence is 0.31 (Table 6.4). There are two control constraints for this development plan, that is, the cost of technology 3 applied in the first stage and the implementing time of technology 7 used in stage 4. It is also comprehensible that modification of the original goal of long-term sustainability improvement is essential in order to apply this development plan.

Table 6.4 Fuzzy grade of constraint satisfaction of the third development plan.

Technology	Budget constraint	Improvement constraint	Time constraint	Total
T3	0.31	1	0.88	0.31
T6	0.40	1	0.56	0.40
T4	1	1	0.50	0.50
T7	0.78	1	0.31	0.31

6.8 Conclusions

Fuzzy dynamic programming is a powerful technique to solve multistage decision making problems. At each stage, the evaluation of decisions can be regarded as a multiple objective decision making problem. In this study, a novel fuzzy dynamic programming (FDP) based approach has been developed for the long-term sustainable development with multiple decisions being applied in consecutive stages. The merits of this methodology are: (i) it combines both fuzzy evaluation and conventional normalization to address the uncertainty and subjective issues in sustainability assessment; (ii) it is sequential in nature and does not need to set exact development plan for each development stage; and (iii) it can provide multiple options for decision makers to choose. A case study of 4-stage sustainability improvement project is used to demonstrate the approach is feasible and efficient in practice. The proposed methodology could effectively identify the optimal

solutions with two alternative options for decision-makers to select with respect to different development scenarios.

CHAPTER 7 CONCLUSIONS AND FUTURE WORKS

Increasing concern with the environmental impact and human welfare accompanied by human economic activities has led to a rising interest in comprehensive sustainable development that is shifted from the traditional two dimensional environmental protection framework. Sustainability is nowadays accepted by all stakeholders as a guiding principle for both public policy making and corporate strategies. Although current studies provide a variety of different methodologies to address sustainability assessment and decision-making, the increasing size and complexity of industrial systems results in the necessity to develop more comprehensive systems approaches to ensure the sustainable development over a long time period for industrial systems.

This dissertation aims at addressing the necessity of systems approaches to decision-making in which economic, environmental and social factors are integrated together to ensure the triple bottom lines of sustainability by generating a number of effective methodologies for sustainable development of various industrial systems. The first part of this chapter summarizes the scientific findings and significant contributions of this dissertation while the second part recommends possible directions to expand the current study.

7.1 Conclusions

To address the challenges associated with the study of sustainability, three fundamental frameworks are developed in this dissertation, that is, life cycle based sustainability assessment (LCBSA) framework, life cycle based decision-making (LCBDM) framework, and fuzzy dynamic programming (FDP) based long-term multistage sustainable

development framework. LCBSA can offer a profound insight of status quo of the sustainability performance over the whole life cycle. LCBSA is then applied to assess the industrial system of automotive coating manufacturing process from raw material extraction, material manufacturing, product manufacturing to the recycle and disposal stage. The following LCBDM framework could then prioritize the sustainability improvement urgency and achieve comprehensive sustainable development by employing a two-phase decision-making methodology. In addition, FDP based long-term multistage sustainable development framework offers a comprehensive way to ascertain the achievement of long time sustainable development goal of complex and dynamic industrial systems by combining decision-making and sustainability assessment together.

In Chapter 2, the life cycle based sustainability assessment (LCBSA) framework is developed to achieve a more comprehensive sustainability assessment comparing to the traditional system-focused sustainability studies. A general hierarchical LCBSA framework includes four consecutive steps which contribute to the achievement of sustainability assessment at life cycle level. Parameter identification, selection of sustainability indicators, stage-based sustainability assessment and final information integration are involved in the methodology.

In Chapter 3, the efforts made towards the life cycle based decision-making (LCBDM) framework are described. Based on the preceding framework of LCBSA, LCBDM involves the two-phase prioritization of sustainability development and resource allocation. The first phase concentrates on the urgent improvement of stage-based “must-be” system variables and the second one prioritizes the sustainability development needs

from the life cycle point of view. Priority order can then be used to guide the resource allocation for sustainability enhancement to achieve life cycle based sustainability improvement.

To accomplish the life cycle based sustainability assessment on nanocoating materials, Chapter 4 provides the details of the multiscale modeling and simulation of paint application process (automotive paint curing process). The modeling of paint curing oven is performed in order to study the effects of nanoparticles addition into coating matrix on the process dynamics, energy consumption and coating film quality. The energy transfer process, solvent removal process, and polymer network formation process are investigated. An energy efficient operational setting is obtained based on with the consideration of coating quality requirement. The data obtained in these chapters could be used for the quantification of some of the sustainability indicators described in Chapter 2 and 3.

Electroplating industry is facing tremendous challenges toward sustainable development largely due to the inherent nature of the industry. In addition, the absence of appropriate sustainability metrics system is also critical. Chapter 5 describes a practical sustainability assessment and performance improvement for electroplating processes in which a systematic method for designing sustainability metrics system from the supply chain perspective is involved. With the selected sustainability metrics system, the sustainability status and possible improvement technology candidates are evaluated accordingly. An effective methodology for identifying optimal decisions for sustainability improvement is also introduced in this work. An electroplating process case study is employed to outline the

proposed evaluation method, which prioritizes improvement measures to guide advances toward sustainability.

In chapter 6, a FDP based multistage decision-making framework designed for long-term development of industrial sustainability is presented. Fuzzy dynamic programming is a powerful technique to solve multistage decision making problems. At each stage, the evaluation of decisions can be regarded as a multiple objective decision making problem. By this methodology, data uncertainty, qualitative sustainability indicators, and subjective judgement are addressed with fuzzy set theory. Decision constraints including budget, time, and improvement achievement are evaluated based on fuzzy set theory as well. A comprehensive fuzzy dynamic programming approach is applied to identify the optimal route to achieve preset long-term sustainability goal. A case study of 4-stage sustainability improvement project is used to demonstrate the approach is feasible and efficient in practice.

7.2 Future Works

The systems approaches generated in this dissertation builds a solid basis for sustainability assessment and decision-making of industrial systems. This section discusses possible directions for future development.

LCBSA framework investigates the sustainability performance of product in the life cycle by heavily emphasizing the stage-based sustainability performance given the assumption that all of the life cycle stages are independent from other stages. However, the life cycle stages of product may have interactions which could affect the sustainability assessment and the following decision-making process. Therefore, it is desirable to develop a new framework that is capable of handling not only the essential system performance

related sustainability within each individual stage but also the interaction among life cycle stages.

Currently, the LCBDM framework focuses on the prioritization of improvement necessity of stage-based system variables and sustainability performance based on the same materials. The product/process performance in the life cycle stages of product may have interactions which could affect the overall sustainability status. A comprehensive sustainability study and product/process performance is expected with the presence of process models and model-based simulation and optimization. Global optimization based on integration of product performance with respect to material design and process performance with respect to critical system variables is key to the evaluation.

The framework of FDP based multistage sustainable development has rendered a comprehensive methodology to design long-term developing plans for simplified industrial systems. Most industrial systems exist in a much more complex form such as hierarchical systems. To make this methodology more effective, it is necessary to involve the analysis of dynamic, adaptive behavior of complex systems, as steady-state sustainability models are too simplistic. Detailed resource allocation plans can then be obtained by improving the methodology. In addition, uncertainty from technology integration is not covered in this study. It would be considerable to add the handling approach of this type uncertainty into it.

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ABSTRACT**LIFE CYCLE BASED SUSTAINABILITY ASSESSMENT AND DECISION
MAKING FOR INDUSTRIAL SYSTEMS**

by

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Increasing concern with the environmental impact resulted from human activities has led to a rising interest in sustainable development that will not only meet the needs of current development but also protect the natural environment without compromising the needs of future generations. This leads to the necessity of a systems approach to decision-making in which economic, environmental and social factors are integrated together to ensure the triple bottom lines of sustainability. Although current studies provide a variety of different methodologies to address sustainability assessment and decision-making, the increasing size and complexity of industrial systems results in the necessity to develop more comprehensive systems approaches to ensure the sustainable development over a long time period for industrial systems. What's more, current research may conduct results based on one or only a few stages of the manufacturing process without considering all the stages of a product's life. Therefore, the results could be bias and sometimes not feasible for the whole life-cycle. In the meanwhile, life cycle analysis (LCA) which has been widely adopted in a variety of

industries does provide an effective approach to evaluate the environmental impact. The lack of life-cycle based economic and social sustainability assessment results in the difficult to conduct more comprehensive sustainability assessment.

To address these challenges, three fundamental frameworks are developed in this dissertation, that is, life cycle based sustainability assessment (LCBSA) framework, life cycle based decision-making (LCBDM) framework, and fuzzy dynamic programming (FDP) based long-term multistage sustainable development framework. LCBSA can offer a profound insight of status quo of the sustainability performance over the whole life cycle. LCSA is then applied to assess the industrial system of automotive coating manufacturing process from raw material extraction, material manufacturing, product manufacturing to the recycle and disposal stage. The following LCBDM framework could then prioritize the sustainability improvement urgency and achieve comprehensive sustainable development by employing a two-phase decision-making methodology. In addition, FDP based long-term multistage sustainable development framework offers a comprehensive way to ascertain the achievement of long time sustainable development goal of complex and dynamic industrial systems by combining decision-making and sustainability assessment together.

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