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CLASSIFICATION AND DEVELOPMENT OF MATHEMATICAL MODELS AND SIMULATION FOR INDUSTRIAL ECOLOGY

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CLASSIFICATION AND DEVELOPMENT OF MATHEMATICAL MODELS AND SIMULATION FOR INDUSTRIAL ECOLOGY

BY

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ABSTRACT

Recent publications call for a higher focus on implementation of the theoretical concept of industrial ecology. It embodies the idea that collaborating companies use each other's waste and byproducts following the example of the natural metabolism. Subject matter of this work is the practical application of this idea, i.e. eco-industrial parks and networks. In addition to the positive impact on the environment due to a reduction of pressure on limited natural resources, existing cases show that benefits can simultaneously be achieved for all three dimensions of sustainable development, including the economy and society.

In order to promote this concept and thus facilitate the implementation of sustainable development in the private sector, this thesis proposes an Interactive Optimized Negotiation Algorithm (IONA) embedding a mixed-integer linear program with weighted achievement functions. This flexible network model supports the establishment of new industrial ecology in practice. It can flexibly be adapted to various circumstances and overcomes major critiques of existing approaches. In addition to the computer implementation of this advanced modeling approach, this work provides a catalogue of requirements to meet when modeling industrial ecology.

The approach considers multiple objectives, different stakeholder interests, and various material flow types. The closing study of two cases shows the comprehensive capabilities of the program. Exceeding the scope of this work, the computer program can be used to conduct studies of existing networks regarding their stability when facing today's increasing necessity to set and meet environmental and social objectives.

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TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

LIST OF ABBREVIATIONS

ABM	Agent-Based Modeling
CP	Cleaner Production
CSD	Commission on Sustainable Development
CSR	Corporate Social Responsibility
EA	Evolutionary Algorithm
EIN	Eco-Industrial Network
EIP	Eco-Industrial Park
GO	Governmental Organization
GPS	Global Positioning System
GRI	Global Report Initiative
GUI	Graphical User Interface
IChemE	Institution of Chemical Engineers
IE	Industrial Ecology
IONA	Interactive Optimized Negotiation Algorithm
IS	Industrial Symbiosis
ISO	International Organization for Standardization
ISWT	Interactive Surrogate Worth Trade-Off

KPI	Key Performance Indicator
LCA	Life Cycle Assessment
MCDM	Multi-Criteria Decision Making problems
MFA	Material Flow Analysis
MILP	Mixed-Integer Linear Program
MINLP	Mixed-Integer Non-Linear Program
MOO	Multi-Objective Optimization
MOP	multi-objective optimization problems
NGO	Non-Governmental Organization
NIMBUS	Nondifferentiable Interactive Multiobjective BUndle-based optimization System
NSGA II	Non-dominated Sorting Genetic Algorithm-II
OECD	Organization for Economic Co-operation and Development
PCSD	President's Council on Sustainable Development
SAEIS	Simultaneous Analysis of Environmental Impacts Sensitivity
SD	Sustainable Development
SDGs	Sustainable Development Goals
TOPSIS	Technique for Order of Preference by Similarity to Ideal Solution
UFLP	Uncapacitated Facility Location Problem

UN	United Nations
UNCSD	United Nations Conference on Sustainable Development
WCED	World Commission on Environment and Development
WLP	Warehouse Location Problem
WSSD	World Summit on Sustainable Development

LIST OF SYMBOLS

I	Number of potential emission points at location (i=1,2,…,I)
J	Number of potential receiving points at location (j=1,2,…,J)
K	Number of flow type (k=1,2,…,K)
$y_{s,I}$	Binary decision variable (1, if a participant emits to the network)
$y_{s,I}$	Binary decision variable (1, if a participant receives from the network)
$y_{l,I}$	Binary decision variable (1, if a participant is part of the network)
x_{ijk}	Transportation flow of type k from location i to j [unit/period]
z_{ik}	Transportation flow of type k from location i to market [unit/period]
w_b	weight of the economic objectives (business)
w_e	weight of the environmental objectives
w_s	weight of the social objectives
z_o	objective function of goal o
$t_{b,1}*,t_{b,2}*$	target values for the economic objectives (business)
t_e*	target value for the environmental objectives
t_s*	target value for of the social objectives
$p_{E,k}$	external market price for flow of type k [$/unit]
$p_{I,ik}$	internal price of receiving location i for flow of type k [$/unit]

d_{ij} distance from location i to location j [miles]

$c_{v,k}$ variable transaction cost for flow type k per mile [$/mile]

$c_{f,I}$ fix cost or incentive for location i as a part of the network [$/period]

$c_{s,k}$ social performance of location i (CSR index of the company)

$e_{max,k}$ maximum network emission for flow type k [unit/period]

$e_{min,k}$ maximum network emission for flow type k [unit/period]

$f_{max,ij}$ maximum flow from location i to j [unit/period]

s_{jk} total input flow capacity of location j for flow type k [unit/period]

q_{ik} total output flow emitted by location j of flow type k [unit/period]

M Big M, place holder for a large number

N_{crit}: Critical number of participants in a network

1 INTRODUCTION

1.1 Background and problem statement

"Nature does nothing in vain and in the use of means to her goals she is not prodigal." (Immanuel Kant, 1784)

The increasing attention paid to the endurance of the earth and its resources is investigated in the field of sustainability. The growing level of resource consumption coupled with a significant increase in population size result in an intense strain on planet earth (Meadows et al. 1972). Based on Meadow's report, "Limits to Growth", the interest in academic research and industrial activities grew exponentially within the last three decades. As one of the first milestones towards sustainability, the United Nations World Commission on Environment and Development promoted the official and urgent call for a greater focus on a sustainable use of resources in 1987 (Brundtland 1987).

As a result of this increasing interest, governments of developed and developing countries and non-governmental organizations started to support an incremental shift towards sustainable development. Many examples show that this shift is in progress: Companies are more liable for their environmental impact in many regions all over the world (Spengler and Walther 2005; Roberts 1994) and some countries, for instance China, are going a step further by promoting a comprehensive legal strategy called circular economy (Yuan and Moriguichi 2006, Yong 2007). Sustainable development meets the needs of current generations without compromising the ability of future generations (Brundtland 1987). Concepts have been applied successfully with a simultaneous increase in economic performance, and a decrease in the impact on the environmental and social deficits.

While the public sector transfers its concerns into action, the private sector still lacks the enactment of sustainable development at a corporate level. In addition to the society-driven change towards sustainable practices of companies, costs will increase dramatically due to environmental concerns supported by politics, forcing organizations to face these new cost structures and react (Ayres and Ayres 2002).

With the concept of industrial ecology, Frosch and Gallopoulos (1989) suggest a holistic approach for companies to efficiently achieve improvements in all three dimensions of sustainable development, i.e. economy, environment, and society. The concept suggests industrial systems to operate like natural eco-systems (Frosch 1994, Allenby 1992, Jelinski et al. 1992). This can be achieved through introducing a closed-loop approach and concepts like recycling and reuse in collaborative circumstances. The waste and byproducts of one company could be the inputs of another (Frosch 1994). Eco-industrial parks or networks, as the practical application of this concept, prove this idea to be a theoretical construct, which can successfully be implemented in industrial practice. Those parks and networks involve the cooperation of companies and communities sharing and using their resources and byproducts, while synergistically reducing waste. Following the example of nature, this promising concept leads to various benefits meeting the fundamental maxim of the German philosopher Immanuel Kant, as initially quoted. Additionally, economies of scale can help to achieve an economic improvement (Tudor et al. 2007). The case of Kalundborg in Denmark is one of many promising examples (Ehrenfeld 1997, Bain 2010). However, recent publications claim that this concept has mainly remained a theoretical concept (Drexhage and Murphy 2012, Fischer et al. 2007). Furthermore, most of the aforementioned successful cases are not setup from scratch, but developed in response to fortunate circumstances. The current situation lacks systematical approaches for analyzing, improving, and generating such industrial parks or networks. Mathematical and computational modeling is the scientific approach to investigate and support the improvement and design of corporative networks. Resulting models can help to support the process of turning into reality the idea of industrial ecology by providing optimal decisions, assessing patterns, and investigating key factors. This methodology has hardly been investigated and applied in this field of research (Gu et al. 2013).

The main problem of this thesis is the large gap between the theoretical concept of industrial ecology and its application in reality. There is an extensive lack of systematic methods to analyze, improve, and create eco-industrial parks and networks.

1.2 Objective and structure

Two guiding questions are outlined in the following in order to pursue main outcomes of this thesis. Overall, this work seeks to investigate the state-of-the-art mathematical modeling and simulation for practical applications of industrial ecology.

The investigation of examples and specific properties of eco-industrial parks and networks, as well as currently existing approaches for systematic analysis, improvement, or design provides a fundamental basis of which important requirements for an advanced approach may be derived. A general classification and evaluation of different approaches has not yet been provided. Thus, the first question is:

> *Q1: What are important aspects and purposes of modeling for industrial ecology and is there an existing approach comprehensively considering these aspects?*

Based on the findings for this question, the thesis provides a more advanced approach to promote mathematical and computational modeling of eco-industrial parks and networks, which apply industrial ecology and thus sustainable development at the corporate level. The developed model will be based on re-creation, transfer, and innovation of currently applied approaches, and will seek to bridge gap and overcome weaknesses of existing approaches. The increasing importance of simultaneous consideration of ecological, social, and economic targets, leads to the second question:

> *Q2: Is it possible to develop an advanced modeling approach in order to close the current gap of implementing industrial ecology?*

The two questions of this thesis will be answered following the structure depicted in Figure 1.1. A quick summary is provided at the end of each chapter.

This introduction includes a description of the field of research and explicitly states the underlying problem (Section 1.1). The main purpose and guiding research questions of this thesis are outlined subsequently (Section 1.2).

The second chapter provides theoretical foundations about the subject matter and methodology to be applied in this thesis.

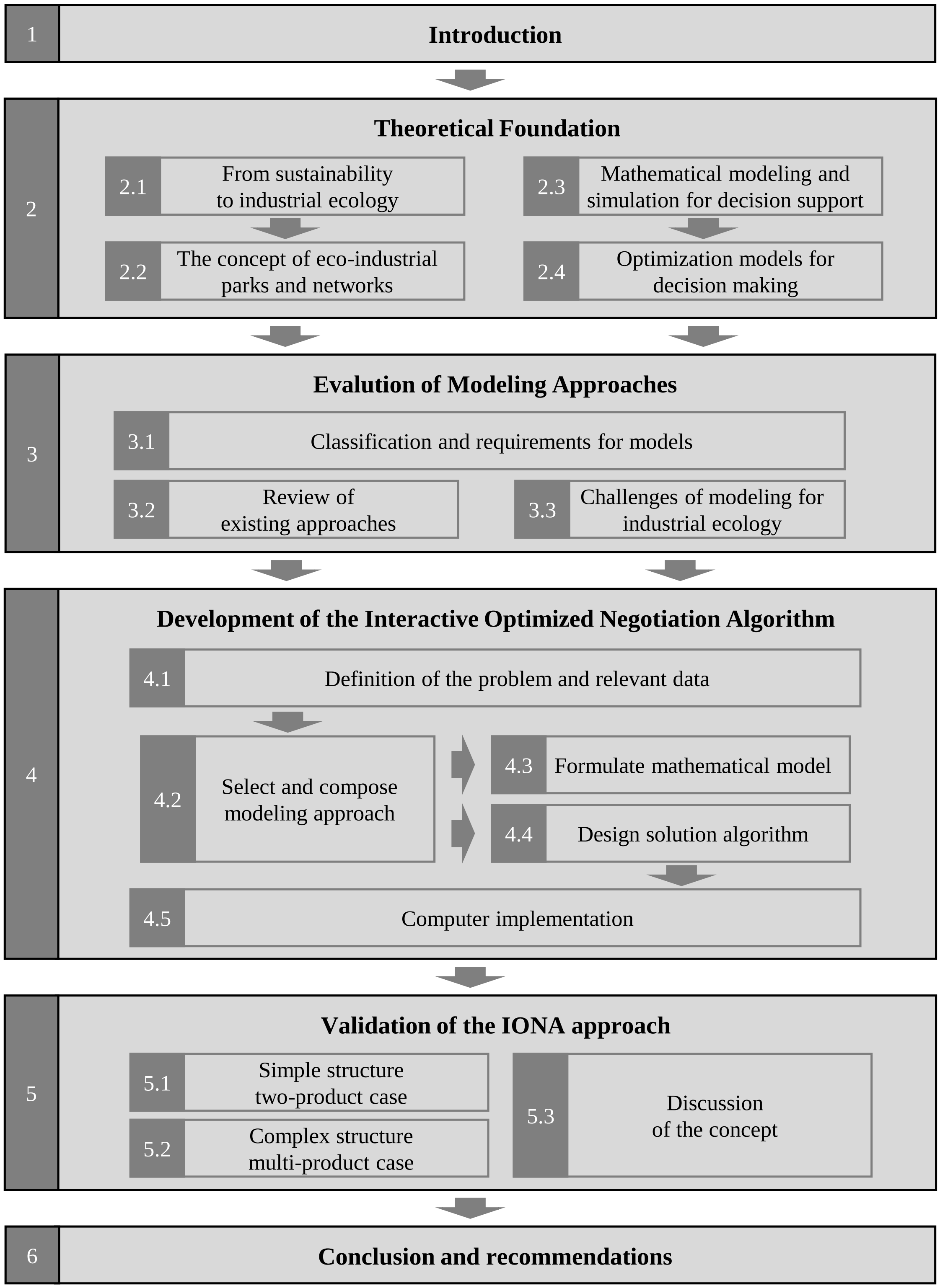

Figure 1.1: Structure and procedure of the thesis research

While Section 2.1 describes the field of industrial ecology, Section 2.2 gives a broad description of industrial ecology's applications within eco-industrial parks and networks. Separately, the methodology of mathematical modeling and simulation for the purpose of decision support is described in Section 2.3. Relevant modeling approaches are finally introduced in Section 2.4.

Based on these fundamentals, Chapter 3 provides an evaluation of modeling approaches. The development of a classification, including requirements for modeling in the field of industrial ecology, is the first step (Section 3.1). A literature review of existing approaches follows (Section 3.2) based on the prior developed classification. Challenges of modeling in this field of research are emphasized in Section 3.3.

After compiling main requirements and special challenges, an advanced mathematical model is developed and its computer implementation proposed in Chapter 4. This development is aligned to a step-by-step process adapted from Meerschaert (2013) for mathematical and Royce (1970) for computer models divided into: problem definition and relevant data (4.1), selection and composition (4.2) as well as construction of the model (section 4.3), design of the algorithm (4.4), and computer implementation (4.5).

In order to accomplish the previously applied development process, chapter 5 conducts a validation of the approach by applying industry related data (5.1 and 5.2) and discusses strengths and weaknesses of the approach (5.3).

Finally, chapter 6 provides conclusions and recommendations by summarizing and reflecting the outcomes of each chapter and their combined uses.

2 THEORETICAL FOUDATION

The second chapter contains the theoretical foundation required to understand, discuss, and develop a mathematical and computational model for an eco-industrial park or network. This chapter is clustered in two parts and has four main sections. The left side of Figure 2.1 shows the first part and the right side illustrates the second part.

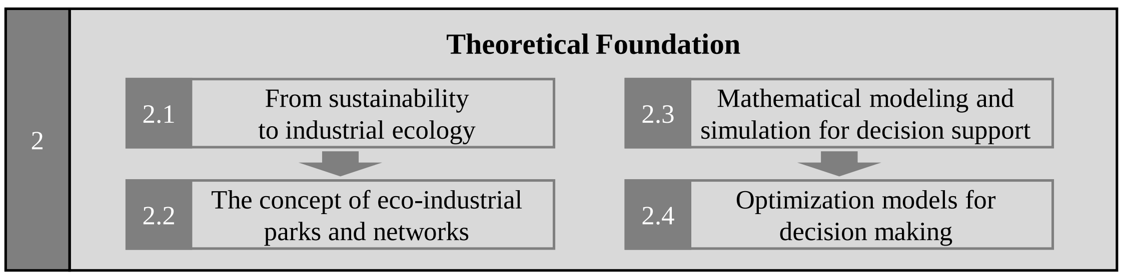

Figure 2.1: Structure of Chapter 2

The first part provides information about the subject matter. Within this first part, Section 2.1 gives an overview of the field of "sustainable development" and the concept of "industrial ecology". Based on the first section, the application of this concept in an "eco-industrial park" is introduced in the second Section 2.2.

The second part describes the methodology of mathematical and computational modeling in the field of industrial ecology. Hence, Section 2.3 introduces relevant concepts and terms for decision making using models. Subsequently, Section 2.4 gives an overview on approaches of mathematical and computational modeling with relevance to this thesis.

2.1 From forest sustainability to industrial ecology

The theme of sustainability has become part of the everyday life in both private and public sectors. Manufacturers, trading companies, and even service providers claim to be "sustainable"; however, in order to gain a common understanding of the term sustainable development, the following subsections provide an overview of the evolution of this topic. Subsequently, keywords such as "industrial ecology" and "industrial symbiosis" are introduced. Subsection 2.1.1 gives an understanding of historical evolutions in this field. An illustration of main historical events helps the reader to understand the origin of the interest in sustainable development by academics and industry.

2.1.1 History and definition of sustainable development

Originating in the German forest industry during the 16th and 17th century, the term "sustainability" has become a huge topic of public interest. The historical development and the focus on different key areas are depicted on a timeline in Figure 2.2.

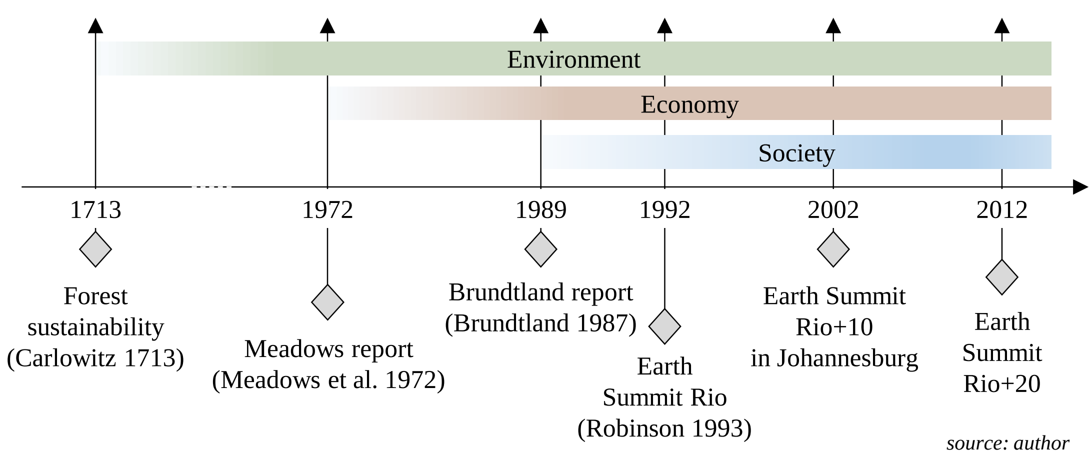

Figure 2.2: Main publications and events of sustainable development

The key areas, i.e. environment, economy, and society, are known as the three pillars or dimensions of sustainable development and are investigated later in this section.

The first documented application of sustainability was the religious driven sustainable use of the forest by Carlowitz in 1713 (Weber 2005). This description and upcoming publications that investigated the management of a forest include concerns about the ecological basis and the technical feasibility (Mosandl and Felbermeier 2001). Carlowitz was mainly concerned about the impact of human being on nature.

With Meadow's report entitled "Limits to Growth" in 1972 a broad discussion arose concerning the use of resources and economic growth. A group of researchers from the Massachusetts Institute of Technology (MIT), funded by the Volkswagen Foundation, predicted the limit of the resources on this planet to be reached within one hundred years of 1972 (Meadows et al. 1972). Using computer simulation, the exponential economic and population growth was investigated and consequences for the environment were predicted. The negative impact of the human being on its environment was not only predicted but also detected by environmental damages, increasing pressure on the existing level of natural resources (Tammemagi 1999), and climate change within recent years (Drexhage and Murphy 2012). Meadows et al. (1972) drew further conclusions and investigated the impact on the world's economy. This report is considered the first official study related to "sustainable development". Followed by this publication, the United Nations World Commission on Environment and Development (WCED) was founded aiming to place environmental topics in political concerns.

The first publication popularizing sustainable development is “Our Common Future” published by the WCED in 1987. Understanding that a growing consumption, linked with increasing urbanization and a rising world’s population results in high pressure on natural resources, this publication, also known as the Brundtland report, calls for a

> *“Development that meets the needs of the present without compromising the ability of future generations to meet their own needs” (Brundtland 1987, p. 398), which was defined to be sustainable development (SD).*

This definition implies that actions of current generations should not impair the opportunities of future generations. This was the first time all three dimensions of sustainable development, i.e. environment, economy, and society, were introduced. Inspired by previous events, the next big step towards sustainability was the first World Summit in Rio de Janeiro in 1992. The main achievement of this meeting was that United Nations member countries are obliged to include the concept of “sustainable development” in their politics. This achievement has been formulated by Agenda 21, which describes an action plan for the next century (Robinson 1993). It includes actions for social and economic dimensions, conservation, management of natural resources, the role of major participants, and means of implementation (Weber 2005; Drexhage and Murphy 2012). In addition, instruments of environmental governance were established at the Rio Summit. One of the outcomes of Agenda 21 is the Commission on Sustainable Development (CSD). With the main goal to supervise and ensure the development towards more sustainability, the CSD developed and continuously improves measurements for sustainability (United Nations 1992, United Nations 2013).

Since the first Earth Summit in 1992, a number of following conferences have been held. The 1997 *Earth Summit+5* in New York, the 2002 World Summit on Sustainable Development (WSSD) in Johannesburg and the very recent *World Summit+20* in Rio de Janeiro. Reviewing the goals set by Agenda 21, it was concluded that the "progress towards reaching the goals set in Rio has been slower than anticipated" (United Nations 2002, p. 4). Amongst many gaps between goals and actual states, the implementation of sustainability was found to be the main problem.

Although Brundtland has introduced the social aspect of sustainable development in 1987, the actual consideration of this aspect was only made after the World Summit 2002 in Johannesburg (see Figure 2.2). Noticing a lack in the consideration of the social side of sustainable development, the WSSD 2002 supported a major shift away from environmental issues towards social development, especially for developing countries. However, as a theme for the *Rio+20* conference in 2012, the "green economy" was criticized by many developing countries because it is expected to be a connection of economic development and environment, significantly neglecting social issues (Drexhage and Murphy 2012). While the WSSD in 2002 did not result in many promising outcomes, the WSSD in 2012 resulted in significant outcomes for the future of sustainable development. The result of this conference was the publication "The Future We Want" (United Nations 2012) which states a common vision as well as explicit sustainable development goals (SDGs) for all members.

2.1.2 Dimensions and goals of sustainable development

In order to understand the relevance of sustainable development to academics and companies, it is important to understand how a higher degree of sustainable development can be achieved and how goals can be defined. The goals are crucial to comprehend the origin of the concept of eco-industrial parks and networks.

Conceptual models. Brundtland's definition implies that actions of current generations should not impair the opportunities of following generations. It further describes the "concept of needs" which contains three dimensions of sustainability. These are environment, economy (also called technological aspect), and society. This determination led to two different models illustrating the relationship between the dimensions. Both the triple bottom line model and the bio-centric view are illustrated in Figure 2.3 and discussed in the following paragraphs.

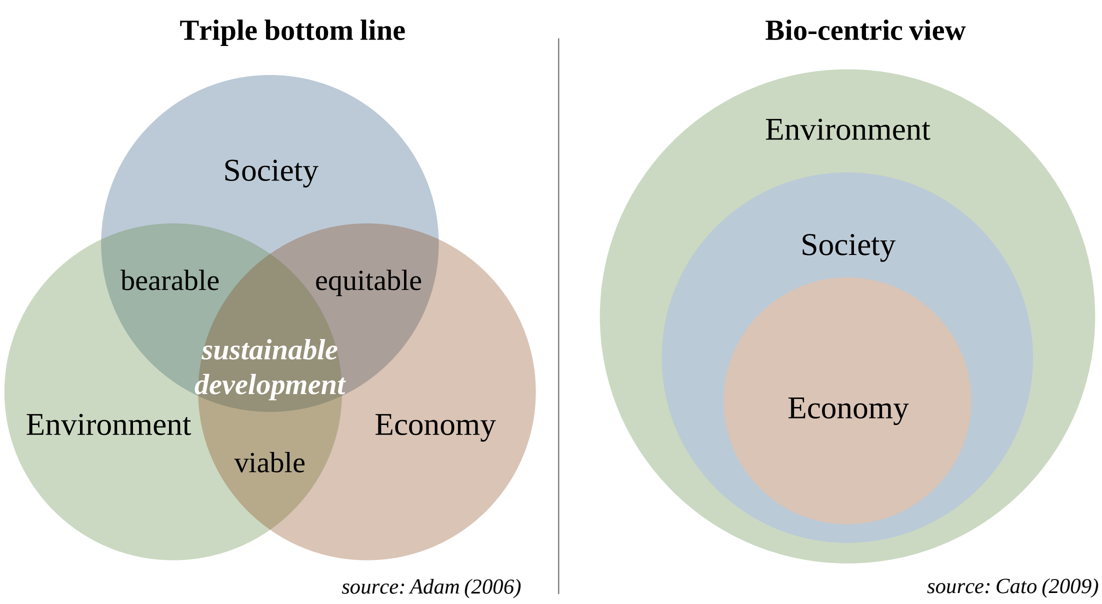

Figure 2.3: Conceptual models for the dimensions of sustainable development

The triple bottom line model represents the classic understanding of how sustainability can be achieved. It shows three overlapping circles of the dimensions “environment”, “society”, and “economy” (Cato 2009). Sustainable development is indicated to be more than the protection and responsible use of resources. The achievement of social as well as economic goals is crucial in order to accomplish sustainable development. According to this model, sustainable development occurs when all three areas of the model are considered in an activity. This model also contains the basic idea that natural capital can be substituted by material or human capital. The simultaneous consideration of environment and economy leads to a viable future. Environmental aspects considered with social aspects lead to bearable actions for human kind. Further, the simultaneous consideration of society and economy leads to equitable solutions for economic needs.

Further development of the triple bottom model led to the bio-centric model, which is depicted on the right side of Figure 2.3. It results in a concept where society is embedded in the environment. Economy is then included and surrounded by social and environmental circumstances. Every action influences both (Adam 2006). Even though this model resulted from the previous concept, it does not replace it. The two models emphasize different focuses. While the triple bottom line focuses more on humankind and an equal role of environment, society, and economy (anthropogenic view), the other model focuses more on the environment, including society and the restricting economy as a subset (bio-centric view) (Weber 2005; Williams et al. 2003). The bio-centric view contains the fact that both environmental and social aspects have to be taken into consideration by companies in order to develop sustainably.

Goals. Derived from these conceptual models and the historical evolution of this topic, the purpose and explicit goals are provided in this paragraph. Fundamental dimensions are determined due to the models described above and the main purpose has been promoted since 1987. However, explicit goals and respective activities have not been defined for a long time. Realizing that the implementation of sustainable development mainly suffers because of a lack of explicitly defined goals, the Millennium Development Goals were developed and adopted by 189 nations in 2000. The goals were set to be achieved by 2015. Examples for these goals are “Eradicate extreme poverty”, “Promote gender equality and empower women”, and “Ensure environmental sustainability” (United Nations 2007). Noticing that these goals are difficult to be turned into single actions, the Summit of *Rio+20* provides guidelines for individual sustainable development goals. Examples for explicit goals are “End extreme poverty including hunger”, “achieve development within planetary boundaries”, and “Transform governance and technologies for sustainable development” (United Nations 2012).

However, these goals including an action plan mostly remain institutional requests with very few ideas for activities to achieve single goals. As the sector with the most impact on sustainable development issues, the private sector lacks ideas, principles, and actions to develop sustainably and contribute to achieve the goals.

2.1.3 The idea of industrial ecology

The defined goals for sustainable development as well as the establishment of international and governmental institutions indicate the extent of political effort. Especially Asian and European countries establish legal limitations for companies in order to promote sustainable development (Yuan et al. 2006, Yong 2007, Spengler and Walther 2005). However, it has been proven to be a much greater task to transfer the theoretical concept into reality (Drexhage and Murphy 2012, Veiga and Magrini 2009).

Industrial ecology. An innovative concept that has emerged within the last two decades is industrial ecology (IE). IE provides the opportunity for improving environmental, business, and social performance by restructuring the industrial system to a closed-loop. It is one of the most influencing concepts of sustainability. The assumption of this concept is that an open, industrial system that takes raw materials and energy as inputs and creates products and waste can unlikely continue indefinitely (El-Haggar 2007).

Inspired by metabolism and many advantages of natural ecosystems, the idea has been introduced and first mentioned by Frosch and Gallopoulos (1989). Traditional industrial models contain manufacturing processes that take raw materials and generate products and waste. Frosch and Gallopoulos suggest a more integrated model such as an industrial ecosystem (Frosch and Gallopoulos 1989). This concept adapts principles of nature like recycling and reuse and claims that economy can work as nature does. Multiple organisms throughout the system share available resources of materials or energies. The system regulates itself and produces everything it consumes, but also consumes everything it produces (Frosch 1995, Korhonen 2002).

Since human beings produce waste, pollutant emission, and overuse resources, the analogy of industrial ecosystems is an approach to copy the natural recycling model in which elements seek to use each other’s waste material and waste energy (Weber 2005). Frosch and Gallopoulos (1989) described their integrated model as one where “the consumption of energy and materials is optimized, waste generation is minimized and the effluents (…) serve as the raw material for another process" (Frosch & Gallopoulos, 1989, p. 146). Many definitions are provided by literature (see Bissett 2014). For this work, industrial ecology will be defined as

> *"a holistic, interdisciplinary systemic, and cyclical approach to optimizing industrial activity inspired by nature's ecological processes for the sake of economic, environmental, and social enhancement."*

Industrial ecology considers the flow of materials and energy from the extraction through manufacturing, product use, reuse, and return to the natural system (Ehrenfeld 1995). It is further essential to this concept that

> *"if materials are cycled through industrial systems as they are in natural ecosystems, the byproducts of one process would become the feedstock of another and (…) waste would cease to exist." (Veiga and Magrini 2009, p. 654).*

Thus, the goal of industrial ecology is to apply the cyclical and cascading flows, which can be found in nature, to the industry and replace "throughputs" by "roundputs" (Korhonen and Snäkin 2005). Veiga and Magrini (2009) further state that current production processes do not take such a concept into consideration, resulting in major damage for the environment and society.

Cleaner production. As a relatively new field of science research, industrial ecology develops from an academic curiosity to a practical tool (Yu et. al 2013, Lombardi et al. 2012). The related field of cleaner production (CP) overlaps with the field of industrial ecology and shares principles and goals. The goal of cleaner production is to implement a production with zero waste (Pauli 1997). Both concepts have the same scope, but the focus of action is differently. Cleaner production focuses more on pollution prevention and reduction of hazard through substitution (Ayres and Ayres 2002). Emphasizing the customers' responsibility Akenji and Bengtsson (2014) promote sustainable consumption as second key factor.

Industrial symbiosis. The concept of industrial symbiosis (IS), also derived from the natural ecosystem, is a part of industrial ecology. The term symbiosis describes a relationship between two or more species exchanging materials, energy, or information for a common benefit, and thus takes advantage of synergies (Starlander 2003). Applied to an industrial environment, this analogy indicates a symbiotic relationship between corporative actors that exchange materials, energy, or information for their mutual economic advantage. Those relationships commonly seek to achieve environmental and social advantages. Lombardi and Laybourn (2012) investigated numerous definitions for industrial symbiosis (e.g. Chertow 2000, Jensen et al. 2011). The first and most cited definition in literature by Chertow will also serve as the definition in this thesis. Chertow explicitly claims that industrial symbiosis is a part of industrial ecology and defines:

> *"Industrial symbiosis engages traditionally separate industries in a collective approach to competitive advantage involving physical exchange of materials, energy, water, and/or byproducts." (Chertow 2000)*

Thus it is the special case of industrial ecology where separate industries work together. Chertow claims that key factors for industrial symbiosis are collaboration and synergetic possibilities offered by geographic proximity (Ehrenfeld and Chertow 2002). The industrial mix, byproduct availability, resource demands, management structures, institutional linkages, and regulatory climate are relevant factors to be taken into consideration when pursuing industrial symbiosis (Chertow 2000, Gertler 1995).

This concept and the key factors, such as collaboration and geographical proximity, have been applied worldwide. The following Section 2.2 defines, classifies, and discusses the different forms of applying industrial ecology in practice.

2.2 The concept of eco-industrial parks and networks

Understanding the need for application of sustainable development and thus industrial ecology, this section provides an overview of current forms of applications (2.2.1). Building up on a classification of these forms, the following discussion will narrow the scope down to the concept of eco-industrial parks and networks (2.2.2) which are the subject matter of this thesis, as well as pursued goals and properties (2.2.3). Examples and success factors (2.2.4) are specifically investigated.

2.2.1 Applications of industrial ecology

Many publications discuss and review different kinds and examples of applying industrial ecology (Lombardi and Laybourn 2012, Gibbs and Deutz 2005, Ayres and Ayres 2002). In order to classify these examples, Chertow (2000) suggested a framework. Based on the operating level, the classification distinguishes three forms, i.e. facility or firm level, inter-firm level, and regional or global level. Building up on this classification, Bissett (2014) developed an extended classification scheme.

Integrating and merging many discussed forms of applying industrial ecology, Figure 2.4 shows the classification scheme proposed in this thesis. It captures the aforesaid classifications and emphasized aspects of relevance to this research. This classification also matches the distinction of geographical approaches, which are opposing to product-based industrial ecology (Korhonen 2002).

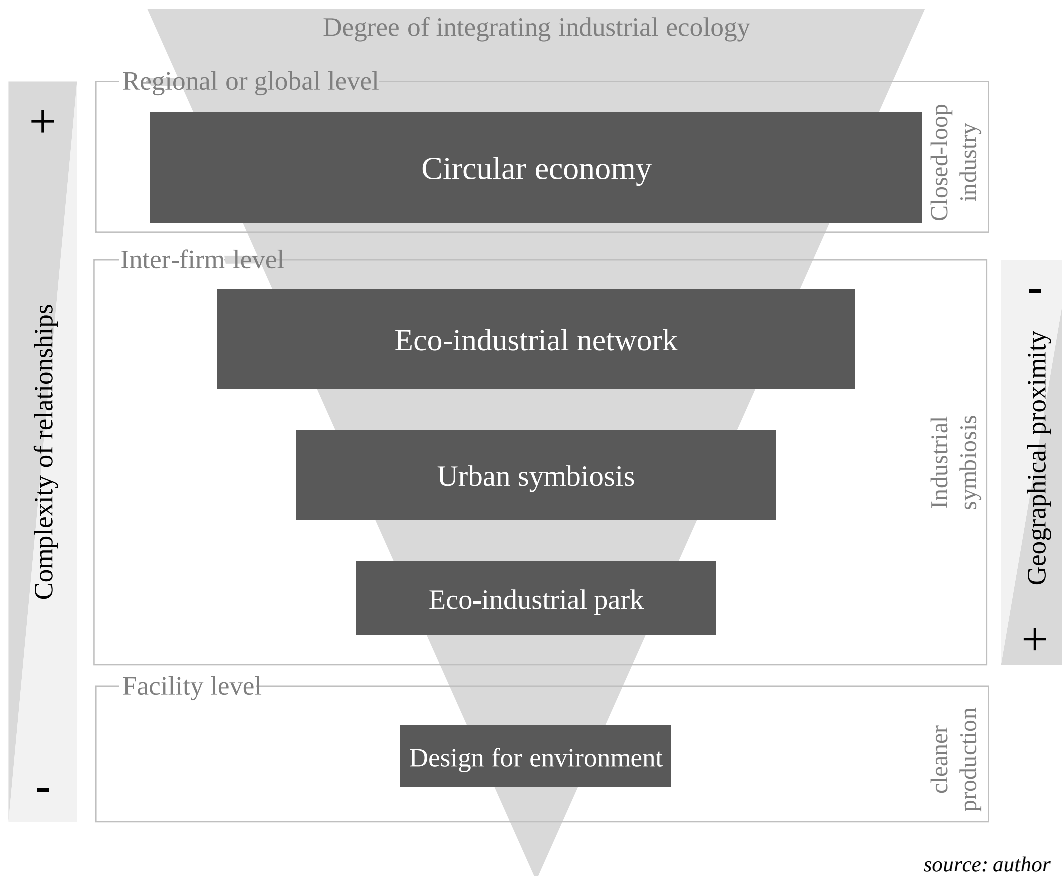

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Figure 2.4: Classification of applications of industrial ecology

The illustration above is based on the three aforementioned levels of industrial ecology by Chertow (2000) extended by the relevant aspects “complexity of relationships”, “degree of integration industrial ecology”, and “geographical proximity”. These aspects are important for the development of a mathematical and computational model in

Chapter 4 of this thesis. While Chertow suggests a very basic classification with operational levels, Bissett (2014) structures a new classification based on spatial scale and temporal existence in literature. The classification of applications of industrial ecology merges ideas of the classification by Chertow (2000) and Bissett (2014).

Starting with the facility level, the main application of industrial ecology is a design for environment that is a part of cleaner production. With an increase of both complexity of relationships between the involved parties and the degree of integrating the concept of industrial ecology, the inter-firm level follows. Industrial ecology at an inter-firm level defines the concept of industrial symbiosis (see Subsection 2.1.3). Applications of industrial ecology at the inter-firm level are eco-industrial parks, urban symbiosis, and eco-industrial networks. The three forms are mainly distinguished through their geographical proximity. While eco-industrial parks are concentrated on a limited region, eco-industrial networks can contain collaboration spread worldwide. Additionally, the complexity of relationships decreases from an eco-industrial network to an eco-industrial park. While eco-industrial parks have a local park management and all members of the park are in one place, members of an eco-industrial network are spread out, difficult to coordinate, can even be members of many different eco-industrial networks, and the degree of autonomous behavior is high. Members can join easily, but the barriers of leaving the eco-industrial network are even lower. The circular economy is the application of industrial ecology on a national or even international or global level. In addition to the industrial and community members, political stakeholders make the task of coordination even more complex.

Fang et al. (2007) apply a similar classification to the Chinese economy based on scale (community level to national level) and industrial sustainability.

This research work focuses on the inter-firm level application of industrial ecology. Hence, the next subsections provide a detailed view on the definitions, goals, drivers, limitations, and properties of the application of industrial symbiosis.

2.2.2 Definition of an eco-industrial park and network

One of the most important goals of industrial ecology, making the waste of one industry the inputs of another, can be accomplished in many different ways (Frosch 1994). El-Haggar (2007) states that “the most ideal way for IE is the eco-industrial park” as it has been introduced previously (El-Haggar 2007, p. 91). It is referred to as the major application of industrial symbiosis (Veiga and Magrini 2009). The classic example of an EIP has evolved in Kalundborg and will be discussed in Subsection 2.2.4. However, many definitions have been proposed, enhanced, and modified over the last two decades in literature (Veiga and Magrini 2009, Lowe 2001, Schlarb 2001, Chertow 2000, Rosenthal and Côté 1998, PCSD 1996; Chertow 1997, Ayres 1995, Lowe et al. 1995, Côté and Hall 1995). Most definitions reflect the focus of research of the respective publication. The following paragraphs discuss the term eco-industrial park and its enhancements to capture core elements and essential properties of this idea.

Industrial park. Peddle defined an general industrial park and points out that in contrast to a network of companies, an industrial park contains “several firms simultaneously, (…) shareable infrastructure and close proximity of firms” (Peddle 1993, p. 108).

Eco-industrial park. Extended by the aforementioned concept of industrial ecology, the eco-industrial park is a special case of industrial park. Côté and Hall (1995) proposed one of the very early definitions, building on the previous definition:

> *"An eco-industrial park is an industrial system which conserves natural and economic resources; reduces production, material, energy, insurance and treatments costs, and liabilities; improves operating efficiency, quality, worker health, and public image; and provides opportunities for income generation from use and sale of wasted materials."*

While this definition defines the term from the company perspective by emphasizing aspects of sustainability on the company level such as costs, worker health, and public image, other definitions are more politically biased.

In October 1996, the President's Council on Sustainable Development (PCSD) recommended "Federal and state agencies assist communities that want to create eco-industrial parks" (PCSD, p. 104). Under consideration of 15 existing eco-industrial parks, the PCSD suggested two advanced definitions. The majority of the council's participants voted for the political draft of a definition:

> *"A community of businesses that cooperate with each other and with the local community to efficiently share resources (information, materials, water, energy, infrastructure and natural habitat), leading to economic gains, gains in environmental quality, and equitable enhancement of human resources for the business and local community." (PCSD 1996).*

This definition has been widely accepted in the field of industrial ecology (Côté and Cohen-Rosenthal 1998). However, a second definition suggested by the same council sets a different, corporate focus on the properties of an EIP. It is "An industrial system of planned materials and energy exchanges that seeks to minimize energy and raw materials use, minimize waste, and build sustainable economic, ecological, and social relationships." (PCSD 1996). Since none of these definitions captures every property of an eco-industrial park, many publications modify and enhance these definitions according to their individual needs. It should be emphasized for the purpose of this publication that all of the introduced definitions share elements. Veiga and Magrini (2009) review contemporary definitions and recall the definition by Lowe (2001) as a further development of previous definitions to capture the full idea of an EIP:

> *"An eco-industrial park or estate is a community of manufacturing and service businesses located together on a common property. Member businesses seek enhanced environmental, economic, and social performance through collaboration in managing environmental and resource issues. By working together, the community of businesses seeks a collective benefit that is greater than the sum of individual benefits each company would realize by only optimizing its individual performance." (Lowe 2001)*

Not only does this definition emphasize all three dimensions of sustainable development, i.e. economy, environment, and the frequently neglected society, it further expresses the need of a systematic method for analysis. Lowe explicitly mentions the aspect of optimization. This emphasizes the need for mathematical and computational methods in order to analyze, improve, and create such an EIP.

Eco-industrial network. It is not always possible to establish geographic proximity. To relax this condition and make the concept of industrial ecology even more applicable, "virtual EIPs" (Ehrenfeld and Chertow 2002) are defined as EIPs without geographic proximity. The terms "industrial symbiosis networks" (Domenech and Davies 2011), and "zero waste networks" (Curran and Williams 2012) are interchangeable. If the participants of a geographically spread virtual EIP are EIPs respectively, this is called an eco-industrial networks (EIN). Roberts defined EINs as

> *"networks of EIPs at national or global levels" (Roberts 2004).*

To achieve the target of this thesis, mathematically and computationally model and optimize such parks and networks, it is necessary to gain a deeper insight into the goals and properties of eco-industrial parks.

2.2.3 Goals and properties of an eco-industrial park

While it is important to the task of mathematically modeling to be aware of the goals pursued by an eco-industrial park, the main properties help to understand the modeled system. Both aspects are investigated in this subsection.

Goals. The overall goal of an eco-industrial park is the application of industrial ecology and the promotion of sustainable development in all of its dimensions. Sustainable development seeks to achieve the following: equity in society, reduction of environmental pollution, and industrial development. Hence, the needs of the present generation can be met without sacrificing the needs of future generations through a sustainable use of resources and preservation of ecological and human health. The primary goal of industrial ecology is to promote sustainable development at the global, regional, and local levels (Keoleian and Menerey 1994). Derived from these general goals, specific goals of an eco-industrial park are more explicit than the goals of higher-level concepts. Lowe (2001) appended the aforementioned definition:

> *"The goal of an EIP is to improve the economic performance of the participating companies while minimizing their environmental impacts. (...). An EIP also seeks benefits for neighboring communities to assure that the net impact of its development is positive." (Lowe 2001)*

The reduction of demand on finite resources by recycling and reusing waste materials is a main accomplishment. Hence, more natural resources are made renewable and waste and emissions are diminished. On the social side, EIPs create new regional jobs and increase the cooperation and participation among different industries. This leads to development in a sustainable manner. The improvement of municipal infrastructure and increased tax payments are further advantages and goals of eco-industrial parks and networks (El-Haggar 2007, Lowe and Evans 1995). These goals can be split further into sub-goals. El-Haggar discusses the goals of an EIP depicted in Figure 2.5.

Following the basic concept of economic activity, i.e. the “homo economicus”, every business transaction is based on rational and self-interested decision makers who attempt to maximize their utility as consumers and benefit as producers (Rittenberg and Tregarthen 2009). Hence, the economic goals of an EIP are of special interest.

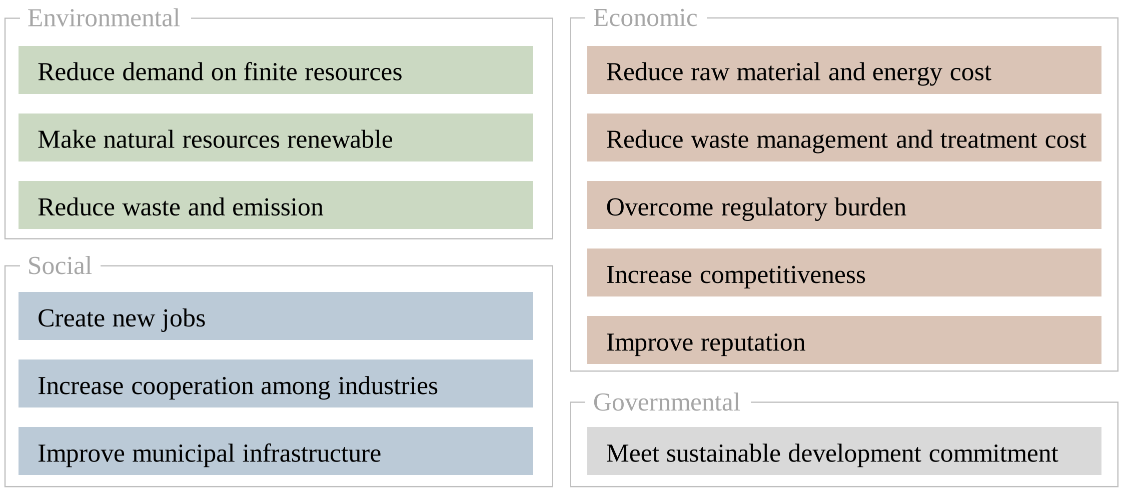

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Figure 2.5: Goals of an EIP clustered by dimensions of sustainable development

A reduction of cost for materials, energy, transactions, waste management, waste treatment, and other factors must be part of the basic goals to convince members to join the EIP (Lowe and Evans 1995). Weber (2008) shows that sustainable behavior of a company, commonly referred to as corporate social responsibility (CSR), can positively affect its success through competitiveness and reputation in short and long term.

Many sub-goals can lead to harmful consequences for the overall goal of sustainable development. Creating new jobs through promoting EIPs in developed countries can lead to a decrease of social sustainability in developing countries. An example is the placement of a new employee in a developed who replaces up to four workers in a developing country due to higher efficiency. Other than the worker in the developed country, the four workers in the developing country commonly do not have an alternative and may become unemployed and end in poverty.

Properties. Pursuing the abovementioned goals, eco-industrial parks have a similar structure and interacting essential elements. Figure 2.6 illustrates the concept of an eco-industrial park, its elements, and their relationships.

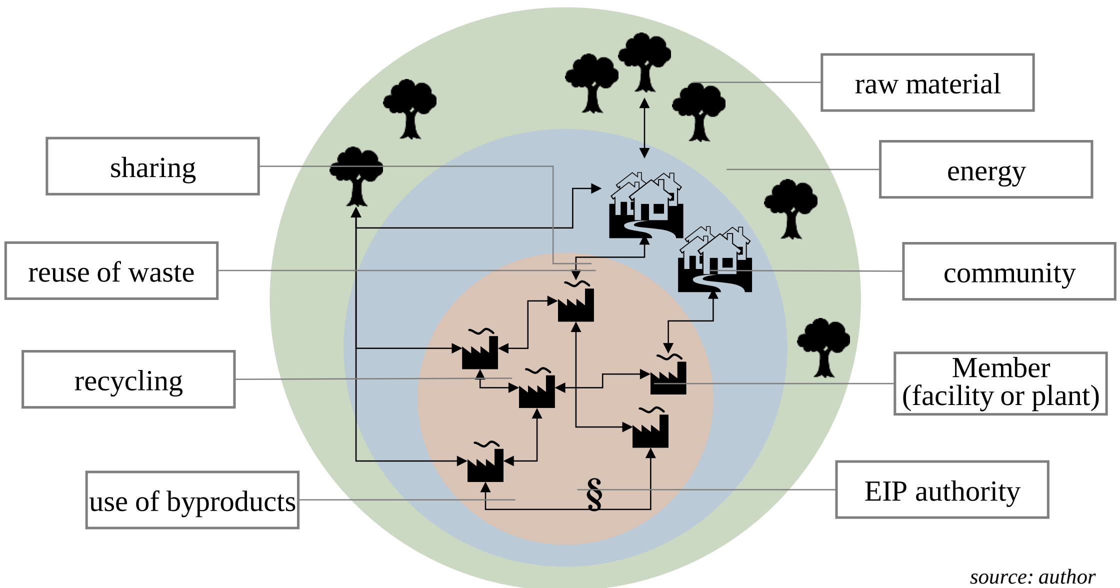

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Figure 2.6: Scheme of an eco-industrial park and its elements and relationships

The figure shows how the previously introduced dimensions of sustainable development (see Subsection 2.1.2) perfectly appear in this form of applying industrial symbiosis. Promoting their economic targets, members of an EIP are mainly faculties or plants from companies of different industries. They collaborate by using their byproducts, sharing utilities and operations as well as reusing and recycling waste materials or products. Pursuing a social benefit, the EIP is also commonly connected to a near community. In the subsequently discussed example of Kalundborg (see Subsection 2.2.4), the community participates by receiving heat and job opportunities. Energy and raw materials are acquired from nature and partially given back. For example, fresh water may be reused and completely recycled back into the environment.

The understanding of the structure and goals of an eco-industrial park is essential for mathematical modeling; however, in order to develop a comprehensive model in the fourth chapter, the main factors of successful, existing examples should be identified.

2.2.4 Drivers and limitations of EIP development

In pursuit of the declared goals, many examples of eco-industrial parks have been established within the last two decades, especially since the beginning of the investigations in the Kalundborg case by Ehrenfeld and Gertler in 1997. EIPs are found in many different countries, including the investigated examples in North America (Côté and Cohen-Rosenthal 1998), South America (Veiga and Magrini 2009), Asia (Zhang et al. 2010), Australia (Roberts 2004), and Europe (Heeres et al. 2004, Costa et al. 2010). Further examples for EIPs in the United States and Canada, as well as key industries were studied by Côté and Cohen-Rosenthal (1998).

The Kalundborg case. The classic example of an eco-industrial park is Kalundborg in Denmark (Ehrenfeld and Gertler 1997). However, the industrial park in Kalundborg was not designed as an EIP, but instead evolved over time and due to fortunate circumstances. Participants discovered the establishment of exchanging byproducts and utilities resulted in both environmental and economic benefits for all the park's members (Lowe and Evans 1995). The total economic benefit is estimated as 12 to 15 million US-dollars annually (Heeres et al. 2004). Figure 2.7 shows the industrial ecosystem in Kalundborg, Denmark, first investigated academically by Ehrenfeld and Gertler (1997).

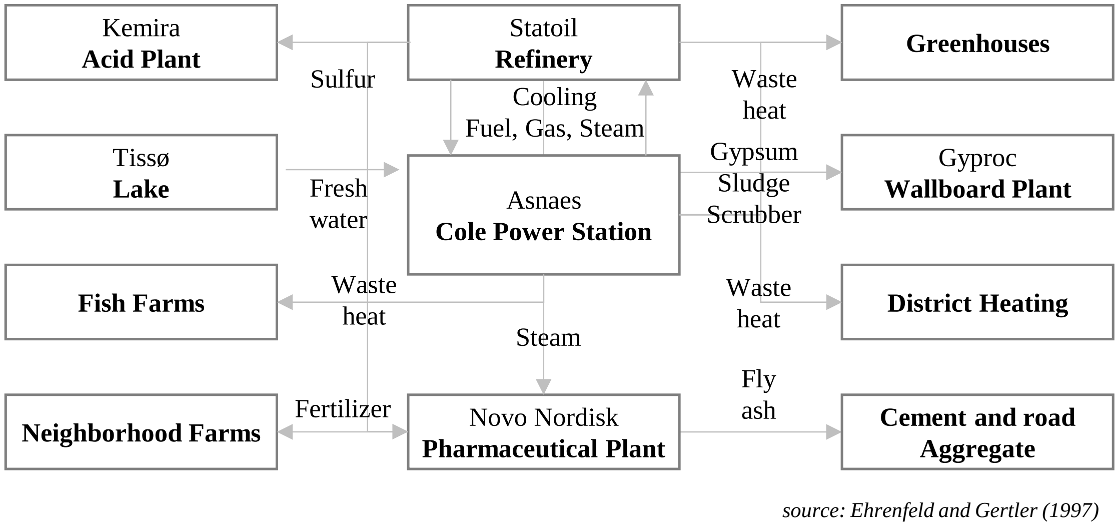

Figure 2.7: The eco-industrial park at Kalundborg, Denmark

This park exchanges materials and energy with companies and a community in the industrial region west of Copenhagen. With the goal of a profitable benefit for their waste products and thus a reduction of the environmental impact, five core companies have evolved a pioneer application of industrial symbiosis. The members are a central power station fired with coal for 1500 megawatts of electrical power, an oil refinery with a capacity of 3.2 million tons, a plasterboard factory with an output of 14 million square meters of plasterboard annually, a biotechnological company, and the city of Kalundborg. The biotechnological company is the largest member of this cooperation and the city of Kalundborg participates via water supply and district heat (Lowe and Evans 1995). The flows of this park can be distinguished in two categories:

- Energy flow (Steam, Fuel, Gas, Heat)
- Material flow (Fly ash, gypsum, sulfur, sludge, fertilizer, water)

This network of recycling and reuse has generated additional revenues and cost reductions for all involved partners and has avoided air, water, and land pollution in the region (Lowe and Evans 1995). However, Korhonen (2004) points out that the park in Kalundborg relies upon non-renewable fossil resources, produces extensive emissions and is thus not environmentally sustainable (Gibbs & Deutz 2007).

The Paracambi case. Unlike the prior case, the EIP in Paracambi, located outside of Rio de Janeiro, Brazil, has been planned and set up completely from scratch as a green field project in 2006 (Veiga and Magrini 2009). Coordinated and supported by the government, this park has been designed to help industries which are looking for ways to cut cost and simultaneously reducing the consumption of natural resources.

It should be mentioned that this concept of environmentally friendly sharing is not entirely new. Many chemical companies and industrial complexes have existed for a long time, leveraging synergies with other companies in the same industry (Clift 2006). However, examples of EIPs are characterized by new, unexpected connections between heterogeneous classes of industries or even outside of industrial production such as a service provider (Heeres et al. 2004).

Investigation of these and other examples of industrial ecology in practice, it is conspicuous that members are mostly chemical companies and power stations. Typically, technological or legal reasons lead to collaboration for the purpose of industrial ecology (Tudor et al. 2007). This makes it difficult to include manufacturers of commodities in such parks. Many parks develop over time and after all, the evolution of the pioneer Kalundborg was commented by Jorgen Christensen, vice president of

Novo-Nordisk as follows: "At the time we were just doing what was profitable and what made sense" (Lowe and Evans 1995). These findings lead directly to the question of how EIPs evolve as well as success factors, and boundaries of their development.

EIP development. Eco-industrial parks can evolve through many different ways. Figure 2.8 shows three different ways which can be observed when an EIP occurs.

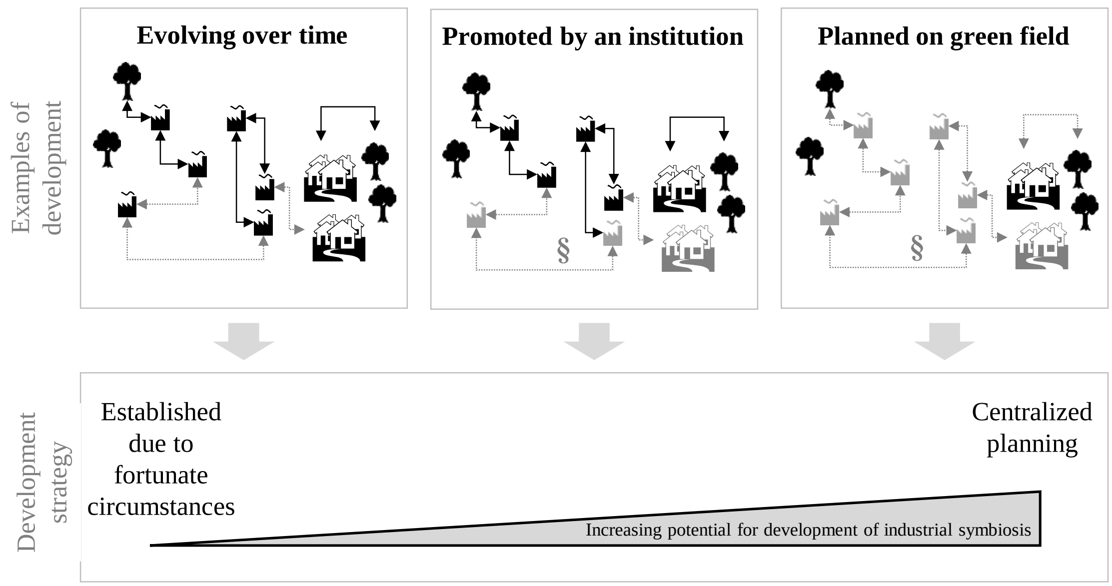

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Figure 2.8: Development strategies of eco-industrial parks

Two extreme development strategies are derived from these observations, i.e. established due to fortunate circumstances and centralized planning.

The case of Kalundborg shows that EIPs can evolve due to fortunate circumstances or suitable business relationships. Common problems and collaboration abet the development of such a park. Over time, more and more connections and members are joining the park for the sake of a mutual economic benefit. In contrast, deliberate planning from scratch can lead to green field projects (Korhonen et al. 2002). An example for this case is the EIP in Paracambi. However, many publications call for more centralized planning and promotion of EIPs to overcome market failure. They claim that unlike biological systems, industrial systems are based on payments and profits to economical markets. Biological systems work without such mechanisms (Ayres 1997, Tudor et al. 2007, van Leeuwen et al. 2003). Successful examples have overcome this barrier by implementing institutions that promote EIPs (Zhang et al. 2010).

Drivers. Regardless of which development strategy has been applied, Tudor et al. (2007) investigated the successful development of eco-industrial parks due to an extensive review of existing EIPs. An extract of the identified major success factors are listed in Table 2.1 below.

No.	Factor of success	Source
1	Cooperation on basis of improving environmental and economical performance	Pellenbarg 2002, Heeres et al. 2004
2	Initiative from firms and not from government	Pellenbarg 2002
3	Active participation from range of stakeholders including public sector, companies, and environmental organizations	Heeres et al. 2004
4	Presence of large firms acting as a ‚magnet‘ for other businesses	Pellenbarg 2002
5	No participation of direct competitors	Dekker 1997
6	Existing level of trust between the participants	v.d. Veeken 1998, Rondinelli and London (2002)
7	An association firm should be created	v.d. Veeken 1998, El-Haggar 2007

Table 2.1: Success factors for development of EIPs (extract of Tudor et al. 2007)

These and many more factors can have a positive influence on the development of an EIP; however, there is no reliable and safe recipe for setting up a successful project.

In reality the contrary is the case, for many known and unknown circumstances have to be matching for the evolution of a new EIP.

Limitation. Despite the presence of many fortunate circumstances, some EIPs do not exist long term. A major cause is the potential fragility of such a system. While large companies can serve as a 'magnet', the small networks and collaborations of businesses are extremely vulnerable when such a company leaves. Sterr and Ott (2004) claim the fluctuation in general of any network partner has a huge impact on the long-term existence of EIPs. Due to the structure and composition of EIPs, additional difficulties through miscommunication and a lack of information dissemination are likely to arise (McIntyre 1998). Chiu and Yong (2004) studied eco-industrial parks in China and found that a lack of a clear understanding of the concept, inaccurate measuring of defined goals, an unclear definition of roles, rights, and duties of participation are common causes for the failure of EIPs. They further claim that in many cases, potential participants do not understand the specific potential of applying industrial symbiosis.

Independently of the performance and effort of the members, a main problem for creating industrial symbiosis is that some contents that may be industrial wastes cannot be economically reused or recycled (Ayres 2004). Ayres promotes a negative attitude towards the success of EIPs stating that "The idea that some industry can always be found (or created) to consume another industry's wastes or even just its solid wastes' is naïve." (Ayres 2004, p. 428) Ayres adds that industrial waste is mostly a mixture that would still be useless for others even if it was separated into pure components. Facing the challenges of the application of industrial symbiosis.

Pellenbarg (2002) even considers the economy and ecology as natural enemies.

And yet, the success of some examples proves the basic idea of applying industrial symbiosis can lead to a simultaneous improvement of environmental and economic performance while supporting a positive social development, and thus generate a win-win-win situation in sustainable development (Gibbs and Deutz 2005, Elkington 1994).

Showing the history and origin of sustainable development and its industrial application in eco-industrial parks and networks, Section 2.1 and 2.2 provide a review of the main concepts, terms, examples, and aspects in this field. Thus theoretical basis is crucial to successfully investigate and develop modeling approaches. Besides the subject matter, the second part of the theoretical foundation, i.e. the methodology of mathematical modeling and simulation for decision support will be reviewed in the following sections.

2.3 Mathematical modeling and simulation for decision support

Many industrial symbiosis relationships are established due to coincidences and fortunate circumstances; however, drivers and limitations have been investigated for EIP accruement (Subsection 2.2.4). In general, supporting proper decisions in order to establish industrial symbiosis can promote sustainable development. Therefore, the second part of the theoretical foundation for this work is a review of the promoted scientific methodology of mathematical modeling and simulation for decision support.

This section introduces main terms in the field of decision-making followed by major distinction of mathematical models and simulations (Subsection 2.3.1) as well as an overview of the occurrence of models in science over the last decades (Subsection 2.3.2)

2.3.1 Terms in the field of decision making

The previous section shows that the concept of an eco-industrial park can provide a variety of environmental, economic, and social benefits. Before this happens, decisions for future actions must be made. These can lead to both potential success and failure. Due to the consideration of many influencing factors on success or failure of a system, decisions based on mathematical models are significantly less likely to fail. Such decision-making problems always relate to an underlying system, called the relevant system. The responsible person or group who make these decisions is called decision maker for the problem (Murty 2012).

Complexity of decision-making problems. Decision making problems can be of various complexities. A problem can consist of just a few variables with very simple conditions to be met. Decisions of those problems can often be made intuitively. On the other hand, extensively large problems with many variables and restrictions have to be included to distinguish between possible alternatives. Two main categories are:

- Simple problems

These problems usually contain a finite, discrete set of possible alternatives. All of them are fully known in complete detail and a choice has to be made by the decision maker. An example for these problems is when a company gets three offers for a request and has to decide on one of these possible alternatives. For these Multi-Criteria Decision Making problems (MCDM), scoring methods are mostly applied in order to support a decision (Triantaphyllou 2000). The second category is called:

- Complex problems

An alternative taken into consideration as a solution for such a problem must satisfy all restrictions given by the problem circumstances. In order to make the best decision, mathematical models are constructed. Depending on the field of restrictions, an infinite number of possible solutions can be possible. Examples of these quantitative analysis problems are the optimization of process parameters and decisions about material flows and locating plants (Murty 2012).

During the process of decision-making, different methods are required. To ensure a comprehensive understanding of terms used in the context of the decision-making process, this subsection provides definitions for important terms and methods related to the process of decision-making, spanning from the original objective to the final decision. The main terms and their relationships are illustrated in Figure 2.9.

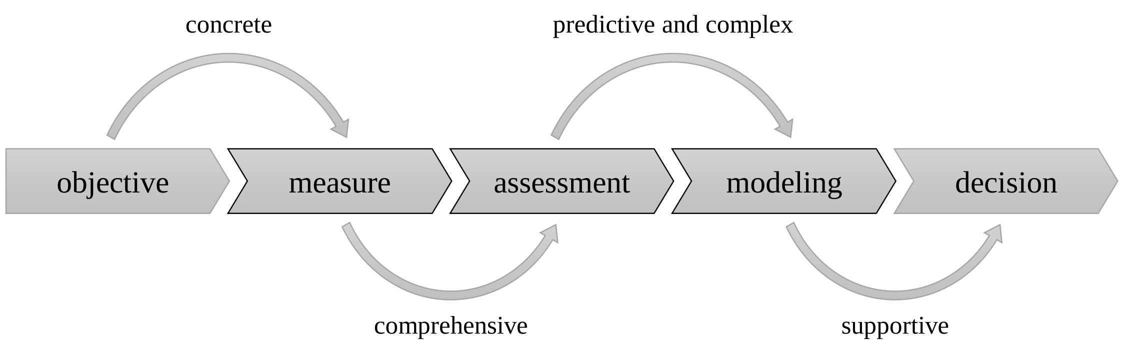

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Figure 2.9: The logic of modeling for decision-making regarding an objective

Objective. The process of making a decision starts with a main goal. In mathematical and modeling related terms, this goal is considered to be the objective of the decision.

Measure. In order to represent an objective in mathematical terms, a measure is constructed to ascertain and assign a numerical value to a property of the relevant system. A measure can be an amount, size, or degree measured by various units.

Assessment. By means of a collection of measurements, the evaluation or estimation of a comprehensive situation can be determined. In this work, such a comprehensive ascertainment is called an assessment. In general, assessments determine a quantitative or qualitative value for a concrete situation and can thus support decision or general conclusions. Assessments are commonly used to capture numerous measures with complex relationships in a single value or attribute.

Modeling. Due to the extensive complexity and uncertainty of today's modern world systems, methodologies to capture the complexity are unavoidable (Velten 2009). In order to reduce this complexity, models can be constructed.

> *"a model is a simplified description of a system" (Velten 2009).*

This system refers to the object of interest. It is crucial that modeling is goal-driven and models are created to answer a specific question or for a defined purpose (Cellier 1991). Stated by Velten (2009),

> *"the best model is the simplest model that still serves its purpose"*

or is still complex enough to help understand a system and solve the predefined problem. The process of creating a model is called modeling. Depending on the purpose, frameworks for modeling are defined in literature (Andradóttir 1998, Benington 1987). Due to the loose definition of the word model, there are many different classes of models. Many approaches for clustering models can be found depending on the field of research and the pursued goal. Eijndhoven distinguished models into four main categories based on the degree of physical implementation in contrast to theoretical construct: physical, schematic, verbal, and mathematical models (Eijndhoven 2014). These categories are subsequently described.

Physical models represent physical properties of an object and are mostly very similar to the modeled object of the real world. A common kind of this category is a physical prototype, which is built to test and learn from during operation in reality. A prototype is a tangible model that can operate as a real system.

Schematic models are more abstract than the first class of physical models. These models look much less like physical reality, but still visually represent a subject of matter. Graphs, charts, and computer programs are examples of schematic models that provide a visual display or relationships and circumstances.

Another step further away from a tangible representation is the third class of models, called verbal models. Verbal models use words to represent circumstances, situations, or objects from the real world. Descriptions and information on a special case can describe the situation of a company such as a business case. Additionally, verbal models contain enough information to later develop a model of the fourth class of models.

Mathematical models are the most abstract of the four model classes. They involve mathematical constructs and formulations to describe reality. Such models can provide a number of insight, for example of dynamic and statistic systems. Their structure allows the modeler to gain insight and clarity about certain aspects in a very accurate manner.

Decision. A selection for one of the possible alternatives is based on the chosen modeling approach. This decision is the core of a decision-making problem.

Eco-industrial parks can be assessed and their performance measured. In the understanding that the development of a modeling approach is a main goal of this thesis, the next section provides a deeper insight into the methodology of modeling.

2.3.2 Mathematical models and computer simulation

Due to the increasing complexity of considered systems and a dramatic improvement of supporting computer technology, mathematical models in the original sense have changed. In addition to mathematical equations, logical constructs and automation have extended the possibilities of recent research. Mathematical models have been extended to computer models. Approaching the modeling task in a scientific manner, Figure 2.10 shows the relationship of these kinds of which are defined in the following.

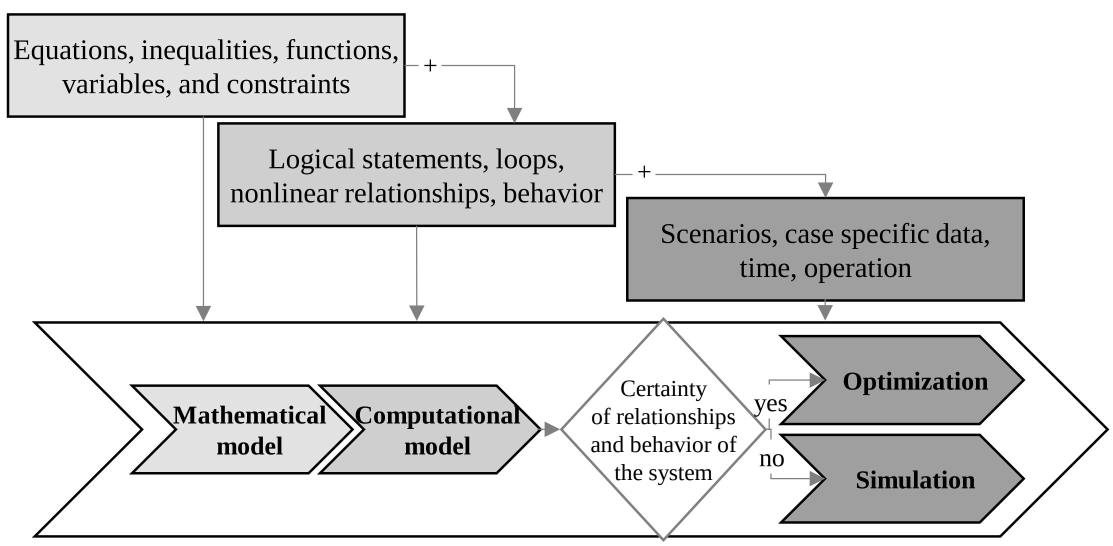

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Figure 2.10: Relationship of mathematical models, optimization, and simulation

Mathematical model. Every model is created to solve a certain problem. Figure 2.10 shows the sequence of extending methodologies depending on the complexity of the considered model. While a model in general is a simplified representation of a real world system, the mathematical model describes the subject matter by means of mathematical concepts and language such as equations, inequalities, functions, variables and constraints. Dym suggests a definition of a mathematical model:

> *“A mathematical model is defined as a representation in mathematical terms of the behavior of real world systems” (Dym 2004, p. 4).*

In addition to this definition, Eijndhoven adds that mathematical models always represent a part of the real world (Eijndhoven 2014).

Algorithm. In some cases, the application of a mathematical model requires more than just a single step. In these situations, a step-by-step procedure for calculations and executions of mathematical constructs is defined. These are called algorithms. As a compilation of mathematical model(s), the implementation of an algorithm is called a computational model and defined subsequently.

Computational model. By adding logical statements, loops, nonlinear relationships and behavior, a mathematical model (or algorithm) can be extended to a computational model. Regarding complexity of a model, mathematical models can be considered to be a subset of computational models. Due to the use of computational resources, the computer model can solve additional problems, which cannot be investigated with mathematical model. Rather than deriving an analytical solution to a problem, computational models are the basis to conduct experiments, adjust parameters of the system, and study the dependent output (Eijndhoven 2014).

Depending on the circumstances and specific situation of applying a mathematical and computational model, these can be used for optimization or simulation. The basic difference between these two forms is that an optimization always determines the best possible solution(s) of a given set of data in order to support a decision, while a simulation is more applicable when the set of data provided is uncertain, relationships within the system are complex and uncertain, and no optimal solution is desired in order to make an optimal decision. Simulation can only put a defined system into operation.

Optimization. With an increasing complexity, mathematical models can be extended and implemented as computational models. A certain type of mathematical models are optimization models, which work to find the optimal solution of a decision problem. Adapted to Murty (2012) optimization models are defined as

> *"mathematical models with an objective function to be optimized (maximized or minimized) to satisfy restrictions on the numerical decision variables".*

Since optimization models are of a very high relevance to this thesis, the next Section 2.4 will introduce and describe relevant optimization models for relevant purposes.

Simulation. In contrast, mathematical models and computer models can be applied to complex and uncertain situations in a simulation, which is defined by Maria (1997):

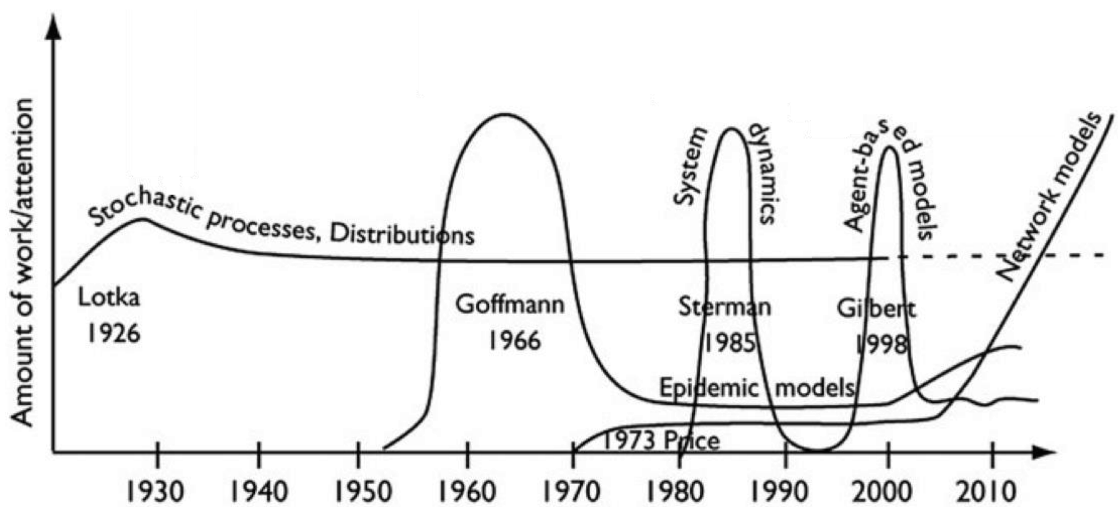
> *"A simulation of a system is the operation of a model of the system"*

The term originates from the Latin word "simulare", which means "to pretend".

The simulation proceeds the input data to a computed output for a computational model which again was built up from a mathematical model. Thus, different scenarios and conditions can be applied to a model. It can be seen as the imitation of a real process (Banks et al. 2013) and puts the model into operation. Other than optimization, simulation represents a deductive practice of investigating a system (Mattern 2009).

2.3.3 Occurrence of mathematical models in science

To provide a state-of-the-art modeling approach in this thesis, existing approaches are essential background information. While the following third chapter provides a deeper insight in the modeling approaches of industrial ecology, this section discusses a broad overview of mathematical models applied in science. Diana Lucio-Arias and Andrea Scharnhorst provide such an overview. The results of their algorithmic-historiography review are illustrated in Figure 2.11.



source: Lucio-Arias and Scharnhorst (2012)

Figure 2.11: Historical overview of the occurrence of certain mathematical models

Lucio-Arias and Scharnhorst suggest increasing capabilities due to computer performance is one reason for increased investigation of network models. Based on these investigations and the development of an advanced modeling approach, network models are described in the following section.

2.4 Optimization models for decision making

Eco-industrial parks and networks are the relevant system to be modeled in this work. While Chapter 3 focuses on both the mathematical model for optimization and simulation approaches, Chapter 4 does not target simulation. This section will thus provide a narrowed selection of modeling approaches focusing on optimization.

The EIP can be generalized as a network of many stakeholders pursuing different goals under a limited degree of certainty. Basic methodologies and problems referred to for these circumstances are network models (2.4.1), multi-objective optimization (2.4.2), and sensitivity analysis (2.4.3). This section focuses on relevant models.

2.4.1 Network models

In order to mathematically describe the structure of an EIP or an EIN, network models are suitable. In addition to their frequent use due to increasing computer performance, network models provide many other advantages:

- Large problems can be solved quickly and allow real-time decision making
- Models can mostly be solved quickly though linear problems (NP-complete).
- Networks are intuitive and eligible for application in industry circumstances

Networks have been described in various ways. Network optimization is a special type of linear programming, which is widely used in production, distribution, project and location planning, and many other fields. The shortest path, maximum flow, transportation, and assignment problem are basic network problems. In order to represent the circumstances given by an EIP or EIN, the transshipment, multi-commodity network, and warehouse location problem are introduced subsequently.

Transshipment model. In the mathematical sense, networks always contain a set of nodes and connections amongst interacting elements of the network. Each connection, called arc, can have a certain weight, which represents the cost or distance from one node to another. The formulation of this problem is the transshipment problem. It contains items being supplied from different sources to destinations. While the transportation problem can only have sources and sinks, the transshipment problem contains additional transshipment points. A shipment can pass through one point for economical, ecological, or social reasons. The model is given subsequently.

$$min \sum_{i=1}^{m} \sum_{j=1}^{n} c_{ij} x_{ij} \qquad (2.1)$$

subject to:

$$\sum_{s=1}^{m+n} x_{is} - \sum_{r=1}^{m+n} x_{rs} = a_i \qquad \forall i \qquad (2.2)$$

$$\sum_{r=1}^{m+n} x_{r,m+j} - \sum_{s=1}^{m+n} x_{m+j,s} = b_{m+j} \qquad \forall j \qquad (2.3)$$

$$\sum_{i=1}^{m} a_i = \sum_{j=1}^{n} b_{m+j} \qquad \forall i \qquad (2.4)$$

$$x_{rs} \geq 0 \qquad \forall r, s \qquad (2.5)$$

The goal is to minimize the sum of all weights (2.1), i.e. distances, times, or costs for the shipped amount from each node to every other node in the network. The objective function is restricted by the following constraints: The first constraint (2.2) ensures that the overall balance of incoming and outgoing amounts of the commodity equals the available amount that can be supplied by each source node. The second constraint (2.3) ensures that the overall balance of incoming and outgoing amounts of the commodity equals the available amount that is demanded by each sink node. The third constraint (2.4) guarantees that the problem is balanced. The total supply equals the total demand. Thus it is possible for goods to enter a certain transshipment point and leave this point so that the total sum equals the supply or demand provided by this node. The last constraint (2.5) is a non-negativity constraint for the amounts transferred (Nering 1993).

Multi-commodity flow. A multi-commodity network is an approach to model the previously mentioned transshipment problem extended by the assumption that not one, but a number of different objects can flow through the network. Such a network contains nodes connected by arcs. The generalized flow problem of multi-commodity networks with a maximum transferred amount of u_{ij} from node i to j can be formulated as:

$$min \sum_{i=1}^{m} \sum_{j=1}^{n} \sum_{k=1}^{h} c_{ij}^{k} x_{ij}^{k} \tag{2.6}$$

subject to:

$$\sum_{j=1}^{n} x_{ij}^{k} - \sum_{j=1}^{n} x_{ji}^{k} = b_{i}^{k} \qquad \forall i, k \tag{2.7}$$

$$\sum_{k=1}^{h} x_{ij}^{k} = u_{ij} \qquad \forall i, j \tag{2.8}$$

$$0 \leq x_{ij}^{k} \leq u_{ij}^{k} \qquad \forall i, j, k \tag{2.9}$$

Each arc has a particular weight. While this problem is based on similar assumptions, as is the transshipment problem, the main scope is to consider the network under a limited capacity on each arc. A bi-directional flow consumes capacity, which is also referred to as the “bandwidth”. Large scale problems can efficiently be solved (Babonneau et al. 2004, Gabrel et al. 1999).

Warehouse location problem. Other than the two previously introduced modeling approaches, warehouse location problem (WLP), or interchangeably termed uncapacitated facility location problem (UFLP), does not make the assumption that each location must exist. In fact, the nodes included into every network are previously defined. However, additional binary decision variables are included into these models in order to determine whether a location is actually open or not. The UFLP involves locating an undetermined number of facilities to minimize the sum of the fixed setup costs and variable costs of serving the market demand from these facilities. It assumes that the alternative facilities and the demand in each customer zone has been previously determined. It focuses on the production of a single commodity over a single period of time. Krarup and Pruzan (1983) prove the NP-completeness of the UFLP by relating this problem to the set packing-covering-partitioning problems. The seminal publication of Erlenkotter (1987) discusses a dual-based algorithm for solving the UFLP that still remains as one of the most efficient solution techniques for this problem (Verter 2011). Erlenkotter defines the uncapacitated facility location problem as follows:

Let I denote the set of m alternative facility locations with the index i and J denote the set of n customer zones with the index j. Then the two decision variables for this problem are x_{ij} and y_i describe the faction of demand of customer zone j satisfied by facility at location I and binary variables that assume a value of 1, if a facility is to be established at location I, 0 otherwise, respectively. Since the demand data in this case is inherent to the decision variable for the faction of customer zone j's demand, only cost data needs to be defined in this case. The fixed cost f_i of establishing, or opening a facility at location i and the total cost for supplying all demands of customer zone j by the facility at location i, c_{ij} are given in order to determine the following formulation:

$$min \sum_{i=1}^{m} \sum_{j=1}^{n} c_{ij} x_{ij} + \sum_{i=1}^{m} f_i y_i \qquad (2.10)$$

subject to:

$$\sum_{i=1}^{m} x_{ij} = 1 \qquad \forall j \qquad (2.11)$$

$$x_{ij} \leq y_i \qquad \forall i, j \qquad (2.12)$$

$$0 \leq x_{ij}, y_i \in \{0,1\} \qquad \forall i, j \qquad (2.13)$$

The objective function represents the total fixed and variable cost. The first constraint ensures that the demand at each customer zone is satisfied. The second constraint guarantees that customer demand can be produced and shipped only from the locations where facilities are opened. The variable costs are assumed to be a linear function of the quantities produced and shipped at each facility and thus do not consider economies of scale. Lu (2010) suggests step functions as an approximation for s-shaped cost functions of production systems. Heuristic approaches were developed to solve such problems. However, WLPs of decent complexity can be solved exact by means of computers and algorithms (Verter 2011, Akinc and Khumawala 1977, Nauss 1978, Beasley 1988).

2.4.2 Multi-objective optimization

In order to face the challenge of many objectives under circumstances due to sustainable development, basics on multi-objective optimization (MOO) are introduced.

Relevant terms in the field of MOO are clarified initially.

General multi-objective optimization problem. The previous section discusses the general term “mathematical model”. Noticing that a model is always made for a certain purpose, optimization models always seek to optimize a goal, i.e. the objective function. In many real life problems, decision-making often requires more than one objective, for example when many stakeholders or decision makers are involved in a decision. Such problems are called multi-objective optimization problems (MOP) and are of the following form (Miettinen 1999):

$$min\{f_1(x), f_2(x), \ldots, f_k(x)\} \tag{2.14}$$

$$\text{subject to: } x \in S \tag{2.15}$$

where the variables are part of vector $x = (x_1, x_2, \ldots, x_n)^T$ restricted by the field of constraints S. Other than a single objective function, the objective functions of an MOP can have individual optimum and thus the set of functions can have more than one optimal solution. Because of contradictions of objective functions, it is impossible to find a unique solution that would be optimal for all the objectives simultaneously.

Pareto optimality. However, some resulting vectors of decision variables have a state where none of the components can be improved without deterioration of at least one of the other components (Miettinen 1999). This state is called Pareto optimality and was defined by the French-Italian economist Vilfredo Pareto (Pareto 1971). In mathematical terms, Pareto optimality is defined as follows: “A decision vector $x^* \in S$ is Pareto optimal if there does not exist another decision vector $x \in S$ such that $f_j(x) \leq f_j(x^*)$ for all I = 1, …, k and $f_j(x) < f_j(x^*)$ for at least one index j.” (Miettinen 1999, p. 11)

Decision-maker and analyst. Mathematically, every Pareto optimal solution is equally suitable for solving a given problem. However, in general there is a desire of determining one unique solution that fits best. Selecting one out of the set of Pareto optimal solutions requires information that is not part of the objective function. For this reason, compared to a single objective optimization, an additional aspect must be added to the multi-objective optimization based on preferences and insight of the decision maker. Thus, multi-objective optimization always requires both

- a decision maker who makes the decision by selecting one of the Pareto optimal solutions by providing additional information such as preferences
- an analyst who supports the decision by optimizing the objective functions regarding the preferences of a decision maker

Depending on the number of decision makers and objectives, decision-making can be categorized as: Single-participant single-objective, Single-participant multiple-objective, Multiple-participant single-objective, Multiple-participant multiple-objective (Hipel et al. 1993). Due to the consideration of preferences for finding the optimum, different methods were developed in order to optimize multiple objectives.

Scalarization. In general, multi-objective optimization problems are handled by scalarization. This means that the original problem is converted into a single or a family of single-objective optimization problems with a real-valued objective function. This specific function is called the scalarizing function and can include additional auxiliary parameters (Steuer 1986, Miettinen 1999). The methods described below include the concept of scalarizing.

Many methods have been proposed in literature for accomplishing multi-objective optimization. None of these methods can be found to be generally dominating over all other methods. Depending on the specific optimization problem and circumstances of the decision, the best suitable method should be selected.

Classification. MOO methods can be classified in many different ways (Cohon 1985, Rosenthal 1985, Hwang and Masud 1979). Emphasizing the influence of decision maker and analyst on the optimal solution, different classes of methods can be distinguished in four different categories depicted in Figure 2.12.

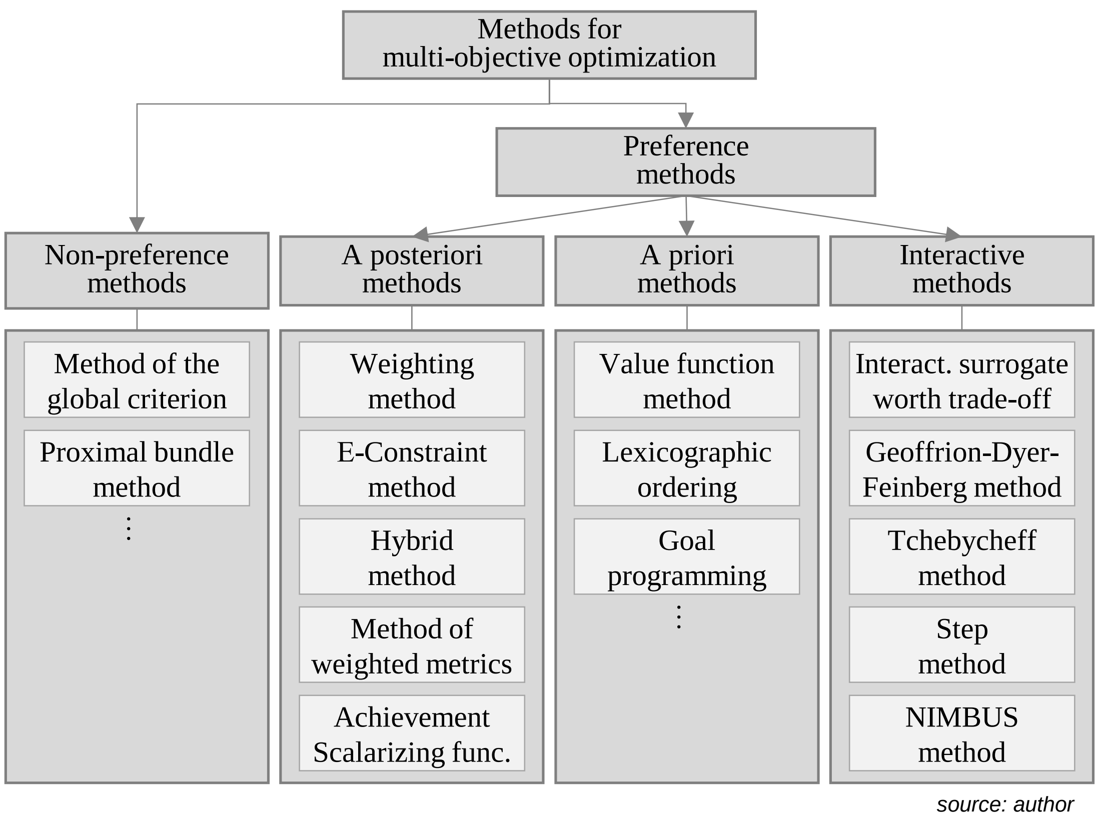


Figure 2.12: Classification of methods for multi-objective optimization

According to the participation of the decision maker in the solution process, non-preference and preference methods are distinguished.

It is crucial to understand that the examples described in the following can be used for the purpose of another category depending on the interpretation (Chankong and Haimes 1983, Miettinen 1999). Since the consideration of multiple objectives is essential in the modeling approach developed in Chapter 4, the categories and examples are described.

No-preference methods do not take opinions of the decision maker into consideration. Decision makers may accept or reject the result in the end and an example is the Method of Global Criterion. The method of global criterion seeks to minimize the distance between a reference point and the feasible objective region. The analyst selects one reference point and a metric for measuring this distance and all objective functions are considered to be of an equal importance to the decision maker (see Yu 1973).

In a priori methods, the decision maker must specify preferences before the solution process. The value function optimization method requires an accurate and explicit mathematical form of the value the decision maker assigns. This function provides a complete ordering in the objective space. Another example is the lexicographic ordering. In this method, the decision maker must arrange the objective functions by their absolute importance. In mathematical terms this ordering means that a more important objective function is infinitely more important than a less important objective. This means every less important objective function will only be taken into consideration if the prior functions don't show a unique solution. Introduced by Charnes and Cooper (1961), the idea of goal programming is that the decision maker specifies an optimistic value for the objective function and any deviation from this level will be minimized (Charnes an Cooper 1977).

A posteriori methods. These generate many Pareto optimal solutions. After the Pareto optimal solution has been determined, the results are presented to the decision maker, who selects the most preferred one amongst the given alternatives. The methods of this category are also called basic methods and are frequently used in practical problems. Many interactive methods have been developed based on these methods.

The most common and intuitive method is the weighting method. The idea is to associate each given set of objective functions with a weighting coefficient and minimize the sum of the objectives. This transforms the actual MOO problem into a single objective optimization and considers, unlike the lexicographic method, all objective function simultaneously, including the relative importance to the decision maker. The weighting coefficients w_i are commonly real numbers such that $w_i \geq 0 \; \forall \; i = 1, \ldots, I$ Also the weights are normalized to $\sum_{i=1}^{I} w_i = 1$. The weighting method is formulated as follows:

$$min \sum_{i=1}^{I} w_i f_i(x) \tag{2.16}$$

$$\text{subject to: } x \in S \tag{2.17}$$

The weighting method can also be used as an a priori method. It can further be extended to an interactive method by allowing the modification of weights by the decision maker after each step or iteration (Batishchev et al. 1991).

The e-constraint method has been introduced by Haimes et al. 1971. In this method, one of the objective functions is selected to be optimized and all the other objective functions are transformed into additional constraints by setting an upper (and lower) bound to each of them. In some cases, the addition of these constraints does not lead to a feasible solution. In this case, a Lagrange relaxation can be applied (Lemaréchal 2001).

The hybrid method combines the weighting method and the ε-Constraint method, and thus weights each of the objective functions chosen to be part of the main objective function and formulates the residual objective functions as ε-Constraints.

The Method of Weighted Metrics is another a posteriori method. There is a general formulation and a specific formulation called the weighted Tchebycheff problem. Since this formulation is an extension of the weighting problem, only the specific problem will be discussed here. This method minimizes the distance between the ideal objective vector and the feasible region.

The Achievement Scalarizing Function approach is related to the previously introduced Method of weighted metrics. Unlike what is suggested by this method, many practical cases cannot offer the global ideal objective vector. If the theoretical optimum is unknown, Pareto optimal solutions may not be found. One possible case can also be when z^* is inside of the feasible region, the minimal distance can be determined as zero and no Pareto optimal solution can be obtained. This weakness can be overcome by replacing the metrics with achievement scalarizing functions (Wierzbicki 1980).

Interactive methods. This class is the most specific out of all the classes. Many of the approaches are only suitable for very specific purposes and based on a priori or a posteriori. This class requires the decision maker to cooperate with the analyst in order to produce satisfying results. Most of these methods contain three steps: (1) find an initial feasible solution, (2) interact with the decision maker, and (3) obtain a new solution. If the new solution is acceptable, stop, if it is unacceptable, go back to step (2). The interactive surrogate worth trade-off method (ISWT), Tchebycheff method, and NIMBUS method. The NIMBUS (Non-differentiable Interactive Multiobjective Bundle-based optimization System) method is an interactive optimization method designed especially to be able to handle non-differentiable functions efficiently. Miettinen (1999) discussed the algorithm and different versions of NIMBUS.

2.4.3 Sensitivity analysis for a limited degree of certainty

For a high degree of uncertainty and complexity of the system investigated, simulation is a suitable approach (see Figure 2.10). However, in cases when data can be given for a defined degree of certainty within specific limits, an optimum can still be determined.

Limited certainty of modeling. While mathematical models are a useful methodology to support decision-making, uncertainty always remains associated with the respective decision. Decisions are rarely made under completely certain conditions. On the contrary, it is frequently the case that assumptions must be made for the considered problem. In the awareness that a formulated model does not represent the problem's circumstances to its fullest extent, the uncertainty of the input data should be considered when drawing conclusions. This can be done by analyzing how sensitive the conclusions are to each of the assumptions made by formulating the model. This concept is called sensitivity analysis (Taylor 2009).

Types of sensitivity analysis. Sensitivity analysis exists in many different ways. The one-way sensitivity analysis is the simplest if only one value of the model is varied by a given amount. The impact of change on the model's results is calculated and evaluated. This analysis could then be repeated with different parameters. While one-way sensitivity analysis is useful for demonstrating the variation of one parameter in the model, it might be necessary to investigate the relationship of two or more parameters by changing them simultaneously. This two-way sensitivity analysis approach contains a combination of each potential deviating value of the uncertain parameters within a determined range. For each combination, the result is calculated. Sensitivity analysis is an important part of mathematical modeling (Meerschaert 2013). When input parameters of multi-objective optimization problems change or contain errors, sensitivity analysis answers the question of how much parameters can vary or alternate without affecting the solution (Rarig and Haimes 1983). Another way of handling the gap between real-world problems and mathematical formulations and results is to consider stochastic or fuzzy problems.

Summary of Chapter 2. With the goal to simultaneously improve economic, environmental, and social performance, eco-industrial parks and networks provide a promising application of industrial ecology and thus promote sustainable development. Industrial ecology is the concept of a company network which reduces the total waste due to collaboration and sharing.

In order to systematically analyze, improve, and create industrial ecology, mathematical and computational models can be used for optimization and simulation. Derived from the optimal results or general insights of an optimization or simulation respectively, decisions in this field can be supported. Existing approaches, such as the multi-commodity flow model and the warehouse location problem, can help to face the challenges of modeling network structures with multiple flows. The lexicographic and weighting method take decision maker's preferences regarding many objectives into consideration. Goal programming allows multi-objective optimization with different quantifying measures.

With an understanding of these theoretical foundations, Chapter 3 establishes an evaluation framework for modeling industrial ecology and investigates existing modeling approaches in literature. Requirements to be met by an advanced approach are a necessary outcome in order to develop such a modeling approach in Chapter 4.

3 EVALUATION OF MODELING APPROACHES

This chapter provides a framework for evaluating approaches for modeling industrial ecology. Existing modeling approaches and their gaps are investigated. Separated into three sections, this chapter seeks to gain insight into important aspects of modeling industrial ecology and the existing approaches in order to answer the first questions Q1 of the thesis (see Section 1.2). This chapter's structure is depicted in Figure 3.1.

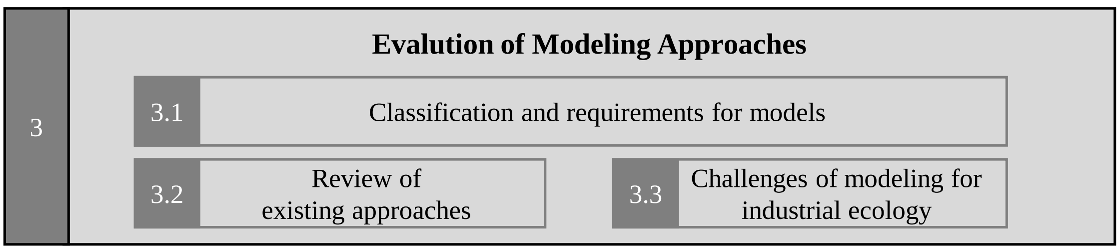


Figure 3.1: Structure of the third chapter

The main outcome of the first section, 3.1, is an evaluation framework for models. A derivation of requirements to be met by models for industrial ecology allows to create classes of approaches. A discussion of major publications follows based on the prior developed framework in Section 3.2. The section ends with a disquisition on the research gap. Finally, the key challenges encountered when pursuing a new, advanced model for industrial ecology is addressed in Section 3.3.

3.1 Classification and requirements for models

Mathematical and computational models are adapted to the field of industrial ecology from different fields of research. In addition to those models which are already applied, other approaches can be suitable to support the process of decision making in eco-industrial parks. In order to guarantee a comprehensive evaluation of all modeling approaches, basic requirements must be defined and classes of models introduced. There is no classification scheme for mathematical models of industrial ecology provided as of now.

A common approach of classifying general mathematical models is the classification in the SQM space proposed by Velten (2009). Velten suggested determining three different dimensions for a mathematical model in order to classify it. The S represents the considered system or subject matter, Q stands for the question to be answered with the model and thus, the purpose of modeling. Further, the letter M in SQM stands for the methodology used in a model. Many mathematical models can be classified by these three dimensions (Velten 2009). Adopted from this classification methodology, models for industrial ecology are classified by their subject matter and their purpose in the following Section 3.2. The first dimension is represented by requirements for modeling the subject matter, i.e. decision making for industrial ecology (Subsection 3.1.1). The second dimension is the purpose of modeling (Subsection 3.1.2).

Approaches are clustered by the mathematical method and evaluated according to this classification scheme.

3.1.1 Requirements for modeling industrial ecology

A model is created in order to represent a system. Certain requirements must be met in order to consider the important properties of the relevant system, i.e. an eco-industrial park or network. Further, the modeling approach needs to provide some inherent properties to capture the process of applying the model. Table 3.1 shows nine requirements, a short description and the source for each criterion.

No.	Requirement: Consideration of	Short description	Source
1	**Economic objectives**	Numerical indices representing corporate performance in monetary earnings and expenses	PCSD 1996, Lowe 2001, Tian et al. 2014, Romero and Ruiz 2014
2	**Environmental objectives**	Numerical indices representing emissions and an impact on the environment	PCSD 1996, Lowe 2001, Tian et al. 2014, Romero and Ruiz 2014
3	**Social objectives**	Numerical indices representing the impact on social matters and individuals	PCSD 1996, Lowe 2001, Drexhage and Murphy 2012, Veiga and Magrini 2009
4	**Multiple flows**	A variety of tangible and intangible flows (e.g. material, information)	Romero and Ruiz 2014, Ayres and Ayres 2002, Gu et al. 2013
5	**Multiple stakeholders**	Different parties with interest in corporate activities (e.g. EIP authority, members, customers)	Gibbs and Deutz 2005, Tudor 2006, El-Haggar 2007, Romero and Ruiz 2014
6	**Negotiation & alternatives**	The possibility to support decision making with given data and allow to generate alternative scenarios	Romero and Ruiz 2014, Drexhage and Murphy 2012 Gu et al. 2013
7	**Uncertainty**	The possibility to support decision making with determined data and depict consequences of changes	Pishvaee et al. 2009, Raymond et al. 2011, Pinar et al. 2005
8	**Optimality & Unique solution**	The possibility to find an optimal solution for the given data (in contrast to heuristics)	Ayres and Ayres 2002
9	**Usability**	The capability of supporting the whole decision making process with GUI and NP-complete	Romero and Ruiz 2014, Miettinen 1999, Drexhage and Murphy 2012

Table 3.1: Requirements for modeling industrial ecology

It is the ultimate goal to accomplish as many requirements as possible. Thus, the comprehensiveness of models for industrial ecology can be evaluated by means of these criteria, which are described in the following paragraphs.

Economic objectives. The basic requirement for mathematical models of any industry-related decision is the consideration of economic objectives. Economic revenue has always been the major driver of corporative activities (Rittenberg and Tregarthen 2009). Further, economic performance is mandatory to achieve sustainable development and is defined to be a requirement for the existence of an eco-industrial park or network (PCSD 1996, Lowe 2001, Tian et al. 2014). Numerical indices and performance indicators, representing monetary earnings and expenses, i.e. fix and variable cost, prices, and revenues, are an essential part of mathematical models for industrial ecology.

Environmental objectives. The main purpose of applying industrial ecology is to achieve a reduction or ultimately the complete elimination of waste (Lifset and Graedel 1997). Hence, it is essential to decision making in this context to consider environmental impacts in models. This can be done in different ways using different measurements. Emissions or waste materials can be measured by standardized metrics, i.e. weight or volume units, and determined by using mathematical models. The increase of ecological performance is demanded by many publications in literature (PCSD 1996, Lowe 2001).

Social objectives. Sustainable development contains the three pillars: economy, environment, and society. While Frosch (1994) focused on economic and environmental advantages of applying industrial ecology when he first used this expression, recent definitions include all three aspects of sustainable development into the concept of industrial ecology and the application in eco-industrial parks (Lowe 2001). To promote comprehensive decisions regarding eco-industrial parks or networks, a contemporary model must include numerical indices of social matters (Drexhage and Murphy 2012, Veiga and Magrini 2009).

Multiple flows. Côté and Cohen-Rosenthal (1998) claim that eco-industrial parks contain more than the exchange of a single byproduct. Companies collaborate by sharing many resources in a network. The most cited definitions of an eco-industrial park, previously mentioned by Côté and Hall (1995), President's Council of Sustainable Development (1996), and Lowe (2001), claim that many different materials, energies, and byproducts are part of the flow in eco-industrial parks. Hence, the consideration of many different tangible and intangible flows is another requirement of modeling industrial ecology.

Multiple stakeholders. Due to the complex and extensive structure of an eco-industrial park or network, many different parties have interest in a decision being made regarding the park. The relationships between parties can be tight or loose, some parties can have more power, and a higher influence on decisions than another, and some parties might not even have an influence on decisions being made. Many stakeholders pursue individual purposes, which makes decision making a complex process. Figure 3.2 shows a stakeholder onion, a visualization of relationships of stakeholders proposed by Alexander (2003). Separated into three different sections, the stakeholder onion shows parties with interest and influence in decision-making regarding an eco-industrial park.

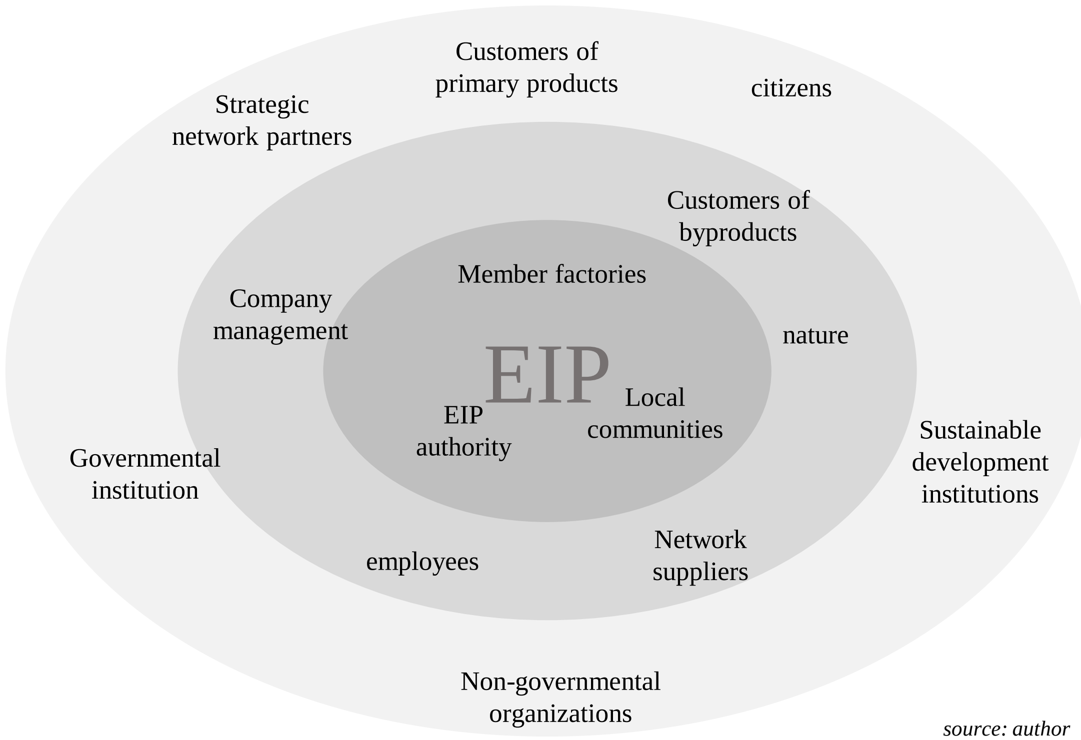


Figure 3.2: Stakeholder onion for an eco-industrial park

The inner circle contains the actual member factories, the EIP authority or management, and local communities. These three parties are directly affected by the consequences of a decision (El-Haggar 2007, Gibbs and Deutz 2005). Customers of primary products and byproducts as well as suppliers have a strong impact on decisions. However, they cannot make decisions directly and are thus part of the second section. The management of the company has an influence on the member factories. Employees as well as nature have to be considered as interest groups for decision regarding EIPs. These groups are directly impacted by decisions made by stakeholders of the inner cycle (Ayres and Ayres 2002, Gibbs and Deutz 2005). Drexhage and Murphy (2012) claim that not only industries, but also governmental, non-governmental organizations (GOs and NGOs respectively), and citizens are related to decisions made about an eco-industrial park.

These stakeholders are indirectly related to these decisions. Strategic network partners of companies may notice changes in their relationships to a company whose facility is part of an EIP (Drexhage and Murphy 2012, El-Haggar 2007, Gibbs and Deutz 2005). The variety of stakeholders of an eco-industrial park or network is a challenging requirement that has to be met by a mathematical modeling approach. The relationships between these stakeholders have to be represented by a mathematical modeling approach. Individual behavior of every stakeholder should be supported.

Negotiations & alternatives. Romero and Ruiz claim that a modeling approach for eco-industrial parks must consider any kind of evaluation of alternative scenarios or individual behavior (Romero and Ruiz 2014, Romero and Ruiz 2013). Due to the complexity of such a system, optimal solutions, if determinable, cannot simply be applied. Parties may change their behavior during the process of decision-making. Taking the above-mentioned variety of multiple stakeholders into consideration, an approach of mathematical and computational modeling must provide the opportunity to include responses to a temporary solution (see Gu et al. 2013).

Uncertainty. In addition to the previous point, a modeling approach must assess the impact of deviation from input data and assumptions. The company, customer, supplier, and other party's behavior are uncertain in real world problems (Pishvaee et al. 2009). A stable model thus considers uncertainty or a defined deviation of certain values.

Optimality & unique solution. Multiple objectives lead to Pareto-optimal solutions. This leads to two different approaches of making a decision (Deb 2014):

1. Find multiple trade-off solutions and choose one based on preferences
2. Estimate preferences and find a single-objective optimum

Since a mathematical model for eco-industrial parks follows the objective of supporting decision-making, a clear preference between economic, environmental, and social objectives can be provided before the optimization takes places. As a consequence, another requirement is that a mathematical model is capable of finding a unique optimal solution. Heuristically approaches are not suitable when pursuing this requirement.

Usability. Implementing sustainable development in industries is one of the largest gaps in this field (Drexhage and Murphy 2012). A mathematical model should be able to represent all the important factors to be considered in a decision. Equally as important as the result is that the modeling approach can be applied to practical cases (Romero and Ruiz 2014). A high degree of flexibility and support of the whole decision-making and negotiation process with a graphical user interface are crucial to an applicable modeling approach (Miettinen 1999).

The definition of the requirements to modeling industrial ecology is a disputable issue. It is difficult to find general boundaries, which satisfy every single opinion existing in literature. However, the requirements are specified to comprehensively satisfy the objective of this work (see chapter 1.2).

3.1.2 Purpose of modeling industrial ecology

Besides the requirements, which a model must satisfy to allow comprehensive decision making, it is specified by a certain purpose it serves. Mathematical models are developed to support a decision-making processes. Decision-making in the field of sustainability concerning eco-industrial parks and networks always relates to the structure of the park or network. Different purposes of models for industrial ecology can be derived from the development strategies distinguished by Tudor et al. (2007) and introduced in Subsection 2.2.4 of this thesis. Relating to Figure 2.8, the following Figure 3.3 shows the logical connection between development strategies and modeling purposes for models of eco-industrial parks and networks.

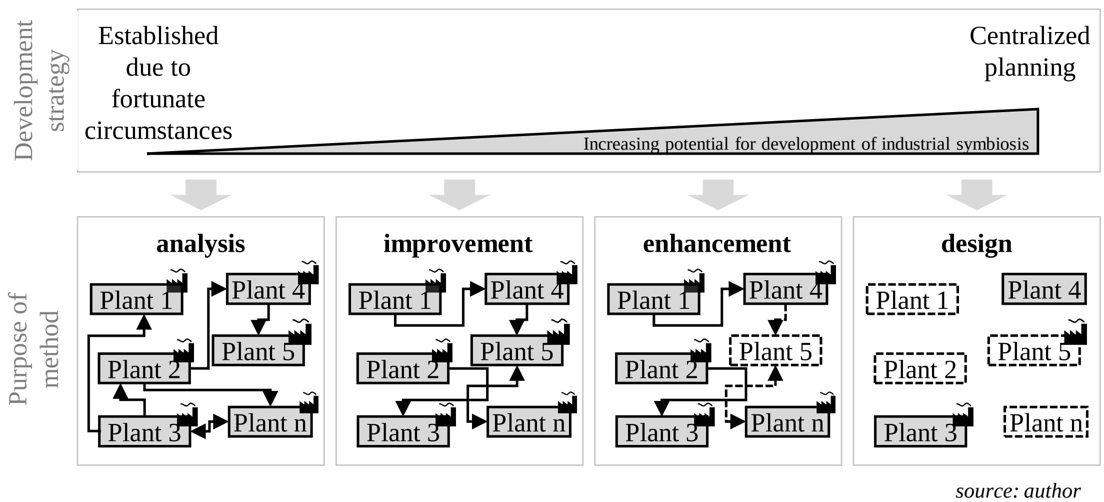


Figure 3.3: Purposes of modeling eco-industrial parks and networks

As mentioned in Subsection 2.2.4, EIPs and EINs can arise in two extreme ways. The one extreme is as the example in Kalundborg, where an eco-industrial park arises 'naturally'. This means that the circumstances are fortunate and result in an efficient way of collaboration that increases the performance in all three dimensions of sustainable development. The second extreme strategy is the completely centralized planning of an EIP from scratch (green field projects).

Depending on the development strategy observed or pursued, models can be set up for a range of purposes. It is essential that models, even if created to serve a certain purpose, can be suitable to other purposes as well. Therefore, the boundaries between the purposes are fading. The four groups of the modeling purpose are analysis, improvement, enhancement, and design. An analysis of an existing system, like the functioning example of Kalundborg, provides a basic understanding of existing industrial symbiosis. Unlike an analysis, improving or enhancing methods can help to identify further potential for changing or extending current structures and achieve even higher performance levels. The most advanced purpose of a methodology is to create completely new industrial symbiosis relationships and EIPs from scratch. In contrast to analyzing existing circumstances, the purpose of creation new EIPs is to predict future developments. By identifying the best possible scenario, a mathematical model can help to design new EIPs and EINs.

In order to make a classification, these four clusters can be seen as a range with an increasing degree of potential development of industrial ecology. While a basic analysis hardly provides any development potential, improvement leads to more advanced industrial ecology practices. Methods that seek to enhance current systems generate even more potential of developing industrial ecology. As the highest degree, methods can pursue the entirely new design of industrial ecology. Regarding the distinction of degree of potential development of industrial ecology relationships, models can only serve the purposes of lower degrees of IE development potential, not higher degrees. A model for designing industrial ecology can, for example, be commonly applied to enhance or improve existing eco-industrial parks, but not the other way around.

The specifications of the different purposes of a modeling approach for industrial ecology and the purpose regarding development of EIPs are summarized in Table 3.2.

Icon	Purpose: Development pot.	Short description	Source
◔	**analyze**	Investigate current relationships in an EIP or EIN developed over time in order to gain insight	Lowe 1997, Chertow 2000, Veiga and Magrini 2009, Tudor et al. 2007
◑	**improve**	Assess current relationships and flows in order to find changes for better performance	
◕	**extend**	Create new relationships and additional flows in an existing EIP or EIN	
●	**design**	Support the setup and establishment of a new EIP or EIN	

Table 3.2: Purposes of modeling eco-industrial parks and networks

Understanding that different models can be classified by their comprehensiveness (see Table 3.1) and their purpose (see Table 3.2), the two introduced dimensions provide a framework of evaluating models. The following Subsection, 3.2, discusses and evaluates existing modeling approaches from literature based on these criteria.

3.2 Review of existing approaches

Different mathematical and computational modeling approaches have been transferred, adapted, and further developed for investigating IE and its application in eco-industrial parks. This section provides a review (Subsection 3.2.1) and evaluation (3.2.2) on existing approaches. The section finishes with the major gaps in current models.

Existing approaches are clustered based on the method used and classified by the framework developed in the previous section. Some proposed models may be part of more than one cluster. The cluster bi-level fuzzy optimization requires, for example, a fuzzy optimization, and an MILP or MINLP, which are clusters themselves. However, the clusters represent main practices of approaching modeling of industrial ecology.

3.2.1 Literature review on models for industrial ecology

Table 3.3 summarizes the existing literature on modeling industrial ecology and assigns every publication to one of the clusters, which are described sequentially.

Cluster	Main publications
Input-output analysis	Ayres and Ayres (2002), Duchin (1992), Martin et al. (1998), Wang (2011)
Material flow analysis	Lee et al. (2006), Suh and Kagawa (2005), Bailey et al. (2004), Bringezu and Moriguchi (2002),Bingezu and Kleijn (1997), Yu et al. (2014)
Mixed-integer linear programming	Gonela and Zhang (2014) , Chae et al. (2009), Sharma and Mathew (2011), Karlsson and Wolf (2007), Tan et al. (2011b)
Lagrange relaxation and penalty functions	Pishvaee et al. (2009), Walter et al. (2008), Walter (2005)
Multiobjective optimization	Gu et al. (2013). , Li et al. (2009), Erol and Thöming (2005) , Azapagic and Clift (1999)
Fuzzy optimization	Taskhiri et al. (2011), Loucks et al. (2005)
Bilevel fuzzy optimization	Tan et al. (2011a), Aviso et al. (2010), Chew et al. (2009)
Evolutionary algorithms	Huo and Chai (2008)
System dynamics and complex network theory	Zhao et al. (2008), Zeng et al. (2013)
Agent-based modeling	Romero and Ruiz (2014), Romero and Ruiz (2013), Bichraoui et al. (2013), Cao et al. (2009)

Table 3.3: Main publications assigned to clusters of approaches for modeling IE

Input-Output analysis. Adapted from Leontief, the input-output analysis was one of the first mathematical analysis methods applied to industrial ecology (Duchin 1992). This analysis considers economic measures and amounts of material to understand and model existing waste flows.

Material flow analysis. The second large cluster of mathematical models and a useful tools to investigate industrial symbiosis based on mathematical expressions is the material flow analysis (MFA). MFA is a systematic assessment of the flows and stocks of materials within a system defined in space and time, also called substance flow analysis (Brunner and Rechberger 2004). An extensive application of the material flow analysis to industrial ecology has been done by Bringezu and Moriguchi (2002). MFA refers to the analysis of throughput of process chains. Bringezu and Moriguchi claim that this is the core of analyzing industrial ecology. This analysis comprises extraction, transformation, manufacturing, consumption, recycling, and disposal of materials. It is based on accounting physical units as inputs and outputs of processes. Bingezu and Kleijn (1997) discuss different types of analysis based on their focus. MFA has mostly been used to determine the main impact factors to environment and processes associated with these emissions. The methodology has become a widely acknowledged approach of assessing ecological impacts of production processes (Barrett et al. 2002). This idea has been adopted and applied by many other publications (Lee et al. 2006, Suh and Kagawa 2005, Bailey et al. 2004, Sendra et al. 2017). However, MFA and life-cycle assessment (LCA) provide an overview of current situations and are thus not eligible for optimization and centralized planning to support decision making.

Mixed-integer linear programming. With objective function and constraints both linear, Taskhiri et al. (2011) modeled energy of EIP water networks by applying a mixed-integer linear programming. They propose a model for minimizing energy, i.e. freshwater, electrical power, capital goods, and wastewater of an interplant water network in an EIP. This approach does not account for any social factors. Chae et al. (2009) propose a MILP to synthesize a waste heat utilization network, including nearby companies and communities. The objective function of their linear model seeks to minimize total energy cost. Social objectives are not considered in this model. Interests of multiple stakeholders cannot be optimized simultaneously. Gonela and Zhang (2014) follow the same approach with a larger extent regarding considered plants, byproducts, waste products, and market products. Many other publications approach industrial ecology with MILP (Karlsson and Wolf 2007)

Penalty function and Lagrange relaxation. Walter et al. (2008) and Walter (2005) develop a negotiation algorithm for the coordination of material flow in recycling networks. The idea of industrial ecology has not been mentioned in these publications. However, based on mathematical models and an interactive negotiation algorithm, new symbiosis can be created. In order to solve the optimization model, Lagrange relaxation is applied. While the original objective function contains economic measurements, the Lagrange relaxation allows a variation of the recycling rate and thus accounts for environmental issues. Penalty functions are a common multi-objective optimization method (Miettinen 1999). Pishvaee et al. (2009) provide a meta-investigation of modeling approaches for reverse and integrated networks considering uncertainty.

While the subject matter of this investigation is a sustainable reverse logistics network, environmental targets or the idea of industrial ecology has not been applied.

Multi-objective optimization. Different methodologies have been developed in literature in order to solve multi-objective optimization (Miettinen 1999). A successful application of the NIMBUS (Non-differentiable interactive multi-objective bundle-based optimization system) method to optimization of eco-industrial parks has been proposed by Gu et al. (2013). They apply the whole process of an interactive multi-objective optimization to both eco-industrial park design and optimization. This composition of computational and mathematical modeling considers multiple waste product flows. Gu et al. consider multiple stakeholders with this interactive negotiation framework, neglecting social performance. Uncertain behavior is also not considered. Since this tool is web-based, it is considered to be highly usable. This methodology supports the improvement and design of eco-industrial parks. Li et al. (2009) consider chemical processes in general for industrial ecology. They apply the TOPSIS (technique for order preference by similarity to ideal solution) and solve this with an NSGA-II (non-dominated sorting generic algorithm). They claim that it is often difficult to find an optimum for a process that satisfies both economic and environmental objectives simultaneously. Instead of finding a set of Pareto optimal solutions, Gu et al. propose to find an optimum based on the decision-makers preferences similar to the NIMBUS approach. Erol and Thöming (2005) combine the simultaneous analysis of environmental impact sensitivity (SAEIS) with multi-objective optimization performed by mixed-integer nonlinear programming (MINLP). They modeled the trade-off between economy and environment under consideration of LCA guide factors. Azapagic and Clift (1999) provided the basis for this approach by illustrating the application of LCA to process optimization. The interactive surrogate worth trade-off method (ISWT) has only been applied to power plants, not to EIPs (Chen et al. 2002).

Fuzzy optimization. Taskhiri et al. (2011) suggest a model to achieve a compromise among the potentially conflicting fuzzy goals of the various EIP stakeholders. Unlike the following approach, this mathematical optimization model does not consider a hierarchical structure.

Game theory and Bi-level fuzzy optimization. A research group from La Salle University and Ohio State University extends the previously mentioned idea of fuzzy optimization by a game-theoretical approach. In order to consider the hierarchy of decision-making in an eco-industrial park the same team of researchers applies a bi-level fuzzy optimization (Aviso et al. 2010, Taskhiri et al. 2011). They consider the participating plants by means of an individual fuzzy cost goal while the upper level and overall goal of an EIP authority is the minimization of resource consumption and generation of waste. Their model thus includes environmental and economic targets but does not consider social issues. The model has been applied to the optimization of the water flow only. By introducing a fuzzy function, lower and upper boundaries are included and provide a range in which alternative economic outcomes are acceptable for participants. The bi-level especially considers the hierarchy of stakeholders. It applies the Stackelberg Game to mathematical optimization. The basic idea of applying game theory approaches has been investigated by the same group of researches a few years before (Chew et al. 2009). This multi-objective bi-level optimization has also been applied to other problems such as transport planning and management problems in the past (Yin 2002, Qu et al. 2014). Aviso et al. (2010) use a nonlinear solver in Lingo to find an optimal solution of an example case. The application of the max-min-concept seeks to maximize the satisfaction of the least satisfied company. New relationships are discovered.

Evolutionary algorithms (EA). Huo and Chai (2008) set up a simulation to understand evolution of industrial ecology patterns and provide new implications on design, improvement, and prediction of structural evolutions. They investigate patterns and apply evolutionary principles as well as nonlinear partial differential equations with boundary conditions and thus computationally implement interacting organisms. Evolutionary algorithms solve many nonlinear programs. However, other than Huo and Chain, most of the nonlinear programs have an underlying mathematical model to be solved. Evolutionary algorithms often occur in order to solve multi-objective optimization problems (Zitzler and Thiele 1999).

System Dynamics. Zhao et al. (2008) investigated social, economic, and environmental relationships in an eco-industrial park in China. System dynamics does not provide numerical information for material flows or explicit information about location decisions. However, it helps to investigate relationships and impacts.

Agent based modeling (ABM). Romero and Ruiz propose the application of agent-base modeling to the optimization and design of eco-industrial parks (Romero and Ruiz 2013, Romero and Ruiz 2014). Due to many advantages of ABM compared to SD, Romero and Ruiz decided to set up a computer simulation. Single companies are implemented as agents with an individual behavior and an individual economic and ecological goal (Cao et al. 2009, Bicharoui 2013). Despite ABM, other simulations have been created for investigating industrial ecosystems via simulation (Reuter 1998).

Other approaches. LCA is product based and not based on company level. However, Tong et al. (2013) applied the method of life cycle assessment to a system for water reuse in an industrial park. In order to determine the correct partners for increasing competitive advantage, many mathematical programming models, such as linear programming (Anthony and Buffa, 1977, Pan, 1989), mixed-integer programming (Bendor et al. 1985, Kasilingam and Lee 1996), stochastic integer programming (Feng, Wang, & Wang, 2001), goal programming (Buffa and Jackson 1983, Karpak et al. 1999, Sharma et al. 1989), and multi-objective programming (Huang et al. 2010). Salema et al. (2009) propose a stochastic model for multi-commodity networks under uncertainty for demands using stochastic mixed integer programming.

The next subsection evaluates the approaches discussed by means of the framework provided in Section 3.1.

3.2.2 Evaluation of reviewed modeling approaches and research gap

Referring to the discussion of publications in the previous section, the capabilities of the approaches are summarized in Table 3.4.

	dimension		Input-output analysis	Material flow analysis	Mixed-integer linear programming	Lagrange and penalty funct.	Multiobjective optimization	Fuzzy optimization	Bilevel fuzzy optimization	Evolutionary algorithms	System dynamics	Agent-based modeling	Desired approach
1	requirement	**Economic objectives**	✗	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
2	requirement	**Environmental objectives**	✗	✓	✓	✓	✓	✗	✓	✓	✓	✓	✓
3	requirement	**Social objectives**	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✓
4	requirement	**Multiple flows**	✓	✓	✗	✓	✗	✗	✗	✓	✗	✗	✓
5	requirement	**Multiple stakeholders**	✗	✗	✗	✗	✓	✓	✓	✗	✓	✓	✓
6	requirement	**Negotiation & alternatives**	✗	✗	✓	✓	✓	✓	✓	✓	✗	✗	✓
7	requirement	**Uncertainty**	✗	✗	✓	✓	✗	✗	✗	✓	✗	✓	✓
8	requirement	**Optimality & Unique solution**	✗	✗	✓	✓	✗	✓	✓	✗	✗	✗	✓
9	requirement	**Usability**	✗	✓	✓	✓	✗	✗	✓	✗	✗	✗	✓
	purpose	**Development potential**	◔	◔	◕	◕	◑	◑	◑	◕	◕	●	●

Table 3.4: Overview evaluated modeling approaches for IE

The table shows that many approaches consider the requirements more or less comprehensively. An approach that does not support decisions and is thus less suitable to the developed requirements is the input-output analysis. On the other hand, there are mixed-integer problems and approaches with penalty functions and Lagrange relaxations, which suit the problem of modeling industrial ecology as defined in this thesis very well. Bi-level fuzzy optimization is a promising approach meeting many of requirements of a suitable model for industrial ecology.

However, some special patterns can be discovered in this overview. While nearly every modeling approach that has been applied by a publication in the field of industrial ecology directly considers economic and ecologic performance indicators in the objective functions, the social performance has not been modeled. It is further conspicuous that most of the publications only consider a single flow of material in a network. Utilities like waste water are mostly the subject matter (Rubio-Castro et al. 2010, Rubio-Castro et al. 2011). Useful byproducts are rarely considered explicitly by any model. There is no current method for achieving an optimized decision for creating new eco-industrial parks and networks. The only approach providing such an idea has been proposed by Romero and Ruiz (2013 and 2014) recently. They use the idea of agent-based modeling that does not provide optimal and unique solutions for decision-making, and are thus not applicable in this thesis.

Since the implementation of industrial ecology in practice is still large gap, two requirements must be emphasized in this thesis. The approach proposed must be easy to use and apply to individual cases and provide an optimal solution for the regarding data.

Optimal modeling approach. The optimal modeling approach seeks to overcome weaknesses of current approaches and leverage potentials by

> *designing an optimal network with many flows under consideration of economic, environmental, and social objectives by providing a negotiation algorithm for multiple stakeholders by means of mathematical models and computer software.*

3.3 Challenges of modeling for industrial ecology

The lack of meeting requirements can occur due to many different causes. Sometimes the effort of considering a requirement is not worth the rewarded benefits. In other cases, the scope of a work does not seek to meet a certain requirement, which is requested by this evaluation framework. Also, interdependencies occur when pursuing multiple requirements, which makes it difficult to meet one requirement, when implementing another. Some requirements are easy to be considered, some are especially challenging.

In order to accomplish the development of an advanced modeling approach and thus answer question Q2, this section provides a discussion of key challenges to be mastered for achieving an advanced methodology. Derived from the experience mentioned by publications and knowledge gained during the investigation and evaluation of these models, three key challenges are emphasized. They are summarized in Figure 3.4.

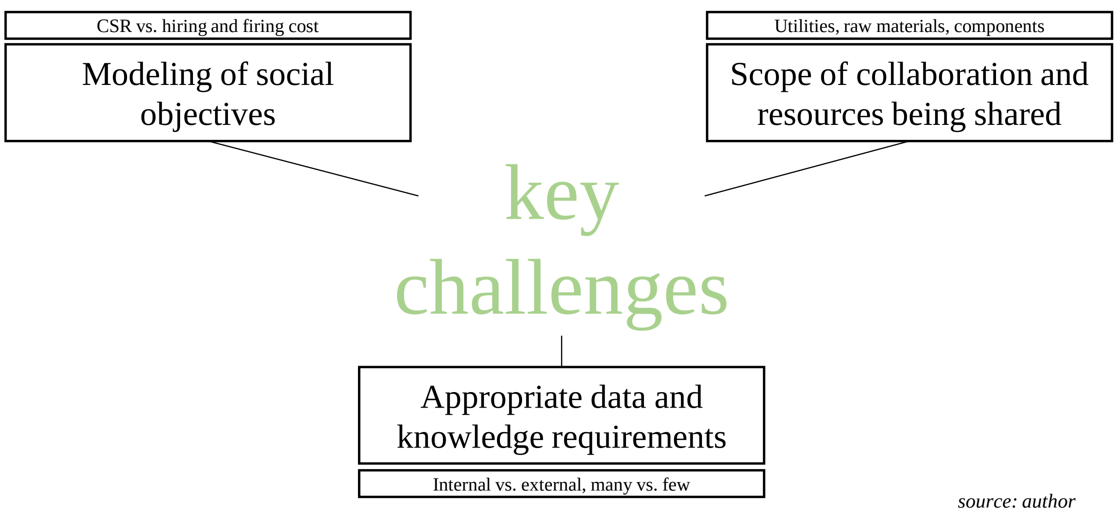


Figure 3.4: Key challenges of modeling for industrial ecology

The following subsections provide a comprehensive discussion of these special topics.

3.3.1 Mathematical modeling of social sustainability

The first of three key challenges to be emphasized in this work is the aspect of modeling social sustainability (Dempsey et al. 2011). Eco-industrial parks or networks are an application of industrial ecology and thus put sustainable development into practice. As part of the definition, the goal of EIPs and EINs is to optimize the economic, environmental, and social performance due to collaboration of all participants (Lowe 2001, El-Haggar 2007). Approaches of mathematical modeling for sustainable development have been successfully applied to many specific problems (see Section 3.2). Mathematical models for optimizing eco-industrial parks and networks are capable of handling multiple objectives quantified by means of various units.

> *However, researched publications consider only the economic and environmental side of the goals of an EIP, neglecting the social dimension of sustainability (see for instance a recent work of Tian et al. 2014).*

None of the investigated modeling approaches explicitly consider the social dimension of sustainable development in the objective function and thus, none of the approaches conduct a mathematical optimization of social performance (see Table 3.4). Following the aforementioned methods required for decision-making, the measure, assessment, and modeling of social sustainable development is discussed subsequently.

Measurement. While measurement of ecological and economic performance indicators have been investigated and developed over years and were considered in the concept of sustainability since the 1960's (McKenzie 2004), the social aspect was introduced decades later (Brundtland 1987). The Global Reporting Initiative has reported that other than economic and ecological indicators,

> *a "reporting on social performance occurs infrequently and inconsistently across organizations" (GRI 2000, p. 33).*

Even a few years later, the Western Australian Council of Social Services (WACOSS) as well as Visser and Sunter (2002) claim that there has been far less work done regarding social sustainability on the company level (Barron and Erin 2002).

However, in recent years, much research has been done in the measurement of social sustainability. This is mainly because of an increasing concern of stakeholders for environmental and social issues (Holliday et al. 2002). Many publications and international committees like the United Nations Commission on Sustainable Development (UNCSD), the Global Report Initiative (GRI), the European Aluminum Association, and the Institution of Chemical Engineers have investigated, defined, and standardized numerous measures. Some examples are: share of households without electricity, proportion of urban population living in slums, life expectancy at birth, immunization against diseases, net enrollment rate in primary education, population growth, and number of international homicides per population (United Nations 2007).

Most of the measures capture sustainable development on a macro-economic level. McKenzie calls for the development of more specific indicators for particular companies (McKenzie 2004). Measures for social sustainability on the company level are mostly used in the field of corporate social responsibility. A meta-investigation for measuring sustainability of factories shows performance indicators depicted in Tab. 3.5.

Field	Performance indicator
Working conditions, health and safety	Occupational and lifestyle health programs
	Records of accidents
	Turnover and absenteeism rates
	Ratio of work force to yearly output tonnage
Employee opportunities and relations	Gender balance
	Equity of wages between firms and positions in the company
	Training programs for employees
Internal communications	Diffusion of information for employees
	Dialogue with the management
Community relationships	Local contribution of the firm
	Employment of local population
	Origins of workers
	Number of mergers and acquisitions

Table 3.5: Performance indicators for social sustainability at the company level (Adapted to: O'Connor and Spangenberg 2008)

The table distinguishes the four fields of working conditions: health and safety, employee opportunities and relations, internal communications, and community relationships. Examples of measurements are working accidents, trainings, and gender balance. These measures offer an alphanumerical qualification and quantification of a company's performance and support the comprehensiveness and reliability of deducted results. Additional measurements are defined by Saling et al. (2001), Global Reporting Initiative (2011), Labuschagne et al. (2005), OECD (2003), United Nations (2007).

Assessment. To provide a comprehensive conclusion about the performance of a nation, an economy or a company, many measurements are put together to generate an assessment. For the assessment of sustainable development in general, many indices have been developed emphasizing more or less the social sustainability. Examples for commonly used indices are Summary Innovation Index, Internal Market Index, Business climate indicator, Human Development Index, Technology Achievement Index, Overall Health System Attainment, the gross national happiness indicator of Bhutan and many more (see Singh et al. 2009 for a comprehensive overview). These indicators aim to reflect the condition for progress, wealth, capital, and development in an economy. Partially including those indices, a broad variety of frameworks have been developed. Amongst other, the frameworks GRI, CSD, IChemE and Wuppertal Sustainability Indicators are used. By means of these frameworks, a multi-criteria analysis for all three dimensions can be performed (Buchholz et al. 2007).

A widely known approach is the assessment of the corporate social responsibility. An abstract of the considered KPIs and possible quantifications are listed in Figure 3.5.

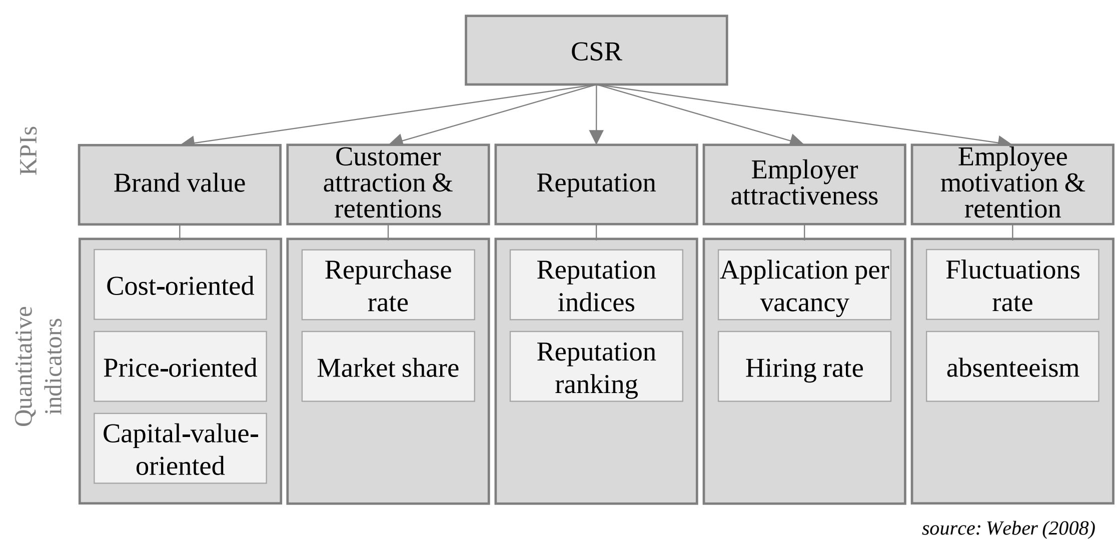


Figure 3.5: Performance indicators of CSR

The listed indicators quantify the five classes of brand value: customer attraction and retentions, reputation, employee attractiveness, and employee motivation. There are several examples of CSR business benefits from current research which prove positive effects on company image and reputation, positive effects on employee motivation, retention, and recruitment, cost savings, revenue increases from higher sales and market share, and CSR-related risk reduction as depicted in Figure 3.6.

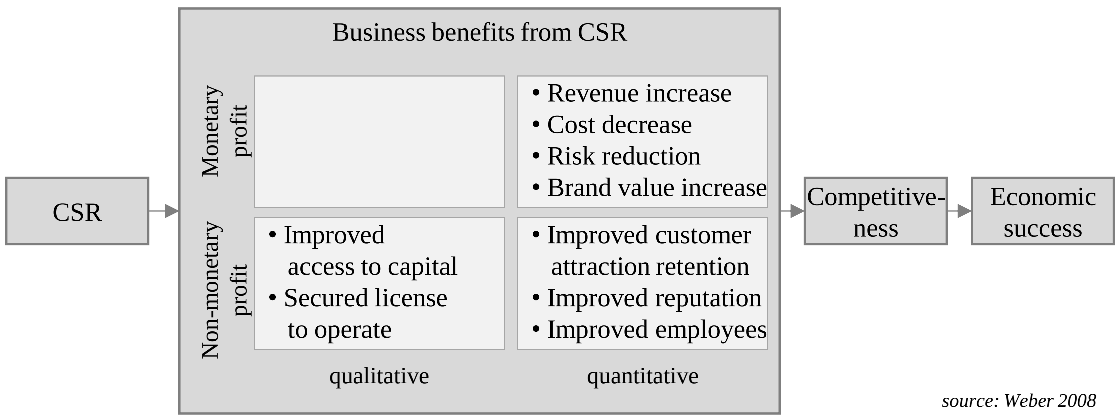
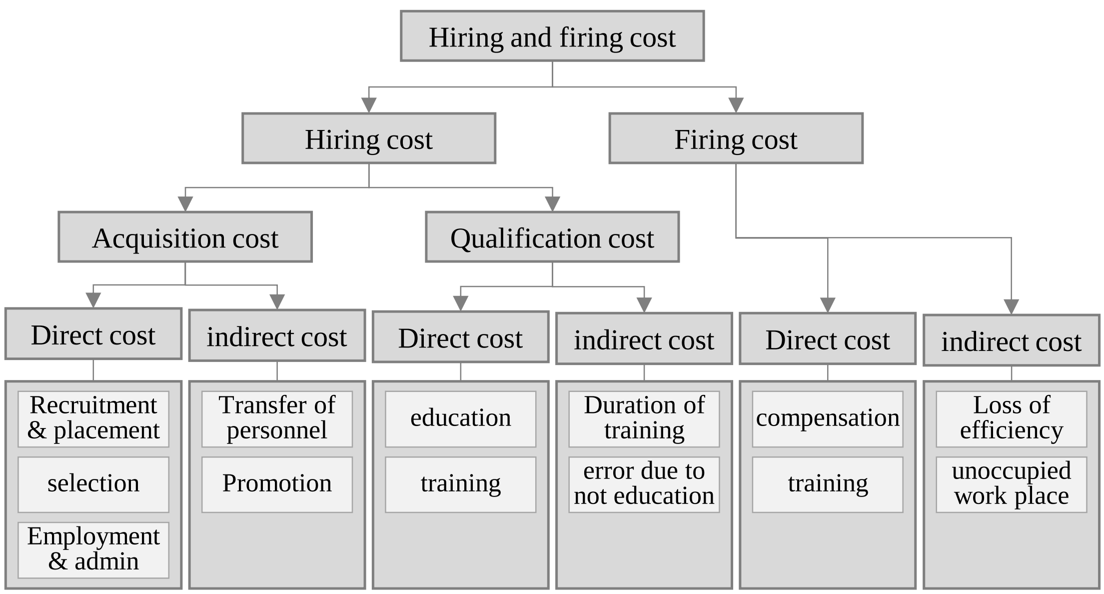


Figure 3.6: CSR Impact model

Investigating the short and long term consequences of company activities in the field of CSR, Burke and Logsdon (1996) found that efforts in this field actually pay off due to several direct and indirect effects such as additional values like a higher productivity, customer loyalty, new markets and products (Burke and Logsdon 1996). Based on this, Weber develops the CSR impact model, which illustrates the relationship between CSR and economic success due to business benefits, both monetary and non-monetary, and improved competitiveness. Omann and Spangenberg (2002) depict further assessments.

Modeling. While assessment gives a comprehensive overview and benchmark of the current situation, companies seek to evaluate their situation in advance. This provides many preventive advantages in comparison to a normal assessment. A model can be used to describe a system using mathematical and computational support, and thus forecast. However, to describe a mathematical model, an alphanumerical representation is required. Besides the aforementioned CSR index, which is a non-monetary value expressing the potential for social sustainability, a monetary measurement could be used for modeling. When dealing with employees, companies have to face cost of hiring and firing. Firing cost is the cost of advanced notice requirements, severance payments, and penalties due when terminating a worker, expressed in weekly wages. Figure 3.7 illustrates the components of hiring and firing costs adapted from Persch (2003).



source: adapted from Persch (2003)

Figure 3.7: Components of hiring and firing costs

The figure shows the different parts of total costs that can occur. When a mathematical model is developed, the decision for a measure must be made based on the availability, usability, validity, and significance of the numerical information to the problem.

3.3.2 Different measures

The second key challenge is the aggregation and collective consideration of different measures. The previous subsection suggest to measure social sustainability by CSR index or monetary values. There are many other possibilities of measuring performance. Common quantification of economic and environmental outcomes have been investigated, neglecting social aspects (Chertow and Lombardi 2005, Atkinson 1997). Figure 3.8 illustrates a classification of quantitative measure applied by Weber (2008).

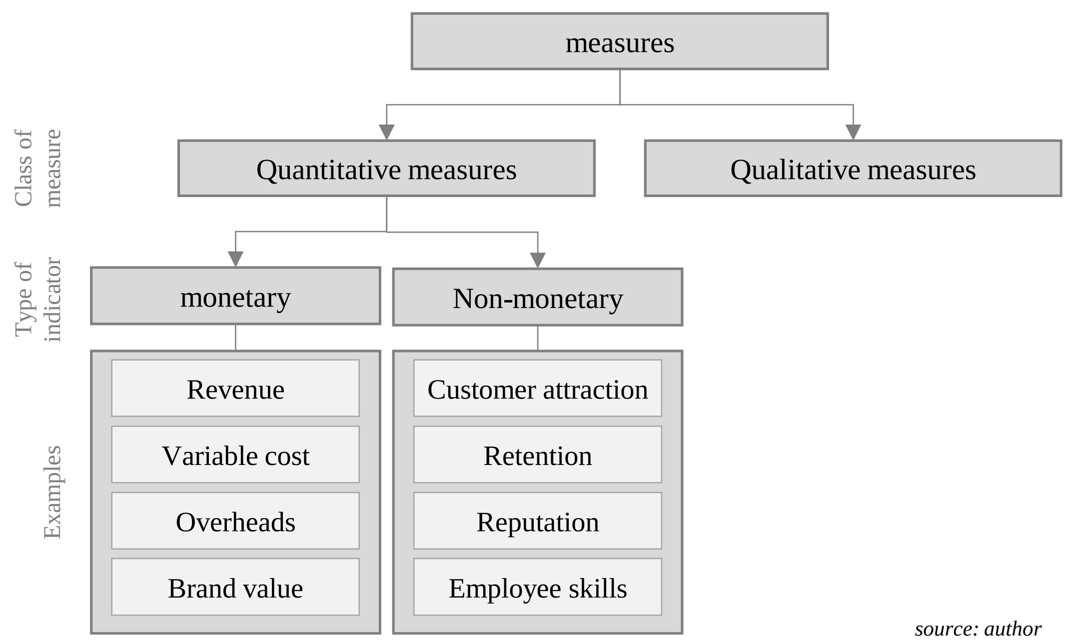


Figure 3.8: Classification of measures for business performance

Since mathematical modeling requires the capability of expressing measures in mathematical terms, it is crucial to a measure to be quantitative. In order to include aspects that are not initially quantified, such as reputation or behavior, artificial measurements have to be developed, such as indices, to allow mathematical models to be applied. Quantitative measures can be divided into monetary and non-monetary measurements (Weber 2008). Monetary measurements, for instance transport costs, and non-monetary measurements, for instance retention, theoretically can be taken into consideration for optimization after they are quantified. In order to consider multiple objectives for business, environmental, and social performance, this classification between monetary and non-monetary measures can be done.

When these performances are considered simultaneously, a common basis for these measures must be provided. Derived from the previously mentioned classification, two strategies are possible.

1. Monetize all measurements

A common approach of aggregating information is to monetize every factor. While this is rather intuitive for general purchase costs, the monetary value of a certain unit of waste material, emission, or social inequality is much harder to capture. Within the last two decades, this approach of monetizing has been much more developed than before. Cost rates for emissions (in general this is measured by a metric ton) have been defined and investigated (Manne and Richels 1992). In many cases, such values are rough approximations and these rates vary from region to region, over time, and sometimes even from company to company so much that estimation does not reflect the real situation at all. However, the general bases for these measurements are usually amounts, weight, or time units so that the can calculation scheme can be formulated as follows:

$$monetary\ value = r \left[\frac{\$}{units}\right] * x\ [units] = y\ [\$] \tag{3.1}$$

The aforementioned hiring and firing costs are one possibility in order to monetize social consequences. The sum of all monetary values then expresses a total monetary value for the described problem under consideration of all included factors.

1. Standardize all measurements

The second strategy is based on non-monetary values. Especially in the field of sustainable development, nonmonetary qualified values for expressing performance have been investigated broadly. Frameworks for indicators of sustainability are, for instance: Global Reporting initiative (GRI 2000), United Nations Commission on Sustainable Development Framework (United Nations 2007), Sustainability Metrics of the Institution of Chemical Engineers (Sikdar 2003), and Wuppertal Sustainability Indicators (Spangenberg and Bonniot 1998). In order to aggregate different materials, the most common approach is to introduce equivalents. For example, the CO2-equivalent is a measure for describing the global warming potential for a given amount and type of greenhouse gas, with reference to the greenhouse gas carbon dioxide (CO2) (Basting 2014). An example for nonmonetary measures of social sustainability is the CSR index, which was investigated broadly and determined for multiple companies (BCCC 2014).

Standardization and normalization. The introduction of equivalents is a valid approach of standardizing many emissions. However, independently to the measure itself, a mathematical formula can provide standardization of various values. In many practical cases, variables or parameters are not given in the same measures. It is advisable to rescale the objective function in order to achieve approximately the same magnitude of objective values. This process is called normalizing. In many cases, this can be done by standardizing every objective function and scaling it between the interval [0,1]. This can be done according to the following formula 3.2

$$f_{i,scal}(x) = \frac{f_i(x) - z_i^*}{z_{nad} - z_i^*} \qquad (3.2)$$

If the ideal vector and a good enough approximation to the nadir objective vector are known, the objective function can be transformed (Miettinen 1999). The optimal value can also be replaced by a value that is desirable. This normalizing is commonly applied in fuzzy optimization and can be a possible scalarizing function in multi-objective optimization (see Section 2.4). Fuzziness is used when boundaries are not well defined and cannot clearly be separated from each other. Loucks et al. (2005) show the application of fuzzy optimization to handle the trade-off between economic and environmental targets for a water resource system.

Another significant aspect of this key challenge is the comprehensiveness of available information. It is unrealistic to change companies' attitude towards sharing of valuable information. A way of convincing companies is to guarantee a responsible treatment of their data and provide incentives. Hence, it is important to establish a model with a minor need of information. The analyst should be aware of the fact that some information is not relevant to the decision and can be neglected.

3.3.3 Scope of collaboration

The third of the three mentioned key challenges of modeling an eco-industrial park is the question about the extent of cooperation and sharing of resources between partners.

Cooperation. The basis of the concept of industrial ecology is that one industry's waste is another's raw materials (Frosch 1994). It implies the cooperation of businesses for the overall reduction (or elimination) of waste. The cooperation or collaboration in a system for a defined purpose is called a network. Cooperation can exist on many different levels. Companies can have a participation of a range from a very loose connection, such as outline contract, to a process integration for delivery or shipments, i.e. just-in-time delivery. Common products orientated from company networks are supply chains. It includes all companies that contribute to the supply, production, and delivery of a commodity. This improves the material and information flow, forecasts reliability, quality, and most importantly the cost for all participants simultaneously. However, the subject for each company is a certain output in a certain quality at a certain time. Even though these networks have many interdependencies, the basic structure is linear. An increasing complexity can be observed for networks of companies, where cycling material or information flows are involved. A common example is a recycling networks or reverse logistics networks (Stock 1992, Kopicki et al. 1993). Reverse logistics encompasses the logistics activities from used products, which are no longer required by the customer to the new product created due to the reuse of the old product (Fleischmann et al. 1997). The following criteria have to be taken into consideration when modeling an eco-industrial park.

- Materials, components, utilities, byproducts, product portfolio
- At a certain process and repetition time
- Integrated processes
- A close geographical proximity

Tudor et al. (2007) states that a commitment to cooperation of companies is a necessary requirement to be fulfilled in order to successfully create an eco-industrial park.

Sharing. Another inherent aspect of a cooperation network with multiple flows is sharing. As well as the aspect of cooperation, this section discusses at first the aspect of sharing of businesses in the context of industrial ecology. Three different stages of sharing are investigated, i.e. sharing of utilities only, sharing of byproducts, and sharing of other resources. The respective next stage contains all the prior stages.

1. Sharing of utilities

It is an essential idea for industrial ecology "to efficiently share resources (information, materials, water, energy, infrastructure, and natural habitat)" (Cohen-Rosenthal 2003). The most quoted and first examples for an eco-industrial park are the Kalundborg case in Denmark (Ehrenfeld and Gertler 1997). The eco-industrial park in Kalundborg evolved to reuse resources that would have been wasted otherwise. With a total of 18 physical linkages in the industrial town at the seaside of Denmark, it is a remarkable example of industrial symbiosis (see Section 2.2.4). The achievements are mainly water and fuels savings as well as a significant reduction of chemical waste (Ehrenfeld and Chertow 2002). The focus is on the material and energy flow exchanges between single companies. A basic utility being shared between companies is fresh and waste water (Rubio-Castro 2010, Sadegh 2011, Chew 2009). Other materials and energy being shared in Kalundborg are Gas, Sludge, Heat, Ash, Steam, Gypsum, Sulphur. Many networks in the field of industrial ecology but also with other purposes share utilities. The advantage about sharing utilities is that many companies often need the same, unspecific kinds of water, steam, or any kinds of energy. It is a common practice to build a network up a collaboration of recycling, for example many companies share a water recycling station. Additional sharing concepts for power plants and similar technologies can also be created due to the potential of IS at EIPs and EINs.

2. Sharing of byproducts

While most of the shared materials and energy forms are classified as utilities, are still a few byproducts involved in the industrial park in Kalundborg. An example for a pure byproduct is gypsum. Conveniently, it is the primary ingredient of wallboard and thus serves as the primary input provided by the power station. Other than the case Kalundborg provides the less famous but larger case of an eco-industrial park in Santa Cruz more cases of byproducts sharing in addition to sharing of utilities. Veiga and Magrini (2009) provide an investigation on byproduct structures and resulting benefits.

3. Sharing of other resources and components

The last and most advanced stage of sharing is sharing of semi-products, modules, or commodities as well as other resources. There are two main causes why this concept of sharing is the most sophisticated in an eco-industrial park: The demand for each semi-product, module, or commodity is very low and the pattern of consumption is extremely volatile. Due to the nature of the market is the last stage of sharing not state-of-the-art. However, some companies are looking to share intangible resources such as computer power, human workforce, office equipment, or information (Lee and Whang 2000). The actual sharing of byproducts for the goal of reducing waste is still not state-of-the-art.

Summary of Chapter 3. Approaches for modeling industrial ecology can be classified by two aspects, i.e. requirements and purpose, and clustered into different groups.

A suitable approach considers all three dimensions of sustainable development, i.e. economy, environment, and society. Multiple flows of resources within a network of many stakeholders are the subject matter of desired approaches. Due to uncertainty and complexity the decision making process requires a negotiation algorithm that provides an optimal and unique solution and allows the variation of initial data. In order to bridge current gaps, an advanced models should be easy and flexible to apply and use.

Some approaches meet the majority of requirements. The approach of bi-level fuzzy optimization and the application of the interactive multi-objective optimization method NIMBUS provide comprehensive models. However, these approaches suffer by inflexibility. Important to note is that none of the existing modeling approaches explicitly consider social objectives in mathematical optimization, and only very few take the new design and creation of industrial ecology into consideration.

The advanced method developed in Chapter 4 considers these gaps, while mastering challenges due to diverse measures and different scopes of corporate collaboration.

4 DEVELOPMENT OF THE INTERACTIVE OPTIMIZED NEGOTIATION ALGORITHM

The previous chapter discusses requirements for and purposes of modeling eco-industrial parks and networks, and evaluates state-of-the-art approaches based on these specifications. The overview of this evaluation in Table 3.4 shows that some approaches partially meet requirements. However, it also shows that some specifications have not yet been taken into consideration for the purpose of modeling in the field of industrial ecology. This chapter proposes a new, advanced modeling approach regarding the specified optimal solution and key challenges discussed in Chapter 3. Figure 4.1 shows the structure of this chapter, which follows a defined process, described below, to develop an Interactive Optimized Negotiation Algorithm (IONA).

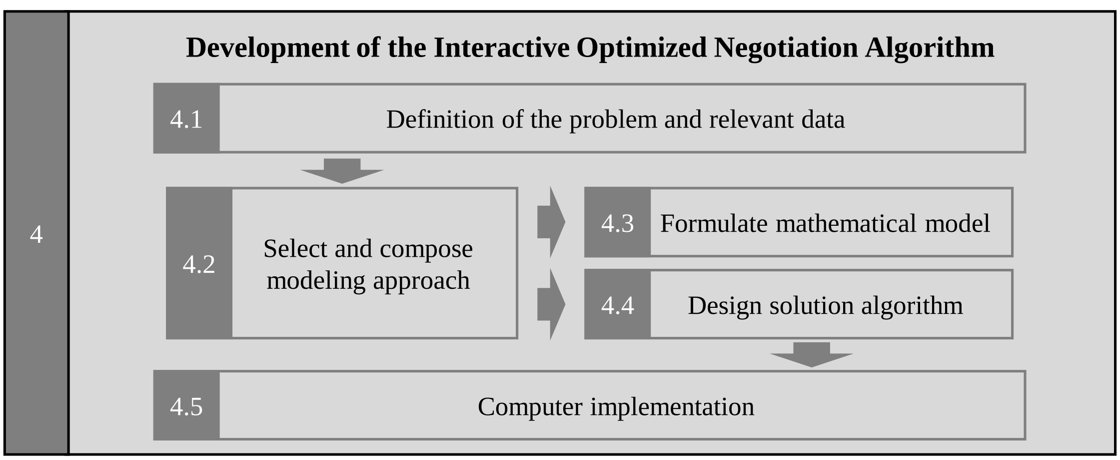


Figure 4.1: Overview of the structure of Chapter 4

The development of mathematical models and computer software often follow a certain methodology. This work will provide both a mathematical model and software in order to apply the solution algorithm established.

Meerschaert (2013) suggested a common approach to decision-making using mathematical optimization models. Meerschaert's five steps are the definition of the problem and relevant data, selecting the modeling approach, constructing the model, solving the model, and lastly, implement the solution. A commonly cited approach for software development has been proposed by Winston W. Royce (1970) and is known as the waterfall model of software development. Royce suggests a subsequent process of defining requirements specification, designing the software architecture, implementing the software, verifying the working system by testing and integrating, and maintaining the system as a final and ongoing phase.

Since this work provides the development of a mathematical model as well as the computer implementation, the following process is a combination of Meerschaert's and Royce's process definitions. The investigation of mathematical modeling approaches and the field of industrial ecology in Chapter 2 and 3 show that every modeling approach has been developed to be used for a specific problem and serve a specific aim. For this reason, the first step of the development process is the initial definition of the problem and relevant data to provide a comprehensive analysis of the initial position. Section 4.1 defines the underlying problem and discusses the relevant data based on the prior defined optimal approach (Subsection 3.2.2) and key challenges (Section 3.2).

Based on the first step, the modeling approach is selected and composed in the following step. Section 4.2 describes the actual process of composing, investigating, and suggesting a modeling approach.

Once the approach and the properties the new model needs are determined, the actual mathematical model can be formulated. A description of this step provides Section 4.3.

In many cases, the simple application of a mathematical model is insufficient in providing a result to support complex and uncertain decisions. Therefore, after constructing a mathematical model, a general algorithm, required to extend and apply this model for practical purposes, is defined in Section 4.4. An algorithm guarantees that the solution provided relates directly to the initial problem and does not only support a part of the comprehensive decision problem. This holistic approach implies that not only mathematical formulas but also other logical constructs can be introduced in order to support a decision being made by means of the proposed approach.

The solution algorithm is subsequently implemented into a computer model resulting in a software program, which is described in Section 4.5.

Finally, the last step of the development process applied in this thesis is the presentation of numerical examples in order to validate the proposed concept. An application and description of the validation step is provided in the following chapter 5. Seeking to overcome the main critique of many models of being too inflexible, various cases are applied and tests conducted.

4.1 Definition of the problem and relevant data

Following the above-described process of developing a mathematical model for the purpose of decision support and its implementation in a solution algorithm and a computer program, this section investigates two aspects, i.e. the underlying problem and the relevant data, as illustrated in Figure 4.2.

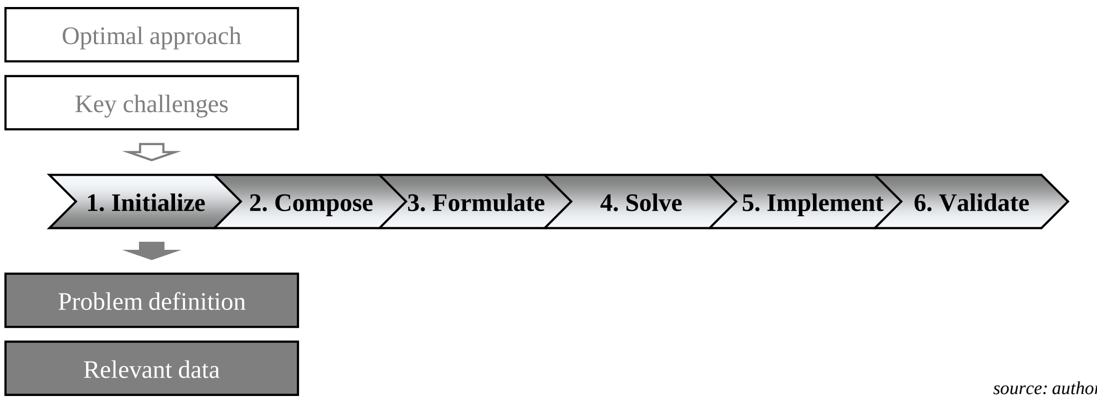


Figure 4.2: Process of developing an advanced modeling approach – step 1

The specific outcomes of Subsections 3.2 and 3.3 provide the basis for the following. The problem definition captures the main goals and significant properties of the initial situation (strategic layer). To supplement this, the investigation about the relevant data provides an overview of the scope and the system considered as well as relationships and the elements to be included in the modeling approach (operational layer).

4.1.1 Problem definition

The initial problem statement of this thesis in Section 1.1 shows that there is a large gap between the concept of sustainable development and its application. In order to provide an approach of closing this gap, academics, governmental and non-governmental institutions all over the world promote industrial symbiosis and eco-industrial parks and networks. The state-of-the-art literature review shows that relationships between companies can be analyzed, improved, extended, and created completely new for the purpose of implementing one of these concepts and supporting the progress of sustainable development. Many running systems have been investigated and success factors derived.

However, theory and practice still lack methodologies for systematically approaching the new design and creation of additional new eco-industrial parks, networks, or simply industrial symbiosis collaboration between companies. Referring to the optimal approach described in Subsection 3.2.2, the problem is stated as:

> *"Support the interactive negotiation process for the design and creation of new eco-industrial parks and networks under consideration of all three dimensions of sustainable development by means of a mathematical model and a computer implementation."*

In order to develop an advanced modeling approach it is important to meet the specific requirements investigated in Section 3.1. These requirement specifications are taken into consideration when the explicit modeling approach is selected and composed in the following section. However, this subsection further promotes ideas of how the major challenges defined and discussed in Section 3.3 are faced.

The first of three key challenges is the mathematical modeling of social sustainability that has not yet been researched. It has been shown that many of the current social goals relate to national effects and can thus hardly be impacted and controlled significantly by a single company. While for example, a company might impact the ratio of women in the work force or the accidents in a plant, a reasonable mathematical optimization cannot be applied. However, possibilities of both monetized and non-monetized measures were introduced. A critique of current models is that artificially introduced monetary values are inaccurate, of a different level of precision, and sometimes even invalid (Costanza and Daly 1987). The discussion of this key challenge shows that the CSR index of a company is an accepted and comprehensive, as well as accurate measure of the social performance of a company. Thus, this index will be essential to the model.

The second key challenge refers to a problem, which is closely related to the previously mentioned challenge. To avoid monetization, different measures are required. Hence, objectives of the proposed model must be comparable. Normalization, standardization, and scaling are important concepts to be included in the mathematical model. This implies that different information must be quantified and accessible to the model in the form of numerical representations.

The third key challenge is the scope of collaboration of the different companies. The companies can collaborate by supplying each other. If two companies do both supply and demand from each other, they share. Companies can share nearly everything. They can share office supplies, utilities, raw and recycled materials, work force, even plants and much more. However, most of the currently existing approaches for modeling of industrial ecology only refer to sharing of resources. Many companies share additional byproducts, which are not yet considered for mathematical modeling. Thus, the approach proposed in this thesis will consider resources in the form of a stream. This does not mean that only continuously streaming material can be modeled. It means that taken as a daily average every kind of resource, from the tangible water to the intangible knowledge (if measureable), can be considered. The model developed should be capable of integrating any kind of flows. The main focuses are utilities, byproducts, and components. It is important that many flows can be considered at the same time.

Besides these three key challenges, many other problems have to be solved and taken into consideration when modeling industrial ecology. Costanza and Daly (1987) discuss further aspects related to this field.

The consideration of economic, environmental, and social issues and performance is an essential part of the problem definition. Derived from the reviewed goals of eco-industrial parks (see Subsection 2.2.2), the modeling approach should include the following three objectives:

1. Minimize total transaction and setup cost of the network

It is crucial to every cooperate activity, that a company makes benefit from its activities. A mathematical model that does not consider the economic side will not provide a practical tool for decision support in sustainable development.

2. Minimize total amount of waste outside of the network

This object applies the main idea of the closed-loop approach. It is not relevant how much waste or how many byproducts are produced in total. The significant measure refers to the waste outside of the defined system boundaries.

3. Maximize social benefits

The consideration of social performance of companies is entirely new to mathematical modeling for industrial ecology. Although many publications suggested to improve the consideration of the social aspect of SD, this has not been captured.

The specific decision provided by the mathematical model must thus be about the optimal set of companies to collaborate in an eco-industrial network in order to achieve a maximum total objective. The result of the optimization model must contain a set of potential companies and an optimized allocation of the resource flows. Since every company can decide autonomously whether or not it is joining the eco-industrial park or network and the optimal solution may vary with every additional company being considered, the mathematical and computational model must provide an incremental optimization and negotiation process.

Even though many companies claim to have sustainable goals in the long run, daily business still mainly focuses on their short-term success, measured in monetary values. In order to investigate different scenarios of performance interests, another aspect of the problem investigated by means of the mathematical model is to allow different preferences to the three dimensions of the objective. However, it is assumed for this problem that decision makers have a general interest in optimizing for sustainable goals.

The next subsection specifically describes the relevant system and data required to be included in a mathematical and computational model.

4.1.2 Relevant system and significant data

The relevant system and data to be considered for the optimization of a network in the field of industrial ecology is described in this subsection.

Relevant system. The subject matter is the structure of an eco-industrial park illustrated in Figure 2.6. Transferring this into a network model, the following Figure 4.3 depicts the boundaries and basic elements to be captured by a mathematical model.

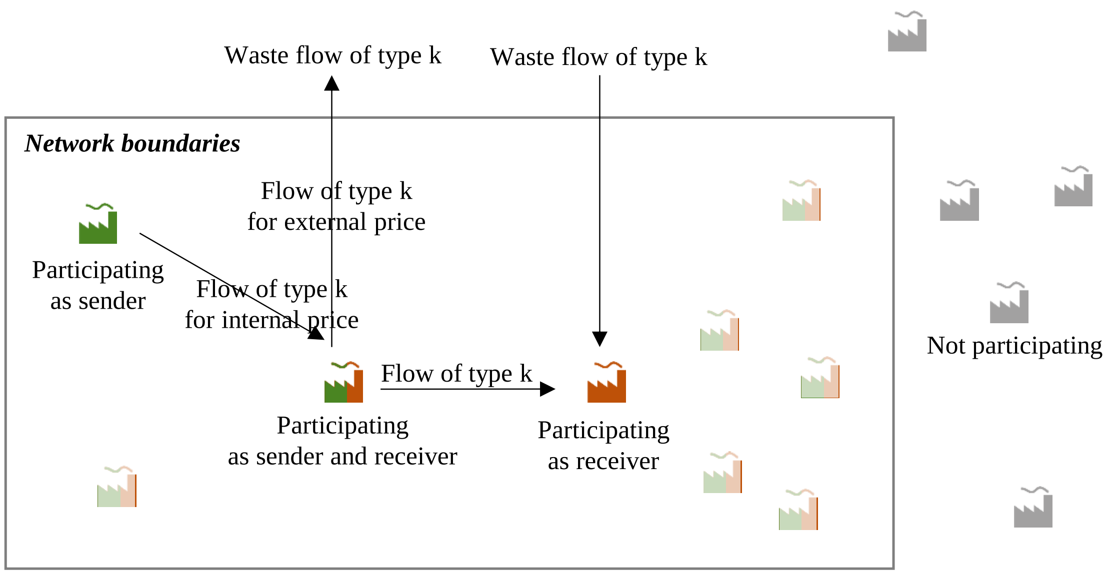


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Figure 4.3: The considered network and relevant information

The figure shows that the units considered are single plants, which are the very direct stakeholders of an EIP (see Figure 3.2). Each of these plants can be a member of the eco-industrial park or network. Furthermore, every member can act in a different way. Member plants can either be receivers, senders, or both. A receiver would be the classical plant emitting waste or producing byproducts with no activity of reuse or recycling. An example for such a company could be a car manufacturer in the classical sense (this does not consider the current development towards a backwards integration as it occurs in the supply chain of car manufacturers recently). A classical sender would be considered to only use waste as an input from the eco-industrial park or network. While these two characters of members are seen in other kinds of networks like recycling networks too, the idea of industrial ecology will be mainly represented. A plant that functions as a receiver as well as a sender in a network promotes the classical interpretation of industrial symbiosis and is thus the most important part of the network. The network also shows other related companies which are not participating in the eco-industrial park or network. Furthermore, the illustration shows possible flows throughout the network. Every plant has an input flow, coming into the plant and an output flow of emissions, waste, or byproducts. A company can receive and send a flow of the same kind of waste. This is practically possible when a plant emits a certain amount but also has a recycling or reuse unit with a limited capacity. If it exceeds the capacity, it has to send something out, if the capacity is higher, it can share this resource and take the waste of other participants of the eco-industrial park or network. Whether a company actually conducts reuse or recycling activities can also depend on the cost per recycled unit. In some cases, it might be more economical to send emissions out to another party, even though this might be less environmental friendly due to additional transportation activities and emissions. In addition to the internal flows between the member companies, every company emits the waste that has not been disposed by any other member to the market for the respective market price of disposal.

The modeling approach requires active inputs from direct stakeholders, i.e. EIP authority, member plants. However, the goals of further stakeholder groups like local communities, governmental institutions, and company management are included in the objectives and represented by the EIP authority.

The mathematical model constructed in Section 4.3 has to consider this general structure of the relevant system and introduce mathematical formulations for the relationships. While the decision about participation of plants and allocation of flows will be calculated by means of the model, data must be provided to investigate the relevant system and optimize the initial situation.

Relevant data. Since mathematical models process the input data into results, the quality of a model depends on both the mathematical model itself and the input data provided by the analyst and decision maker. In general, there are three different types of information classified by its accessibility. The internal, external, and public information is illustrated in Figure 4.4.

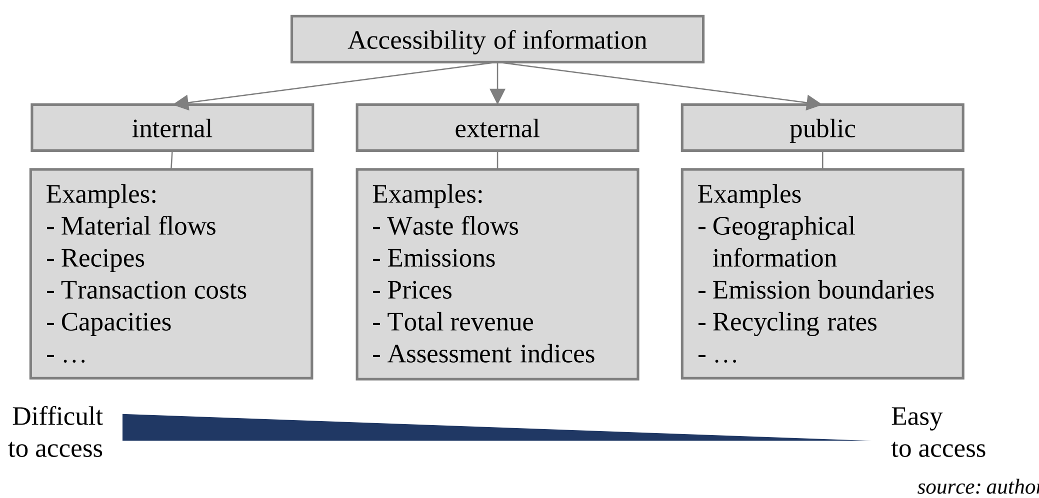

Figure 4.4: Three classes of accessibility for information

The first kind is internal information. This data is difficult to access and usually part of the company's decision-making processes. It is unlikely that the company will share this information with any other party. Internal data is not accessible by any outside parties without permission. It relates to information, facts, and data stored in company internal systems. This data is mostly created by the operation of the organization and includes numerical values about inventory, transactions, material flows, and capacities.

The second kind of data is the external data. This data is commonly an aggregation or the result of internal data. Examples are market prices of the company's products, assessment indices that are published, as well as the overall (annual) business results. This type of information is usually collected by surveys and accessible for money or entirely free to everyone. Depending on the information the accessibility is difficult.

The third kind is public information. This relates to data that is published by the government or any other non-governmental information. Examples are geographical data, and socio-demographic information. Some information like distances between two potential locations can even be calculated and are thus always accessible to everyone.

Since relevant data is the second largest influencing factor in the successful application of a modeling approach, it is crucial that a successful modeling approach require the least information possible. Additionally the rule is to prefer public data over external data and external data to internal data in order to generate a model. On the contrary, internal data provides a more accurate result regarding the real world problem. There is a trade-off between advantages and disadvantages of using internal data in a model.

The more internal data is required for a mathematical model, the more specific are the findings and recommendations from an optimization. In contrary, the less internal information is required, the more accurate and the better accessible is the relevant data.

The mathematical modeling approach should thus allow the application with a varying degree of accessibility of information. While the objective function and the main constraints must be based on external information, internal information can be introduced by adding constraints to the basic model.

Table 4.1 shows the minimum required information to be integrated in the model, including measures, accessibility, and the provider for each set of data.

No.	Data	Measure	Accessibility	Provider
1	**coordinates of the plant location**	longitude, latitude	public	EIP authority
2	**distances**	miles	public	EIP authority
3	**maximum emissions**	kg per period	public	EIP authority
4	**market prices for each flow type**	$ per kg	external	EIP authority
5	**transaction cost**	$ per kg and mile	external	EIP authority
6	**reduction rate of int. transaction**	%	internal	EIP authority
7	**input of each flow type**	kg per period	external	companies
8	**output of each flow type**	kg per period	external	companies
9	**CSR index**	[0,100]	external	companies
10	**network price**	$ per kg	internal	companies
11	**fix cost or incentive for joining**	$ per plant	internal	EIP authority

Table 4.1: Relevant data for the modeling approach pursued in this thesis

The coordinates of the potential plants must be given. Based on this, the distances can be approximated, calculated, or determined by any other way. This data is easily accessible through various sources like Google Maps or OpenStreetMap and can be determined very accurately. Depending on the circumstances and scope of the model, some national and regional requirements must be considered as maximum emissions. This restriction may only apply to certain participants. In order to determine cost differences and mathematically optimize the economic objectives, a price for disposal to the market should be provided for each of the considered types of waste, emission, byproduct, or component (incl. Shipping, taxes, and fees). This price can be negative if companies get money for a certain output stream. For instance, if the output was freshwater, companies can achieve a negative payment or income by emitting materials. Clean air and granulate material are common examples for a byproduct in the chemical industry, which is sold to the markets. The price could also be zero. In this case, the disposal does not cost anything. An example is the emission of polluted air. However, the target of this thesis is to provide an environmentally friendly approach to the creation of networks. Hence, this will not be an optimal behavior due to the consideration of additional environmental related objectives. Transaction cost can be estimated from logistics companies and experiences. The critical information is the input and output flow of a certain kind of waste, emission, or byproduct. Even though this information is difficult to get, it is more likely that companies will share this information than publishing their internal processes. Unfortunately, the documentation of waste products is still not required by any ISO standards. The network price for every type of flow may vary by the receiver and has to be determined. This is the most critical information since companies will try to maximize this price during the negotiations. Constancy and forecast reliability as well as reduced transaction cost will decrease the shipment costs compared to the market prices. This is a main assumption for the modeling approach.

In order to improve the consideration of economic targets of single plants, an EIP authority must determine a fixed cost or provide incentives to companies for participating in the eco-industrial park or network. Incentive payments could be given by the government.

Under consideration of the defined problem and the relevant system and data, the next section provides a comprehensive description of the actual development process for the main ideas of modeling for eco-industrial parks and networks.

4.2 Select and compose modeling approach

The second step in the development processing of a new mathematical and computational model, for decision-making in the field of industrial ecology, is the selection and composition of the appropriate modeling approach. This section describes the main ideas and aspects of the new approach and where they originate. As previously stated, some modeling approaches and ideas have been developed and can be suitable to the afore-stated problem. The objective of this step is to develop a new approach under consideration of the desired targets and requirements for models investigated in Section 3.1. Figure 4.5 illustrates this step along with the inputs and outcomes.

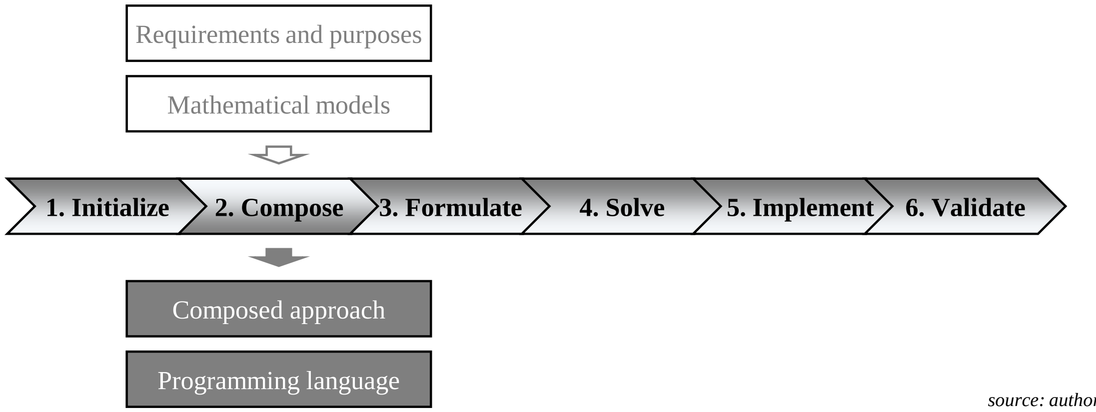

Figure 4.5: Process of developing an advanced modeling approach – step 2

Complex subjects require complex solution methods. In order to create a new network, many decision makers have an influence on the factors, and many objectives must be considered regarding the different tangible and intangible flows through the network. Unlike many suggested approaches, this work seeks to propose a tool to improve negotiations and thus the interaction process between the EIP authority and companies.

1. A mathematical model to support decisions based on current parameters

is one part that leads towards a new approach of creating EINs. In order to allow interaction during the optimization process, the second part is complimentary:

2. A computational model to support the negotiation process

with updated parameters and different weights on objectives provided by the EIP authority and companies. Since the decision is so complex, a new optimization loop after every negotiation step should be provided. Subsection 4.2.1 discusses the selection and composition of the idea for the mathematical model, and Subsection 4.2.2 describes the computer model to be applied within this modeling approach.

4.2.1 Main ideas for the mathematical model

The general scope of the proposed model is to create and design entirely new eco-industrial networks. Figure 4.6 shows an overview of the necessary requirements in order to develop an advanced mathematical modeling approach, which is suitable to model for IE. The targeted state as described in Section 3.2.2 is to meet all requirements.

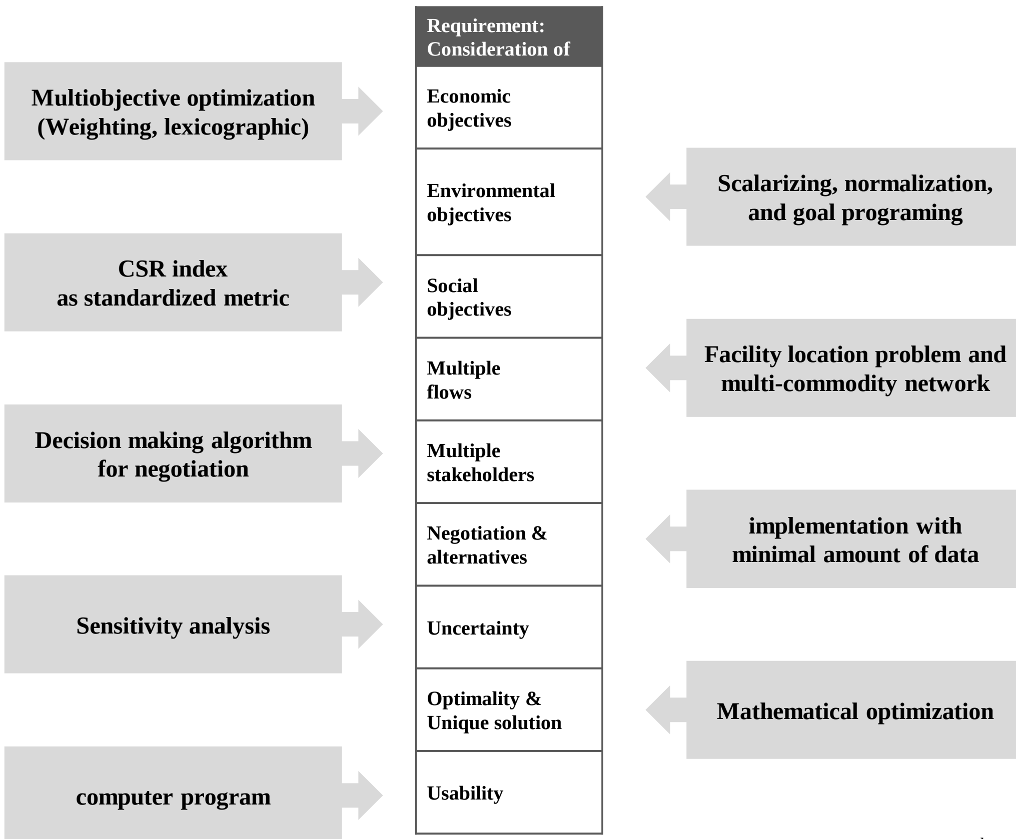

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Figure 4.6: Main concept for an advanced model of eco-industrial networks

Main structure. The main goal of this thesis is to propose a mathematical model for industrial ecology. Because the application of industrial ecology and industrial symbiosis is commonly approached through eco-industrial parks or networks, the main idea is to apply a network model. Network models are powerful tools to support the process of decision making and supply optimal activities (Alhajj 2014). Since the relevant system is a network with locations of plants, the problem narrows to a strategic location decision. Within a network of potential participants, the mathematical model seeks to optimize the allocation of given input and output flows of every plant the

basic formulation is a Multi-commodity warehouse location problem.

Binary decision variables determine the status of locations and amounts of flows are calculated continuous decision variables. This builds the basis of the advanced approach. It can capture existing as well as planned locations. Since there is more than one objective and many different stakeholders with controversial interests to be considered, the model needs to include approaches from the field of MOO.

Multiple objectives. Real world problems are characterized by more than one goal. Many mathematical approaches simplify situations by making assumptions and emphasizing one goal which then will be optimized. For example, the traditional transshipment problem (see Subsection 2.4.1) considers the cost of transportation, neglecting the emissions, transportation times, and other factors. However, a main property of industrial ecology is the simultaneous consideration of all three goals described in Section 2.2.3. Thus multi-objective optimization must be applied. MOO methods can be classified by the degree of participation of the decision maker in the optimization process (see Figure 2.12). In this case, the decision makers are the EIP authority and the potential plants. However, the only decision maker who has an influence on the objectives is the EIP authority and it can express its preference before the optimization happens. An achievement function can be applied to the respective objectives. The total optimum can then be calculated by means of the weighted sum of all achievement functions. Different metrics can be measured relative to their target value and simultaneously optimized. No hierarchal order of objectives is required.

> *Suitable multi-objective methods are the weighting method and the lexicographic method for a relative and an absolute priority respectively and solve those problems applying the idea of goal programming.*

Entirely new to mathematical modeling is that the fix cost of a location will be replaced by its CSR index. Optimizing this aspect, the social impact of the entire network can be indirectly defined.

Since bi-level optimization is applied where a leader and a follower make a decentralized decision, it is not suggested to be applied here. The individual companies do not have an initial need to follow the EIP authority.

Multiple flows and stakeholder. Multi-flow: The main goal of industrial ecology is to introduce the concept of what Korhonen et al. (2003) calls a "roundput". The main idea is to introduce circulating material and energy flows and thus avoid the generation of waste (Korhonen et al. 2003). The network model, which describes the flow of many commodities at the same time, is called multi-commodity flow network (see Subsection 2.4.1); this serves as the very basic model. In addition to this model, the facility location problem provides the opportunity to make a binary location decision. The result of such an optimization provides information whether a certain location should be opened or closed. In the problem of designing eco-industrial networks, the circumstances are similar and the logic of decision-making can be adapted. However, the decision in this case is not if a potentially new location should be opened, but if a potential plant to be included in the network should be included or not, considering the pursued targets. This allows the consideration of many stakeholders, i.e. the plants, at the same time. The EIP authority will be the analyst and one of the decision makers for the modeling approach. Additional decision makers are the potentially participating companies. The rest of stakeholders is considered in constraints, for instance government due to recycling rates and emissions.

Negotiation and alternatives. Today's real-world problems are characterized by both high complexity and extensive uncertainty. Processes cannot simply be assumed to be linear anymore and the solution of a linear model can only sometimes be directly transferred into the real world. Properties of EIPs require more than a one-step model. While the network optimization determines a global goal, every single participant has its own individual set of goals. Considering every single goal in the initial optimization would be an extensive work and the data, as stated in the previous section, would be very difficult to be collected by a single individual or group. Thus,

> *a stepwise interactive optimization of alternating optimization and negotiation steps is defined as a main algorithm.*

Uncertainty and optimality. In order to find an optimal solution to a set of data, this set of data must be determined. However, adapted from sensitivity analysis, the negotiation algorithm should allow to account for a deviation from the initial data provided by the company. The impact of changes from this initial data should be investigated. Since multi-objective optimization often leads to Pareto optimal solutions (see Section 2.3), it is important to implement an algorithm that leads to a unique final solution. Pareto optimal solutions are undesirable in large decision problems.

Usability. The last criterion derives from the call for providing more practical and relevant solutions to promote sustainable development. The mathematical and computational model proposed in this work should be applicable to practical case data. Many of the currently existing interactive optimization approaches, for example NIMBUS, lack flexible use and user-friendliness. Negotiation requires interaction. Computer models with graphical user interfaces can promote user interaction. Due to a minimal amount of accessible data and an implementation with a programming language, a high degree of usability is achievable.In order to guarantee a maximum freedom in the design of the algorithm, an individual program is preferred over a standard software package.

4.2.2 Implementation of a computer program

Many different methodologies have been implemented to solve decision-making problems for eco-industrial parks. Figure 4.7 shows possible methodologies of solving a defined problem by means of computer models. A discussion of these methods and a suggestion is provided in the following paragraphs.

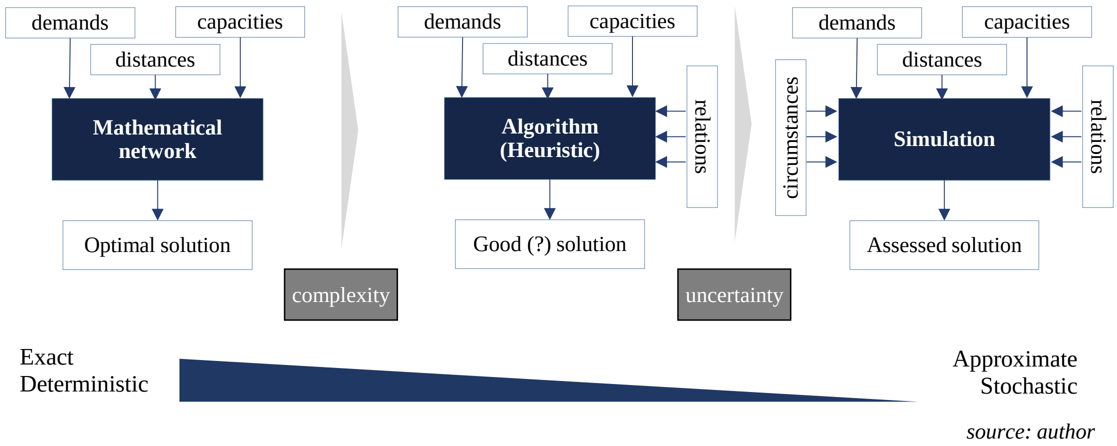

Figure 4.7: Basic methods for solving a problem using a computer model

Optimization program. Optimization has been applied for finding the best possible allocation of material flows within defined networks. For the application of optimization, data must be determined and the behavior and relationships within the network must be known. Many of the applied mathematical models have been proven to be NP-complete and can thus be solved in polynomial time. The advantage of applying optimization to the design of EINs is that the solution discovered provides the best setting for parameters that have an influence on a generated network. The significant disadvantage of optimization is that if the relevant system becomes too complex and the input data is uncertain or inaccurate, the optimal solution is invalid and can even lead to very bad results once it is applied to the real world problem. Additional constraints may lead to models, which are no longer solvable in polynomial time. Since the creation of a new EINs is characterized by a certain level of uncertainty, these advantages may occur by applying such model. An optimization approach is proposed Taskhiri et al. (2010). Standard software like LINGO, GAMS, and AIMMS can be used to implement a mathematical model into a computer model and solve it.

Simulation. Another method for implementing a computer model is to set up a computer simulation. A simulation considers the behavior und additional circumstances in order to understand a complex system under uncertain conditions. Other than an optimization, a simulation does not provide an optimal solution. On the contrary, it is possible to assess the final solution, but it is usually not the goal of a simulation to find a good or a bad solution. Simulations help to understand the behavior of a complex and uncertain system. The advantage of a simulation is that under complex and uncertain behavior, many cases and outcomes can be investigated and patterns extracted. Because the purpose of this work is to find an optimal or at least suitable solution for the design of a new EIN, it is not suggested to apply simulations. Romero and Ruiz (2013, 2014) proposed an example for an agent-based simulation for the design of new EINs.

Numerous common simulation environments such as Plant Simulation, Matlab Simulink, Promodel, and Anylogic support simulation of networks.

Algorithm. While simulations are used in well-structured and under deterministic circumstances and a simulation helps to understand complex and uncertain systems, algorithms are useful to include advantages of both methods. Algorithms allow user interaction in the decision making process. They can be used to introduce a certain degree of uncertainty and allow investigation of the impact of changes in data. Other than a simulation, the data provided needs to be determined, but changes are applicable. However, it is possible to find the optimal solution to the given conditions if desired. Further, if an optimal solution is not required, algorithms help to find a good solution. In this case, heuristics are techniques for solving a problem based on experience. These methods solve problems faster but therefore are not guaranteed to be optimal. Supporting interaction requires freedom in design of the process.

Gu et al. (2013) provides an example for an algorithm that has been implemented to design eco-industrial parks (see Section 2.4). Programming languages like Java and C# can be used to automate algorithms and implement user-friendly computer models. A powerful programming language is Python. Due to its popularity in the field of science, many pre-developed modules can be included. Many optimization and simulation packages provide interfaces to Python. For the purpose of optimization, Gurobi Optimization provides an extensive functionality. SimPy is a process-based discrete-event simulation framework based on the programming language python. The module wxPython provides a large variety of classes for a graphical user interface.

> *This thesis proposes an algorithm based on an optimization of a mathematical model implemented in Python programming language. These three elements will subsequently be described in the following 3 sections.*

A network model with binary decision variables for optimizing the participating locations and continuous variables for optimizing the flows within the network are essential to the modeling approach. Achievement functions guarantee the simultaneous simulation of all objective dimensions. An interactive sensitivity analysis and algorithm as well as the computer implementation of this algorithm provide a useful tool for modeling the design of eco-industrial parks or networks. The following Section 4.3 describes the mathematical formulation and the subsequent Section 4.4 describes the computer implementation.

4.3 Formulate mathematical model

Following the process of developing the mathematical and computational modeling approach, the third step is to develop the basic mathematical model.

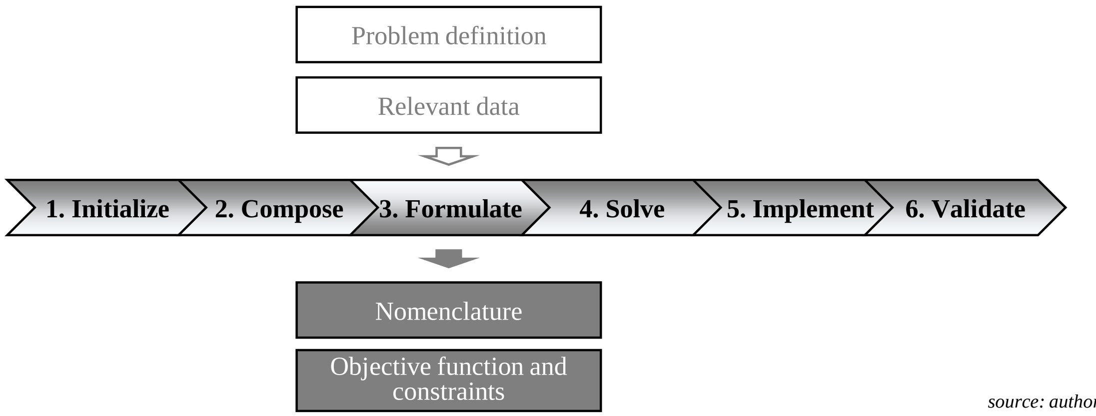

Figure 4.8: Process of developing an advanced modeling approach – step 3

The previous Section 4.2 discusses and suggests ideas of existing approaches. This section integrates all the aforementioned ideas and proposes an entirely new and advanced mathematical model for optimizing the design of new eco-industrial networks (see Section 4.1). Therefore, basic assumptions (Subsection 4.3.1) are examined initially, followed by a description of the model itself.

The description of a mathematical model is given in three steps. The definition of sets, variables, and parameters (Subsection 4.3.2), the objective function (Subsection 4.3.3), and the constraints (Subsection 4.3.4) of the basic model are the focuses of this section.

Subsequently, extensions of the model are promoted in Subsection 4.3.5.

4.3.1 Model assumptions

Every model is a simplified representation of a real world problem. The best model is the simplest possible representation that is still complex enough to serve its purpose (see Section 2.3 and Velten 2009). When simplifications are made, the conditions under which the results of a model are investigated must be concisely defined. Table 4.2 summarizes the assumptions made for the proposed model.

No.	Assumption
1	**All dimensions of sustainable development are relevant to decision makers**
2	**A plant can either be inside or outside of the eco-industrial park**
3	**The output and input flows can be estimated by a high degree of certainty**
4	**The total output of a type of flow is either emitted**
5	**All plants have a capacity within certain boundaries**
6	**Plants are currently setup and no additional costs occur**
7	**Transaction costs within the network are different than outside**
8	**Distances between two locations are determined**
9	**Prices can be determined for a defined period of time**
10	**The decision of one plant is not affected by a decision of another**

Table 4.2: Assumptions for the mathematical model

Decision makers who have an influence on the outcomes must generally have an interest in designing a network under consideration of all three dimensions of sustainable development in order to exclude trivial solutions. A trivial solution, for instance, is a network with no members and no allocation of resources leading to zero cost and no pollution. This case cannot occur when the companies are interested in creating a network. Every plant could potentially have both functionalities, receiver and sender, but must have only one functionality. Since the purpose of the model is to promote industrial symbiosis, the targeted company should act as both receiver and sender.

A plant can either be inside or outside the eco-industrial park. Every plant can estimate its approximate output flow for each of the considered types of flow and the respective input capacity. Flows can be equal to zero and the optimization does not consider partly included plants. However, due to the provided data, a company can determine its own degree of participation by specifying certain ratios of the total output or input as the output or input flows for the negotiation. Further, if a plant does not seek to participate with a certain product, it does also have the opportunity to not announce this to the analyst (EIP authority). In such a case, the optimization is based on hidden information. This can lead to extensively negative results of the optimization and should be avoided or even punished if possible (Soberman 2003). All plants have a capacity within lower and upper boundaries. The decision of one plant is not affected by a decision of another.

The total output of a type of flow is either emitted to a plant that reuses this material type or as waste to the market (balanced problem). The reusing plant can also be the emitting plant itself. It might not be optimal for a company to treat its own emissions when other companies have cost advantages due to economies of scale and better technologies or when the transport distance is considered to have a negative impact on the environmental performance of the network.

This is caused by additional emissions due to the transportation of waste.

The model is further based on the assumption that plants are currently setup and no additional costs occur due to the integration of a plant into the new eco-industrial network. Transaction costs within the network are different than outside of the network. These costs are expected to be lower due to economies of scales and forecast reliability.

As well as the input and output data, the additional data is assumed to be determinable to a high degree of certainty. Distances between two locations are determined. Additional cost due to traffic, delays, loss, and detours are neglected. Prices can be determined for a defined period of time. These prices can be averages.

Only one period of time is considered in this model. All data must be valid for this period. Since this assumption limits the applicability of the results to practice, the algorithm should be used to investigate deviations of data while optimizing.

4.3.2 Nomenclature

The initial step for composing a mathematical model is the definition of required sets, decision variables, and parameters, which represent the provided data.

Sets. The proposed model contains three sets. One set defines the locations and one set defines the flow types. Every location or plant is separated into two parts: the emission point (which emits the output flow) and a receiving point (which reuses the input flow). Flow types can be waste, emissions, and byproducts. The sets and indices are defined as follows where I and J have the same cardinality:

$$I: Number\ of\ potential\ emission\ points\ at\ location\ (i = 1,2, \dots, I)$$

$$J: Number\ of\ potential\ receiving\ points\ at\ location\ (j = 1,2, \dots, J)$$

$$K: Number\ of\ flow\ type\ (k = 1,2, \dots, K)$$

Variables. Decision variables are essential to the mathematical model. These variables will determine the actual solution, which leads to an optimal suggestion for a decision. This model requires two types of decision variables, i.e. binary and continuous variables. The binary variables are defined as:

$$y_{s,i} = \begin{cases} 1, if\ location\ emits\ one\ or\ more\ flows \\ 0, else \end{cases}$$

$$y_{r,j} = \begin{cases} 1, if\ location\ receives\ one\ or\ more\ flows \\ 0, else \end{cases}$$

$$y_{l,i} = \begin{cases} 1, if\ location\ is\ part\ of\ the\ EIN \\ 0, else \end{cases}$$

Besides the binary variables, there is another positive continuous variable representing flow streams of a type k from an emitting location i to the receiving location j. As mentioned before, i can be equal to j if not restricted by any of the provided constraints:

$$x_{ijk}: Transportation\ flow\ of\ type\ k\ from\ location\ i\ to\ j\ [unit/period]$$

$$z_{ik}: Transportation\ flow\ of\ type\ k\ from\ location\ i\ to\ market$$

In total, this model contains a number of variables H:

$$H = (3 * I + I2 * K) = I * (3 + I * K)$$

The introduction of binary variables leads to a mixed integer linear problem.

Parameters. As previously mentioned, the mathematical model proposed seeks to require as little information as possible. However, in complex decision making processes it is always necessary to have an input of some determined data. The following parameters are relevant to this approach:

$$w_b: weight\ of\ the\ economic\ objectives\ (business)$$

$$w_e: weight\ of\ the\ environmental\ objectives$$

$$w_s: weight\ of\ the\ social\ objectives$$

These weights must be determined before the optimization. This method suggests a standardized distribution of the weights with $\sum w = 1$ since achievement levels are introduced in order to simultaneously optimize different measures. Therefore, achievement target values have to be defined for each of the three objectives:

$$t^*_{b,1}, t^*_{b,2}: target\ values\ for\ the\ economic\ objectives\ (business)$$

$$t^*_e: target\ value\ for\ the\ environmental\ objectives$$

$$t^*_s: target\ value\ for\ of\ the\ social\ objectives$$

According to the achievement measure approach, these targets can be utopian or realistic. However, the final objective requires this parameter in order to minimize the distance of the objective to the prior determined value t. All of the above-mentioned parameters have to be determined by the analyst, i.e. the EIP authority.

The following parameters refer to the actual network data:

$p_{E,k}: external\ market\ price\ for\ flow\ of\ type\ k$

$p_{I,ik}: internal\ price\ of\ receiving\ location\ i\ for\ flow\ of\ type\ k$

$d_{ij}: distance\ from\ location\ i\ to\ location\ j$

$c_{v,k}: variable\ transaction\ cost\ for\ flow\ type\ k\ per\ mile$

$c_{f,i}: fix\ cost\ or\ incentive\ for\ location\ i\ as\ a\ part\ of\ the\ network$

$c_{s,k}: social\ performance\ of\ location\ i\ (CSR\ index\ of\ the\ company)$

$e_{max,k}: maximum\ network\ emission\ for\ flow\ type\ k$

$s_{jk}: total\ input\ flow\ capacity\ of\ location\ j\ for\ flow\ type\ k$

$q_{ik}: total\ output\ flow\ emitted\ by\ location\ j\ of\ flow\ type\ k$

Internal prices should be equal to the operation cost of a company by treating the input flow, i.e. waste material. These parameters are used in the objective function and constraints, which are described in the following subsection.

4.3.3 Objective functions

The basic problem is formulated as a composition of a capacitated warehouse location problem and a multi-commodity network, resulting in the problem being categorized as a mixed-integer linear problem (MILP). In order to apply multi-objective optimization, which is required due to the relevance of all three dimensions of sustainable development to the design of an eco-industrial park, two approaches are suggested in the following, i.e. the weighting method (equation 4.4) and the lexicographic approach (equation 4.5). The original methods are described in subsection 2.4.2. The algorithm will allow the analyst to choose between relative and absolute objective preferences.

Weighting method. The objectives for the weighting method are defined as follows:

$$z_1 = \frac{t_{b,1}^* - \sum_{i=1}^{I}\sum_{j=1}^{J}\sum_{k=1}^{K}(p_{E,k} - d_{ij} * c_{v,k} - p_{I,ik}) * x_{ijk}}{t_{b,1}^*} + \frac{t_{b,2}^* - \sum_{i=1}^{I} c_{f,i} * y_{e,i}}{t_{b,2}^*} \tag{4.1}$$

$$z_2 = \frac{t_e^* - \sum_{i=1}^{I}\sum_{j=1}^{J}\sum_{k=1}^{K} x_{ijk}}{t_e^*} + \frac{1}{M}\sum_{i=1}^{I}\sum_{j=1}^{J}\sum_{k=1}^{K} d_{ij} * x_{ijk} + y_{e,i} \tag{4.2}$$

$$z_3 = \frac{t_s^* - \sum_{i=1}^{I} c_{s,i} * y_{l,i}}{t_s^*} + \frac{1}{M}\sum_{i=1}^{I}\sum_{j=1}^{J}\sum_{k=1}^{K} x_{ijk} \tag{4.3}$$

The total objective of the weighting method approach is as follows, neglecting the light grey parts of the equations or setting all Big M's equal to infinity:

$$minimize\ z = w_b * z_1 + w_e * z_2 + w_s * z_3 \tag{4.4}$$

The objective is to minimize the distance to the previously defined target values. This allows the optimization of different metrics. A requirement for the target values of each objective is given below. The economic objective (4.1) reduces the total transaction cost towards a maximum saving target. For every unit, the saving due to transferring a unit within the eco-industrial network instead of disposing this unit as waste, is calculated.

This saving equals the difference of the market price and the sum of transfer costs and the internal network price for type k of a receiver location j. Transfer costs are calculated by multiplying the cost rate per mile and the distance.

The optimization seeks to minimize the difference of the total savings over all units to the maximum savings target. This value is normalized in order to provide a relative measure. If applied, the sum of the participation cost or incentive multiplied with the binary decision value of every location seeks to minimize the difference to the previously determined goal for these costs. Theoretically, the maximum possible savings occur when all output flows of potential plants are transferred the minimal distance and minimal network cost of each product type compared to the most expensive market price. The second objective (4.2) seeks to minimize the difference of the actually internal transferred amount of flows to the absolute goal. If the goal is to reduce waste, the target is to transfer all the flows within the eco-industrial network. In this case, the target value for this objective is the total output of all potential plants.

The third objective (4.3) defines an achievement level for the corporate social responsibility. Plants are accounted by the CRS index investigated for their managing company. The distance from the target value is minimized. The target value can be set within the range of the CSR index [0,100]. While a value of 100 is utopian, an expected value of 80 or 90 has proven to be a suitable target value. The total distance for all weighted objectives from the target values is minimized.

Lexicographic method. The second version of an objective function can be applied when preferences for objectives are not given relatively, but the decision maker can provide an absolute preference. The formulas are slightly different, including the light grey part of the equations (4.1) to (4.3). The total objective of the model is:

$$lexmin\,\{z_1, z_2, z_3\} \tag{4.5}$$

Function (4.5) shows the lexicographic graphic order, where primarily the first objective is optimized, and then subsequently additional objective functions with a decrease of the priority to the decision maker. The order of the objectives may vary, for example to $lexmin\,\{z_2, z_1, z_3\}$ if environmental objectives are more important than economic objectives, and these are more important than social targets.

The following subsection describes the constraints of the mathematical model.

4.3.4 Constraints

In order to add conditions that must be satisfied by the solution of this problem, constraints are introduced in this subsection. The full set of constraints is listed below:

$$\sum_{j=1}^{J} x_{ijk} + z_{ik} = q_{ik} \qquad \forall\, i, k \tag{4.6}$$

$$\sum_{i=1}^{I} x_{ijk} \leq s_{jk} * y_{r,i} \qquad \forall\, j, k \tag{4.7}$$

$$\sum_{j=1}^{J}\sum_{k=1}^{K} x_{ijk} \leq M_2 * y_{e,i} \qquad \forall\, i \tag{4.8}$$

$$y_{r,i} + y_{e,i} - (y_{r,i} * y_{e,i}) = y_{l,i} \qquad \forall\, i \qquad (4.9)$$

$$x_{ijk}, z_{ik} \geq 0 \qquad \forall\, i, j, k \qquad (4.10)$$

$$y_{r,i}\,, y_{e,i}\,, y_{l,i} \in \{0,1\} \qquad \forall\, i \qquad (4.11)$$

The first constraint (4.6) ensures that for every emitting location and product a mass balance is guaranteed. Masses are not interchangeable and can either be transferred within the network or waste outside of the network. This can be seen similar to a demand that has to be satisfied in the classical WLP.

The second constraint (4.7) provides the capacity limit of a receiving company. The maximum amount that can flow for each product cannot be exceeded by the sum of all incoming streams. This constraint has to be met by each location for each product. As soon as one flow is greater than zero, the location is determined to be a receiver location.

The next constraint (4.8) is a big M condition, requiring an emitting location to be open, indicated by the binary variable. The big M must be larger than the maximum value of the sum over all products.

Constraint (4.9) implements an "OR" condition. The binary variable for the location $y_{l,i}$ equals one, if either $y_{e,i}$ or $y_{r,i}$ or both variables are equal to one and thus if a location acts as either or both a receiving and an emitting party. This constraint is a non-linear constraint. It can be replaced by the following three constraints (4.12), (4.13) and (4.14) in order to linearize this constraint.

$$y_{e,i} \leq y_{l,i} \qquad \forall\ i \qquad (4.12)$$

$$y_{r,i} \leq y_{l,i} \qquad \forall\ i \qquad (4.13)$$

$$y_{r,i} + y_{r,i} \geq y_{l,i} \qquad \forall\ i \qquad (4.14)$$

However, this linearization will not be applied for the computer model since the state-of-the-art solvers can easily handle such a nonlinearity and the advantage of the reduced constraints overweigh the disadvantages of the nonlinearity.

Constraint (4.10) ensures non-negativity for the flow variables and constraint (4.11) allows the open/closed-decision variables to be only binary.

These conditions are applied to the negotiation algorithm described in Section 4.4. However, additional constraints can be added to the model without major changes.

4.3.5 Expansion

These constraints relate to additional conditions that occur when decisions must be made under impeding circumstances in the field of eco-industrial networks.

$$\sum_{i \in G_1} z_{ik} \leq e_{max,k} \qquad \forall\, k \qquad (4.15)$$

$$\sum_{i \in G_2} z_{ik} \geq e_{min,k} \qquad \forall\, k \qquad (4.16)$$

$$\sum_{k=1}^{K} x_{ijk} \leq f_{max,ij} \qquad \forall\, i, j \qquad (4.17)$$

While the basic model does not include extra boundaries and constraints for regarding the network emissions, this might be an important expansion of the basic model to consider in the future. Constraint (4.15) considers maximum emission for each flow type regarding a defined region. For example, different countries have different laws or limits for emitting a certain kind of flow. This leads to a maximum boundary for the sum of all waste flows of a kind emitted from certain locations of a subset of locations G_1 (for example Germany, China, or USA). In opposite to this constraint, the next suggested extension of this model (4.16) suggests a minimum constant emission. This constraint is the mathematical formulation of the positive occurrence of the shared byproduct, heat, which is part of the Kalundborg concept (see Subsection 2.2.3). Once an eco-industrial network is setup, it may be required in specific cases to guarantee the supply of a byproduct for a certain group of external customers. Derived from the multi-commodity network, where usually the network flow on each arch is constrained due to a certain capacity, this might be a useful consideration (4.17). A practical case is commonly restricted by a maximum capacity of a truck or a pipe.

The last extension for the basic mathematical model presented in this thesis is the introduction of economies of scales. Lu (2010) discusses this effect for the common facility location problem. As the most useful case for linear programs, a step cost function is suggested depending on the number of open facilities. Transferred to this problem, the objective function as well as the set of constraints must be extended by:

$$minimize\ z = z_{old} + c_f * \alpha \tag{4.18}$$

$$s.t. \sum_{i=1}^{I} y_{r,i} - N_{crit} \leq \alpha \tag{4.19}$$

$$\alpha \in \{0,1\} \tag{4.11}$$

Equation (4.18) shows that an additional amount can be added to the objective function when $\alpha \geq 0$. The additional constraints (4.19) and (4.20) ensure that $\alpha = 1$ when the number of participating receiving companies exceeds a critical number N_{crit}. This can also be implemented as a negative cost for the case of critical numbers of participating companies. This method can be interpreted as a negative penalty objective function and global cost benefit can be considered. In practice, this can occur when the government supports eco-industrial parks or networks starting at a certain number of participants.

4.4 Design solution algorithm

Following the process of developing the modeling approach in this thesis, the next step is to construct an algorithm in order to solve the complete underlying problem, as Figure 4.9 illustrates.

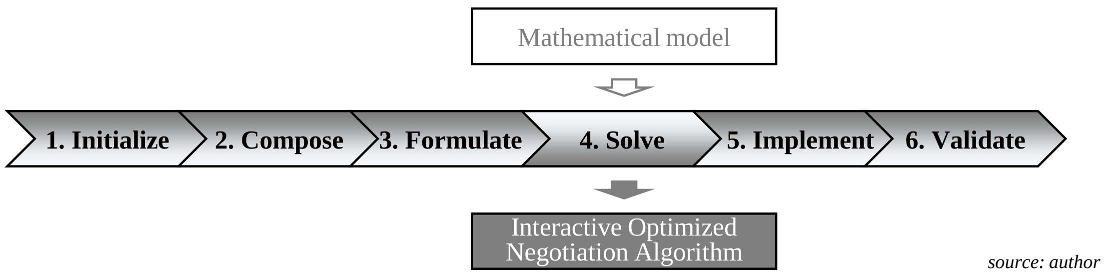

Figure 4.9: Process of developing an advanced modeling approach – step 4

A mathematical model cannot always catch every issue of the entire decision making process. Many decision makers with without a hierarchical structure and involved in situational issues characterize the considered problem. Thus, an interactive and stepwise approach helps to give the main analyst an idea of the initial situation and helps to support the process of negotiations towards the implementation of an eco-industrial network. This aspect is very important since many publications call for more implementation of the concept of industrial ecology as prior investigations show. In order to support the decision making process, the

Interactive Optimized Negotiation Algorithm (IONA)

is defined embedding the previously developed mathematical model. The 10-step algorithm is illustrated in Figure 4.10.

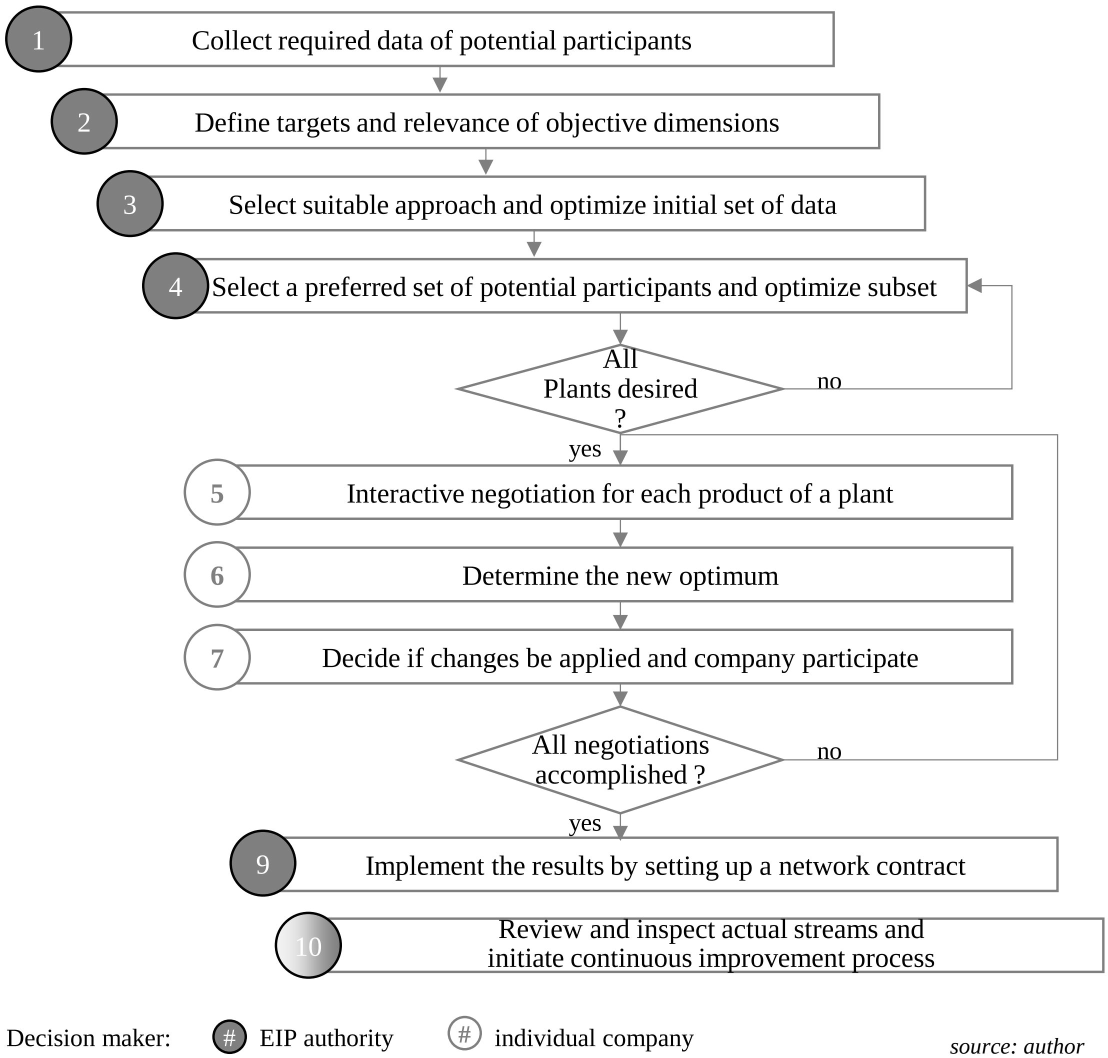

Figure 4.10: Algorithm for interactive negotiation embedding the model

As a main requirement for the suggested modeling approach, the model must be applicable and useful for practical cases. In order to meet this requirement, this thesis does not only provide a mathematical model to create industrial ecology, but also a whole process that embeds this model and, when applied, leads to the implementation of industrial ecology in industry. The algorithm distinguishes 10 steps.

It has been stated before that it is not satisfying to have a single decision maker nor to consider results of decision independently of each other.

Thus, for every step there is a different leading decision maker, which is either the EIP authority as the main initiator of the optimization or one of the individual companies.

The first step contains the collection of relevant data, which is listed in Table 4.1 and classified in Figure 4.4. It is important that potentially participating companies contribute the demanded data. Without accurate data, the optimization cannot be initiated. It is essential in this stage for the EIP authority to decide which companies and plants could be possible participants. Due to the loose definition of flows, many companies from different industries should be taken into consideration.

The second step consists of the general optimization strategy pursued by a project. The target values for the mathematical optimization models and the details of the relationship between objective functions must be determined. Suitable values are crucial to the overall outcome of the optimization.

The optimization allows the trial of different strategies before starting the negotiation steps. With the determined target values, a decision about the multi-objective optimization strategy must be made in step 3. The two strategies weighting method and lexicographic ordering are suggested in Subsection 4.2.1. The weighting method allows the determination of the relative importance of objectives in relation to each other, while the lexicographic ordering requires an absolute rank. The absolute ranked order optimizes hierarchy without compromises between more than one objectives.

After the initial optimization, the EIP authority, the decision maker at this stage, must provide a pre-selection of potentially participating companies. This step can be implemented as an incremental process excluding one or more plants at a time, and is completed when all desired plants, of the initial set, are selected. This is the starting solution for the mathematical model even if there are theoretically more participants possible. This stage expresses the preference of the EIP authority towards collaborating companies and industries.

The role of the decision maker changes with the beginning of step 5. The individual negotiation partners (plant or company management) can now decide, based on the current optimal solution, how their initial provided data should be varied. This practice allows the company to investigate changes of their inputs and output without knowing no the overall objective function or individual restrictions from other companies. However, the company can discover changes of its individual situation. Values are determined after every negotiation.

The sequence of negotiations is highly relevant to the final optimal result. However, this algorithm does not dictate a certain practice. Best practices will be found after applying the tool over time. To start the negotiation with the largest companies measured by their input flow or revenue is a promising strategy suggested here. The negotiation about the input and output flow for every product contributed by a company is accomplished in step 5. Step 6 is to determine the new optimum including the additional constraints provided by the previous negotiation, and step 7 is to finally decide whether a company participates in the newly designed eco-industrial network or not.

Steps 5 to 7 are looped with all previously selected participants individually.

Under consideration of all individual preferences of companies, the model provides the optimal solution for the given data. It is the final step for the EIP authority to draft a contract for the participating companies with a total exchange matrix. The amounts determined in this contract cannot always be exactly met. It will thus be an essential part of every contract to define adjustment payments between companies.

The EIP authority and the individual companies are responsible for the last step. As an ongoing step, the review and inspection of actual streams must be part of a continuous improvement process. Especially in dynamic networks, flows and thus the optimal solutions change quickly. A permanent review is highly recommended for a long term existence of the designed eco-industrial park.

This algorithm provides a guideline for using the mathematical model developed in the previous section. Also the process and interactions of different stakeholders are required. To allow the structured proceeding of this suggested algorithm, a computer program is presented in the following section.

4.5 Computer implementation

The fifth and most relevant step for the application in practice is the implementation of the algorithm to a computer model. The basic input for completing this step is the mathematical model, including both versions of the objective function as well as the algorithm. It should be kept in mind that the implementation of an algorithm embedding a mathematical model was found to be the most suitable approach of solving the underlying problem stated in Subsection 4.1.1. The computer model supports the process that is determined by the algorithm. Figure 4.11 shows this development step.

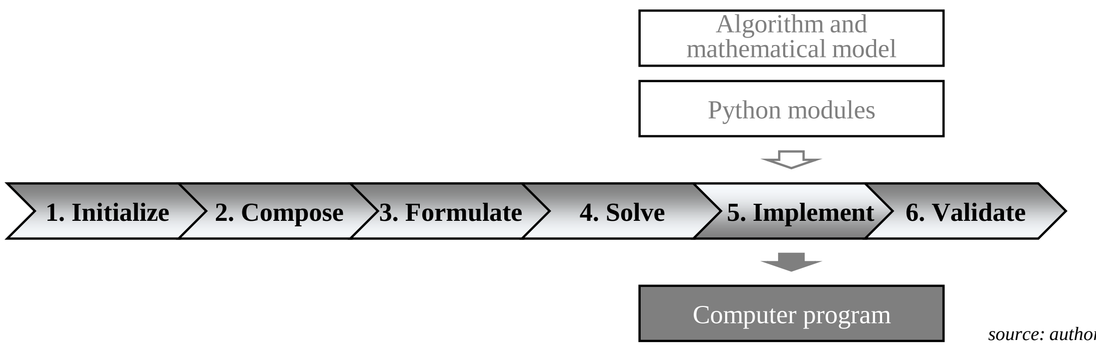

Figure 4.11: Process of developing an advanced modeling approach – step 5

The aspect of supporting an interactive optimization, user-friendliness, and visualization are emphasized due to the use of a graphical user interface (GUI).

> *"It is evident that the user interface play a crucial role in realizing interactive algorithms." (Miettinen 1999, p. 205)*

This section provides a comprehensive description of the graphical user interface that guides through the interactive optimized negotiation algorithm (4.5.1), the technical functionalities and program specific implementations (4.5.2), followed by a description of the solver specification used for the optimization (4.5.3).

4.5.1 Graphical user interface for IONA

The graphical user interface allows the decision makers to interact with the computer program and intuitively navigate through a defined process allowing it to change depending on the user's interaction (Martinez 2011). The GUI has thus been defined reflecting the previously defined ION-Algorithm. This subsection describes the general graphical user interface depicted in Figure 4.12.

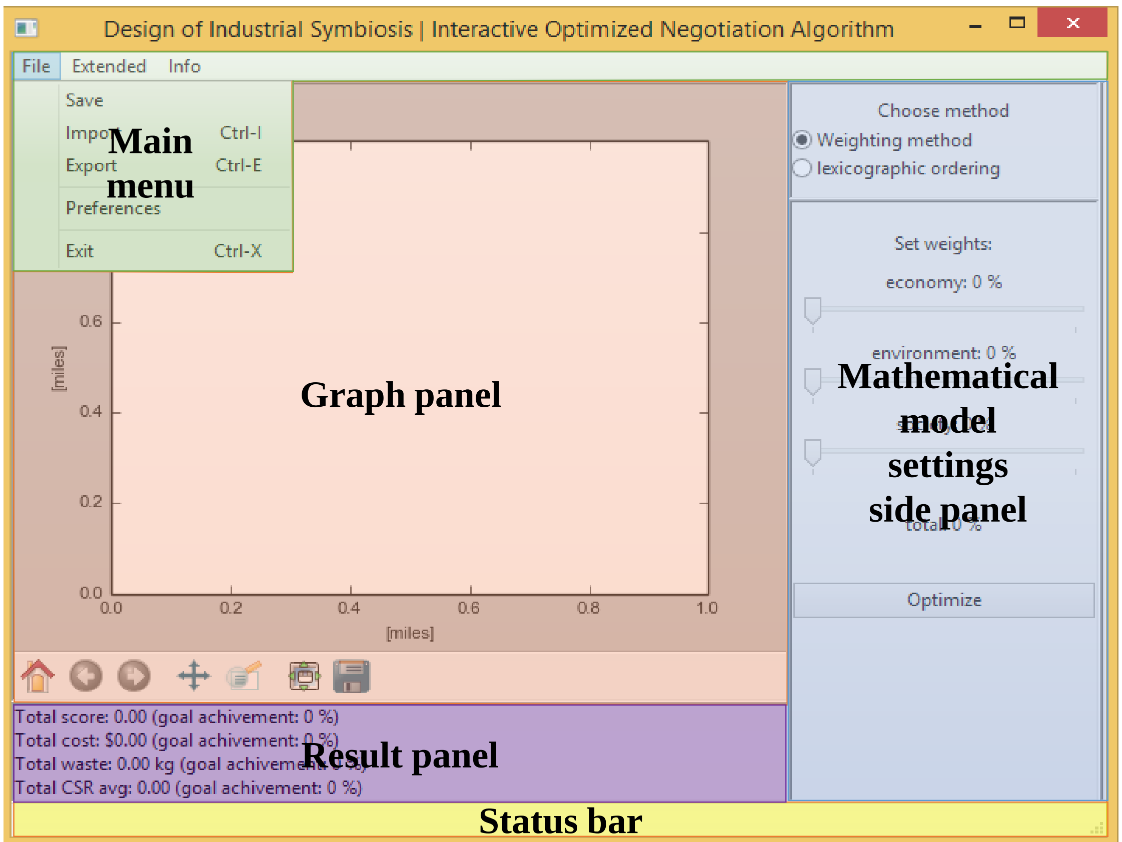

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Figure 4.12: The initial graphical user interface for IONA

The initial surface contains five different sections. The first section is the main menu. This allows the user to save the current investigation, import and export case data and results provided by the interactive optimization, set preferences, and exit the program. Extended functionalities and a user guide are accessible via the main menu at any time.

The second part is the graph panel. This section provides a plot of the results (see also the following Figure 4.13). Due to the use of the pre-defined canvas provided by an external module, a toolbar can be provided, allowing the user to zoom in and out and navigate through the plot.

In addition to the graphical representation of the results, the result panel shows main numerical results for the total achievements, costs, wastes, and the overall average CSR index achieved by the current solution. With additional optimization runs, the delta to previous results will be provided in this section.

The fourth section is the side menu. The user has to provide preferences regarding the objectives, economy, environmental, and society respectively. In order to allow absolute and relative preferences, the user can choose between the two methods weighting method and lexicographic ordering before starting the optimization.

As the fifth element, the status bar always keeps the user updated about the current activities of the program and provides guiding information throughout the whole interactive optimized negotiation algorithm.

In the following section, a step-by-step description of the guided process is provided. The negotiation algorithm starts with the initial surface shown in Figure 4.12. The figure shows subsequent steps of the program following the logic of the algorithm.

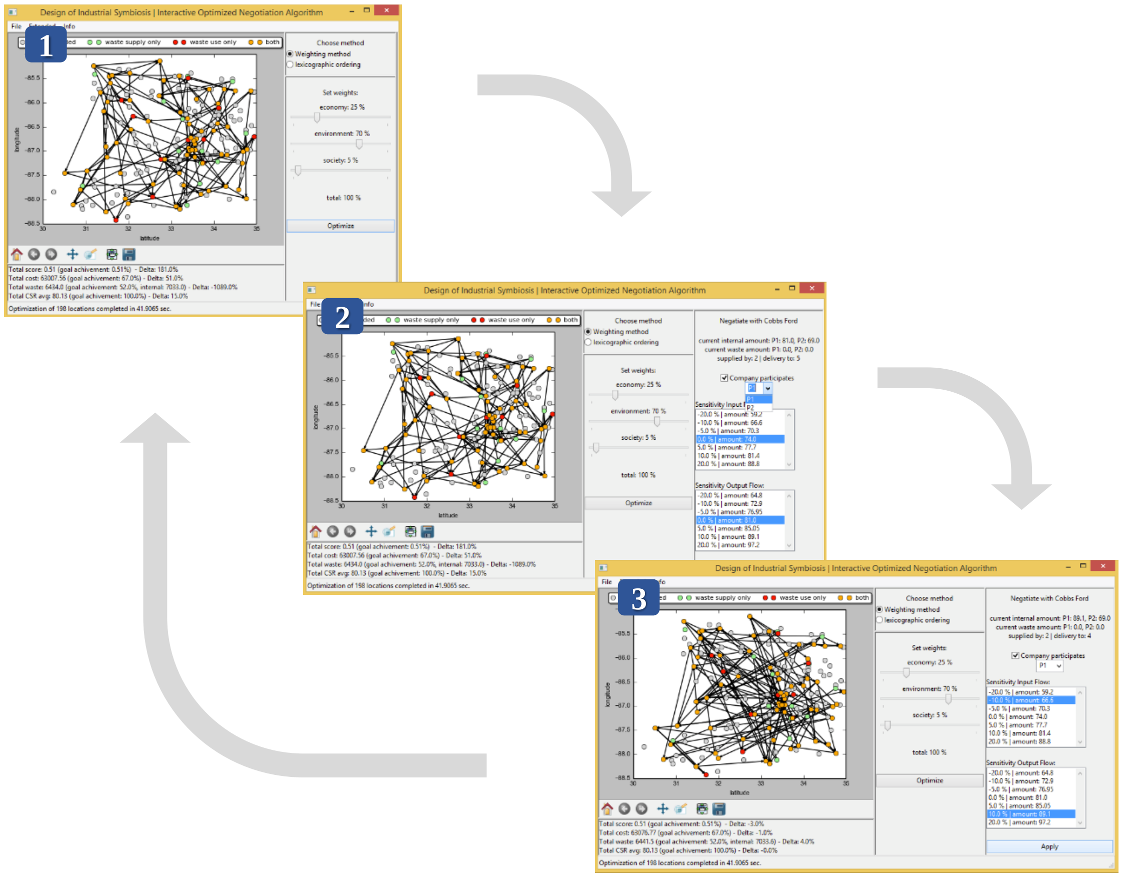

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Figure 4.13: Phases of the individual negotiation represented by the GUI

The first state in Figure 4.1 shows the situation after step 4 in the defined algorithm (see Figure 4.10). The user has chosen the weighting method and chose to set the weights to 25%, 70%, and 5% for economic targets, environmental targets, and social targets respectively. The total achievements, waste amounts, and the solution time are given in the status bar. The network is plotted in the graph panel and different colors of dots indicate if a plant is part of the optimized network, and which function (receiver, sender, or both) every location has.

The second state shows the individual negotiation step. For every location, the user clicks on a dot at the plotted network. Another section shows the name of the selected network, the current number of suppliers and demanders as well as streams within the network and total waste of each material category. The company may vary the previously declared input and output flows within certain limits. Changing the maximum input and output streams may lead to different optimal networks. These changes can be done and recalled for every participating company.

After these changes are applied, the optimal network may change. However, the previously determined negotiation results are fixed and cannot change once negotiated. An example for changing of initially supplied values can be seen in step 3 of Figure 4.13. Not only does the number of suppliers and demanding plants change due to these changes, but small changes can also have a large impact on the whole network.

This process can be seen as an interactive sensitivity analysis where every company can investigate deviations when its own behavior changes, without having to publish the complete set of data.

4.5.2 Technical structure and implementation

The surface is mainly structured in order to support the process described in the previous subsection. Independently of the GUI, the source code is structured following another logic. This subsection seeks to explain the main structure of the source code without referring to an in-depth knowledge on computer programing. The complete source code has more than 1000 lines and can thus not be provided at this point.

The first section of a program includes main parameters that allow the program output to vary. It is possible to provide both, a text output and a graphical user interface. The path of the source file for the network data and additional information are provided in this first section.

The programming language, Python, has been developed so that functionalities can be added to a program by importing external modules. This method follows the open source strategy of Python and allows users to add minor additional functionalities like the calculation of vector addition to extensive large functionalities, such as establishing a graphical user interface. Thus, the second section of the source code contains required imports, which are quickly described in the following. In general, there are three main modules illustrated in Figure 4.14.

source: author

Figure 4.14: Illustration of the interrelation of modules used to implement IONA

The main structure of the program follows the GUI package of wxPython. Using classes, methods, and predefined attributes of this class, the main Window, frames, and panels can be designed. Labels, buttons, checkboxes, radio buttons, sliders as well as dropdowns and list boxes can be created, customized, and arranged. The main frame contains the menu bar, the main panel, and the status bar. The main panel contains the graph panel, the results panel, the side panel, and the optional negotiation side panel. Elements can be hidden and actions bound to every individual element.

The graph shown in the graph panel is another import that allows exploitation of the advantages of the largest scientific package in Python called Matplotlib. Matplotlib is an extensive module allowing to plot graphs and process mathematical operations. This network model is visualized as a vector plot representing the flows between two locations, which are plotted depending on their geographical location. A toolbar allows navigation through complex networks. It provides additional functions like zooming. Further, the Matplotlib module provides an interface to wxPython, which is the largest and most applied GUI package in Python. This interface allows the user to embed graphs into wxPython GUIs. Further, it is possible to implement a picking function, which provides information about a chosen object in the graph and forwards these information to wxPython-objects.

The third and most important part of the implementation is the solver of the mathematical model using the well documented Gurobi Optimization interface. The solver takes inputs provided by the program and calculates respective results. These results can be plotted in Matplotlib graphs and later be revised by picking elements from this graph and changing values at the wxPython surface. The program supports decisions based on the applied solution method about the regarding problem.

Figure 4.14 indicates starting at the top that the visibility of a program module to the user decreases from wxPython elements through Matplotlib functionalities to the Gurobi solver module. However, while the visibility decreases, the comprehensiveness of the functionality and importance to the results increases from the top to the bottom.

Additional modules for mathematical (math) and random functions (random) are required in order to allow additional mathematical operations like determining square roots and geometrical functions.

Besides the aforementioned functionalities, this program requires a function that approximates the distance between two locations given in GPS coordinates. This function has been implemented manually. File reading and writing functions have also been implemented in order to allow import and export of network information.

4.5.3 Specifications of the solver package Gurobi Optimizer

Large mathematical models can be solved using standard optimization software or individual programming languages. Independently of the interface, solver packages have been developed that can be accessed by both standard and individual software. These solvers or solver packages are capable of processing many different solution methods like simplex and various heuristics. Developed over the last decades, the capabilities of such solver packages exceed these of the individual implementation of a single method due to variety and complexity, and are thus more efficient than programming an individual solution method.

The most commonly used solver is IBM CPLEX, which is accessible through a Python interface. However, license costs are very high compared to other solutions. The proposed model in this thesis is a linear problem and does thus not require extraordinary heuristics. Another possibility is to apply solver packages directly implemented through open source projects in Python. Examples for this are SciPy and pyOpt. However, the runtime, efficiency, and capabilities are not as advanced as those of professional solvers. Former developers of CPLEX have developed a good option called Gurobi Optimization. This solver package is entirely free for academic purposes and can easily be integrated into Python programs. The solver package provides a large documentation of predefined functionalities. Another advantage of using a non- Python based solver is that in the case of further development of the negotiation algorithm into another environment, the same solver can be continually used. It provides interfaces to all main programming languages including C++, Java, and Python.

Applying a mixed-integer linear programming problem, the standard solver output provided by the solver shows the information depicted in Figure 4.15.

The solver output provides information about the number of variables, a pre-solving process, which is automatically applied in order to reduce the solution complexity. Following up on the previous information, the solution method is described. For this linear program, a simplex is applied in order to find the optimal solution. Finally, the best objective found in the solution process is provided, including gap information referring to the determined boundaries. The solver output is specific for every solution method. The method supplied by the solver is a version of simplex method.

```
Optimize a model with 990 rows, 79398 columns and 236035 nonzeros
Presolve removed 391 rows and 54183 columns
Presolve time: 0.96s
Presolved: 1193 rows, 25413 columns, 75684 nonzeros
Loaded MIP start with objective 1
Variable types: 24621 continuous, 792 integer (792 binary)
Root relaxation: objective 4.146646e-01, 2590 iterations, 0.25 seconds

    Nodes    |    Current Node    |     Objective Bounds      |     Work
 Expl Unexpl |  Obj  Depth IntInf | Incumbent    BestBd   Gap | It/Node Time

     0     0    0.41466    0    2    1.00000    0.41466  58.5%     -    2s
H    0     0                      0.4152738    0.41466  0.15%     -    2s
H    0     0                      0.4146446    0.41464  0.00%     -    2s

Explored 0 nodes (3130 simplex iterations) in 2.53 seconds
Thread count was 1 (of 1 available processors)

Optimal solution found (tolerance 1.00e-04)
Best objective 4.146445731100e-01, best bound 4.146445731100e-01, gap 0.0%
```

Figure 4.15: Gurobi solver output provided for the mathematical model

All decision variables, constraints, and the objective function including the determined values are accessible. Additional information like runtime and number of iterations is automatically stored in the model class object.

Summary of Chapter 4. This chapter describes the development of one of the main outcome of this thesis that help to answer research question Q2: An Interactive Optimized Negotiation Algorithm (IONA) for Industrial Ecology embedding a mixed-integer linear location problem.

Considering the prior investigated requirements, the mathematical model seeks to optimize the achievement of targets for minimal transaction and purchase cost, minimal amount of waste outside of the network and maximum average CSR index of participating companies by using a minor amount of information. Without entirely publishing these information, every company can investigate its individual impact on the network. Companies can conduct a multi-way sensitivity analysis by varying input and output streams.

Current publications claim that theoretical concepts developed in order to promote industrial ecology suffer by a lack of implementation. For this reason, a flexible MILP was developed, being easily adaptable to different cases. A further result of this thesis is a computer program, which makes the algorithm developed more applicable and user-friendly. The program supports the step-by-step negotiation process between EIP authority and potentially participating companies.

Providing an optimal solution for the multi-commodity warehouse location problem, this mathematical and computational model provides a comprehensive tool to promote the implementation of industrial ecology into practice and thus to support a sustainable development initiated by the private sector. In order to prove this statement, the fifth chapter applies the findings to two case studies.

5 VALIDATION OF THE IONA APPROACH

This previous chapter proposes a mathematical model and embeds this into a computer program for the purpose of creating industrial ecology called Interactive Optimized Negotiation Algorithm (IONA). Following the suggested approach of developing a mathematical and computational model, the final step is a validation of the developed approach. Figure 5.1 depicts an overview of Chapter 5.

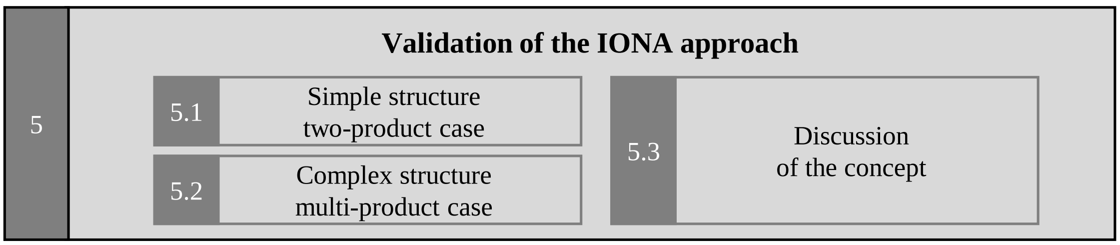

Figure 5.1: Structure of the fifth chapter

The first section, 5.1, discusses and applies a simple structured case with six companies sharing two waste materials or byproducts.

Section 5.2 investigates a more complex case study. This section does not primarily seek to provide results for a specific case. It rather provides an overview of many complex cases in order to test the flexibility of the approach.

Finally, general findings, strengths, and weaknesses of the models developed in Chapter 4 are discussed in Section 5.3. In order to process the final step of the development process, Figure 5.2 introduces required inputs and outcomes.

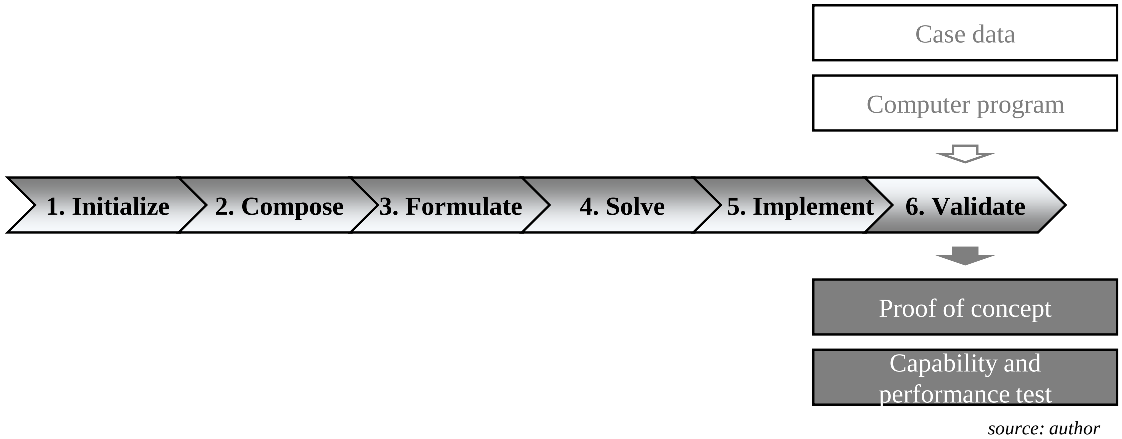

Figure 5.2: Process of developing an advanced modeling approach – step 6

For validating the proposed concept, case data is applied to the computer program. Two cases are investigated: A simple case with two products and few locations and a collection of complex cases with multiple products and locations.

While the first case provides the proof of concept, the cases in the second part investigate the capabilities of the proposed computer program. The simple case contains data and provides decisions within the limits of logical thinking: Two products and six locations with simple relationships are optimized with different preferences regarding target dimensions. The complex cases with many locations and is used to research the model performance. A main critique of promising approaches like Gu et al. (2013) and Romero and Ruiz (2014) is inflexibility. To prove the flexibility of this program, various case data is tested.

5.1 Simple structure two-product case

The simple two-product case is set up according to the investigation of recycling networks in northern Germany by Walter (2005). While the scale, units, and additional information are adapted from the data in Walter (2005), explicit data points are arbitrary. The input data is described in the following Subsection 5.1.1. Investigation of different weights for the objective function and negotiation with companies provide the exemplified test runs (Subsection 5.1.2).

5.1.1 Input data

Walter provides data for a recycling network of electronic components and thus captures more than just the exchange of utilities. Other than for the concept of industrial symbiosis, companies do not have an ambiguous role as receiver and sender. However, this set of data serves as a suitable example for estimating scales for actual data. The locations, distances, prices, and amounts are adapted from Walter (2005). However, the explicit data points are completely arbitrary and show how decisions can be made within the network. Table 5.1 shows the potentially participating companies.

Location Name	X-Coordinate	Y-Coordinate	Status	CSR index
Company A	10.00	200.00	Open	90.0
Recycling company	210.00	200.00	Open	85.0
Company B	50.00	150.00	Open	70.0
Company C	90.00	50.00	Open	80.0
Eco-industrial park B	180.00	90.00	Open	90.0
Eco-industrial park C	20.00	20.00	Planned	50.0

Table 5.1: Data of potential participants for the first case study "Proof of concept"

The table shows a mix of three companies, two eco-industrial parks and one recycling company within a radius of 265 miles. Five of the locations already exist, while one is planned for operation. For each of the locations, coordinates are given in a Cartesian form. The computer program automates the transfer from Cartesian to GPS data so that both measurements can be used interchangeable. An estimate of the corporate social responsibility index is provided in this table. The given data in Table 5.1 is public and external data, which is not difficult to access (see Subsection 4.1.2). However, an estimate of the corporate social responsibility index requires an extensive effort and can be difficult. It is important to mention that an exact value for the defined index is not required, and the determination of this value should be conducted in a similar way for every potential participant to guarantee a practical solution by applying an optimization.

Adapted from the average prices for a considered component and the capacity of recycling companies investigated by Walter (2005), Table 5.2 shows further data required. It is crucial to the concept that this set of data is not accessible by all potential participants. Even though this information is provided in a table for this case study, it can be hidden in model and not accessed by other negotiation partners, making it more likely for companies to share their internal information. The network considers two components to be flows within the network. The following table contains company internal data, which is usually difficult to access. Each company provides data for every waste material or byproduct. Companies determine the average input and output flow for a defined period of time (in this case one year). The amounts are given in metric tons and prices are estimated for one unit of the respective component.

Location Name	Input flow Product 1 [t/a]	Input flow Product 2 [t/a]	Output flow Product 1 [t/a]	Output flow Product 2 [t/a]	Price for Component 1	Price for Component 2
Company A	0.0	0.0	1200.0	850.0	$0.00	$0.00
Recycling company	2000.0	600.0	0.0	500.0	$3.00	$4.00
Company B	0.0	2000.0	500.0	800.0	$0.00	$6.00
Company C	120.0	0.0	100.0	900.0	$5.00	$0.00
Eco-industrial park B	400.0	0.0	300.0	100.0	$9.00	$0.00
Eco-industrial park C	0.0	0.0	5000.0	3000.0	$0.00	$0.00
Transport rate	-	-	-	-	$0.05	$0.06
Market	-	-	-	-	$8.00	$6.50
Total Σ	2520.0	2600.0	7100.0	6150.0	-	-

Table 5.2: Internal and external data required for the "Proof of concept"

Besides the information provided by the company, external information must be researched by the EIP authority, i.e. transport rate within the network per unit and market prices for disposal. Market prices can be zero if a waste can be disposed for no cost. However, this case should not be considered in this model since the main purpose is to reduce and eliminate waste and thus companies should be accounted for any kind of output. If a component is sold at the market, prices can be negative. Inputting this minor amount of data into the model, follow up negotiation steps and a general optimization can be initiated and improvements achieved.

The optimization of the model proceeds in regards to an achievement function. Target values for each objective must be defined properly. Following the suggestions in Subsection 4.3.2, the target values in this case are defined as:

$$t_{b,1}^{*}, = max\{8.00, 6.50\} * (7{,}100 + 6{,}150) = \$106{,}000 \tag{5.1}$$

$$t_{e}^{*}, = 7100 + 6150 = 13{,}250\ t/a \tag{5.2}$$

$$t_{s}^{*}, = 80.0 > \frac{90.0 + 85.0 + 70.0 + 80.0 + 90.0 + 50.0}{6} = 77.0 \tag{5.3}$$

Equation (5.1) shows the first economic target value. This model does not consider setup costs or incentives for participating companies. Thus, the second business target value is zero. However, the first target value is defined to be the maximum possible savings due to disposal within the network instead of outside the network. Savings are determined by the product of the total amount of output flow over all locations and the maximum market price. This value could theoretically achievement if every output flow was disposed for no transportation and operation cost (prices of receiving companies), assuming that every output was of the type with the most expensive market price.

The environmental target value is defined as the total amount of waste and byproducts coming out of the locations (equation 5.2). This target can be utopian. In order to create a more accurate and achievable target value, a waste reduction of a certain percentage could be pursued. This case pursues a waste reduction of 100%.

The target for corporate social responsibility should be determined due to the purpose and achievements of the planned eco-industrial network. It is suggested to choose a value which is slightly above the average value of the whole set of data. For this case, the value of 80.0 was found to be a good achievement as stated by equation (5.3).

Based on the provided set of data, the computer program, the implementation of the algorithm described in Section 4.4 and embedding the mathematical model developed in Section 4.3 is applied. Exemplified results from using this program are described in the following Subsection, 5.1.2.

5.1.2 Optimization and negotiation results

The computer program supports the whole process of IONA. This section summarizes major findings of applying the above-described case data to the algorithm and program.

Finding of initial optimization. As an initial step, the behavior of the system can be researched by setting up different preference scenarios. The scenarios and the resulting graphs are shown in Figure 5.3.

The figure shows the vector of the target weights with the weight for the achievement of the economic, environmental, and social objectives respectively. The results show how the network changes due to a variation of target weights.

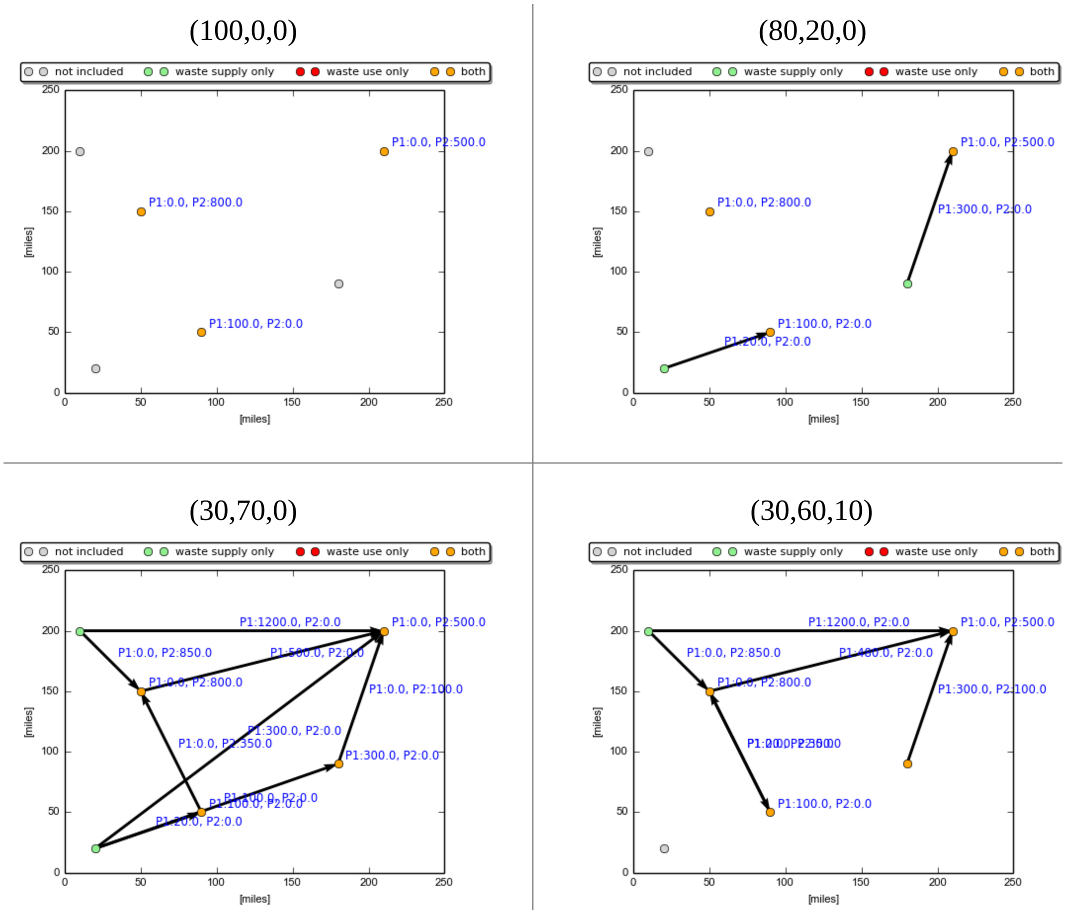

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Figure 5.3: Resulting network of four different weighting vectors scenarios

Other than the original warehouse location problem, this model does not contain demands to be satisfied. If the economic dimension is weighted by 100%, it is not worth transporting anything at all within the network (Figure 5.3, left top). However, three companies show it is the best economic decision for them to treat waste themselves up to the total capacity. The other plants should dispose their whole output to the market price. A network does not exist under these conditions. The score of a solution relates to the previously set goals. Even though the achievement of the environmental dimension is 11.0%, the total score of this solution is at 98.0 %.

The average CSR index is 78.3 and slightly above the total average of 77.0 for all plants.

With an increasing relevance of the environmental dimension, additional links between two plants show up in order to reduce waste due to internal treatment of other network partners. Additional members join the network.

Since the optimization considers the least amount of plants as is necessary, the network grows from the second scenario from three to four members. Even more savings are possible. Additional network partners achieve an increase of 3.0% compared to the previous solution. This results in a decrease of the average CSR index down to 75.0.

In contrast, scenario 3 puts the main focus on the environmental targets resulting in a large network with a total of all six considered plants. The increase of considered plants leads to an increase of savings, even though the relevance of economic goals has been lowered. The high relevance leads to a significant decrease of waste from 11,530.0 t/a down to 8,130.0 t/a, which corresponds to a 26.0 % increase of achieving the goal of zero waste.

Introducing the third dimension of social sustainability, the network changes in scenario 4 towards a higher average of the CSR index. The social goal is now overachieved at 104.0 % with an average index of 83.0. However, accounting the social objective by 10% leads to a decrease of savings to $108,067.8 (-3.0 % goal achievement) and an increase of total waste to 8,550.0 t/a (-4.0 % goal achievement).

Table 5.3 summarizes the major outcomes of the four scenarios. The full solver output and numbers for decision variables are provided in the appendices.

Scenario		Score	Savings [$]	Waste [t/a]	CSR index
Scenario 1 (100,0,0)	**Total**	0.98	94825.0	11850	78.3
	Goal achievement	98.0 %	89.0 %	11.0 %	98.0 %
	Delta to previous	0.0 %	0.0 %	0.0 %	0.0 %
Scenario 2 (80,20,0)	**Total**	0.96	95051.4	11530.0	75.0
	Goal achievement	0.96 %	90.0 %	13.0 %	94.0 %
	Delta to previous	-2.0 %	+1.0 %	+3.0 %	-4.0 %
Scenario 3 (30,70,0)	**Total**	0.77	111592.5	8130.0	77.5
	Goal achievement	77.0 %	105.0 %	39.0 %	97.0 %
	Delta to previous	-19.0 %	+15.0 %	+26.0 %	+3.0 %
Scenario 4 (30,60,10)	**Total**	0.70	108067.6	8550.0	83.0
	Goal achievement	70.0 %	102.0 %	35.0 %	104.0 %
	Delta to previous	-9.0 %	-3.0 %	-4.0 %	+7.0 %

Table 5.3: Numerical results to the four initial optimization scenarios

Findings of a negotiation. Building up on this initial solution for a new designed EIN, negotiations can begin. Figure 5.4 shows changes of the network when a negotiation step is conducted with the recycling company as a representative example. The depicted case shows how the network changes when the recycling company reduces its initially stated capacity for waste or byproduct “P1” from 2,000 t/a to 1,600 t/a. The company still serves all four suppliers, including itself, as before. However, in order to reduce waste, company C now ships an amount of 80 t/a to eco-industrial park B. In addition to company C, the eco-industrial park B is impacted too. Now, the park does not ship its waste product “P1” to the recycling company, but recycles itself instead.

This leads to a total increase of cost of $472.00 for the total network.

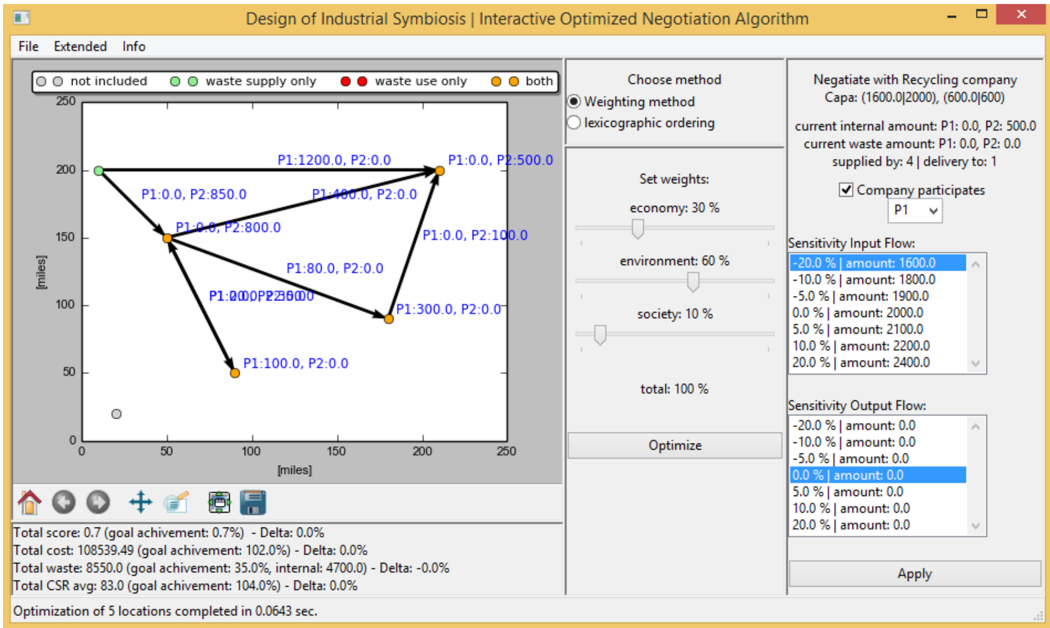

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Figure 5.4: Negotiation of reducing the initial capacity of the recycling company

In order to support decisions regarding industrial ecology, the decision variables leading to the provided objective of the achievement functions have to be translated back into real world decisions. After negotiation with participating companies, a network contract must be set up to establish a common and binding basis. The contract contains sections about contents exemplified by the following phrases:

- The information provided to optimize the network is not shared in its pure form with other potential participants and is thus hidden in the model.
- The network partners Company A, Company B, Company C, Eco-Industrial Park A, Eco-Industrial Park B, and Recycling Company agree to collaborate for the duration of at least five years.
- Company C provides the recycling company with a total amount of 400 t/a. A deviation from this amount is penalized with a rate of $x per t/a.

As a proof of concept, this simple two-product case has shown that the computer program can successfully be applied to create a new eco-industrial network. The following section provides testing of behavior and capabilities of the mathematical model and computer program when applying larger sets of data.

5.2 Complex structure multi-product case

The applied data in the previous case exemplifies the application of the computer implemented IONA to practical data. However, the complexity of data could be handled without computer support. With an increase of potential locations and types of material or components included, the model becomes more complex, and computer support is required. While Section 5.1 proves the feasibility of using the approach for practical purposes under the provided assumptions, this section provides studies of the properties, capabilities, and flexibility of both the mathematical model and computer program. The individual data points generated for testing are described in Subsection 5.2.1. The results of test runs are depicted and described in Subsection 5.2.2. The investigations include model scope, specific phenomena, and runtimes.

5.2.1 Input data

In order to investigate the properties and capabilities of the model and program, numerous sets of data must be considered collectively. These sets of data have not yet been collected nor researched. Hence, sets of random data must be generated. For this purpose in addition to the data given by Walter (2005), a collection of 3,173,958 sets of data serves as the basis for generating potential locations. The open-source data base

GeoLite2 Data for worldwide geographical data is provided by the company MaxMind and includes data of many countries and almost every city in the United States (MaxMind 2014). This set of data allows a biased generation of random locations for participants. This biased generation is even more practical relevant than completely random data. Out of this data set, 3,598 cities in the United States with a population of over 10,000 people are selected. Depending on the population, which ranges from 10,003 to 8,107,916, the shared amounts of products are generated biased but randomly. Bigger cities indicate bigger companies or EIPs. However, the type of participant, e.g. manufacturing company, recycling company, or EIP that exists is irrelevant to the following cases. For this purpose, a random data generator has been developed. The source code and an exemplified output protocol are appended. Due to the extensive amount of data points, the full data is not provided in this work. The generator requires the desired number of locations and products, then randomly generates all desired data for an optimization case study. The scenarios randomly generated by means of the generator for the computer program are described in Table 5.4 and Table 5.5.

Set of data	Avg. Distance	Avg. Input flow	Avg. Output flow	Avg. Product price n	Avg. Product price m	Avg. CSR index
Scenario 100-2	1123.69	238.98	222.50	4.03	6.00	70.2
Scenario 200-2	1075.41	269.45	259.49	3.97	6.50	69.3
Scenario 300-2	1078.30	196.96	218.34	4.01	5.50	70.3
Scenario 400-2	1070.22	213.36	222.87	3.95	8.00	68.9
Scenario 500-2	1104.29	213.42	216.07	3.97	5.50	69.8

Table 5.4: Generated data with a variation of the number of locations

The tables show the average values calculated from the random sets of data for each of the ten considered scenarios. Table 5.4 shows the first five exemplified cases generated with a variation of the number of locations. Every scenario considers two products. While the first scenario consists of 100 locations, the next four scenarios contain additional 100 locations, up to 500 locations for scenario five (Scenario 500-2).

Set of data	Avg. Distance	Avg. Input flow	Avg. Output flow	Avg. Product price n	Avg. Product price m	Avg. CSR index
Scenario 100-2	1123.69	238.98	222.50	4.03	6.00	70.2
Scenario 100-4	1123.69	200.95	234.13	3.96	5.75	69.3
Scenario 100-6	1123.69	257.31	232.30	3.98	6.83	69.7
Scenario 100-8	1123.69	237.68	228.78	3.96	6.75	67.0
Scenario 100-10	1123.69	231.98	236.32	4.04	6.20	69.7

Table 5.5: Generated data with a variation of the number of flow types

The number of locations is constant for every case shown in Table 5.5. These five scenarios vary by the number of flow type changes with an increase interval of two from 2 to 10. The average input flows and output flows over all locations and flow types are also provided as average distances between and CSR indices of locations for all ten randomly generated cases. The average distance is given in miles. The mostly uniform distributed data does not show any systematic deviations or patterns. The average distance for the cases with a variation in flow types is only expected to be the same due to the consideration of the same locations. For further investigation on the randomness of data, a Diehard test can be applied (Marsaglia 1998, L'Ecuyer 1992). However, this thesis focuses on the processing and output of the provided data.

Every scenario is named following the scheme: “Scenario”, number of locations, dash “-“, and number of flow types. Test runs are made for each of these ten scenarios. The test machine was an Intel Duo Core processor (1.86 Ghz) with a total memory of 1 GB running Windows 8 in 32-bit-mode. A configuration of a common personal computer ranges between 4 and 16GB. Different results are expected depending on the machine.

5.2.2 Properties and capability of the approach

The examples for case studies are used to conduct the IONA approach. This section describes the outcome of applying the optimization to the ten previously generated sets of data. The results are summarized for two perspectives. At first, the resulting network properties and average values of the numerical input of the program processed is described and discussed. Following this input- or content-related description, implementation-related aspects are researched. The program behavior and the reaction of the program to certain parameters is studied by varying properties of input data sets.

General findings are discussed in the following section (5.3). This subsection focuses on the program behavior and capabilities rather than on individual data and is thus a performance-related study.

Content-related findings. The findings for the ten conducted studies are shown in Table 5.6 and Table 5.7 for the variation of the number of locations and flow types respectively. To summarize the results, the number of participating locations, connections between network partners and avoided waste due to establishing industrial ecology are provided in absolute and relative values. Other than in the previous case, only one setting of weights will be applied to all ten cases, which consists of 20%, 75%, and 5% for the economic, environmental, and social dimension respectively.

Set of data	Total open Open vs. Total number			Total connections of total possible in the network			% of waste avoided		
Scenario 100-2	70.0 | 100	100	70%	221	200	110%	5685.05	44500.41	13%
Scenario 200-2	116.0 | 200	200	58%	361	400	90%	24724.24	103794.55	24%
Scenario 300-2	173.0 | 300	300	58%	523	600	87%	45049.93	131005.88	34%
Scenario 400-2	216.0 | 400	400	54%	633	700	79%	64114.87	178294.84	36%
Scenario 500-2	282.0 | 500	500	56%	882	1000	88%	69750.29	216066.20	32%

Table 5.6: Content-related results five cases with a different number of locations

This table shows different results when varying the number of potential participants of an eco-industrial network. The total number of participating relationships ranges from 70% down to 54% of all considered locations. There is a tendency of a decreasing percentage of participants included in the optimal network with an exception of scenario 400-2. The individual decision for a certain company as well as the determined flow amounts are too extensive to be provided in this work. However, the total number of connections between two locations has been determined for all case studies. A connection is counted if the material flow between two companies is greater than zero. The total possible number of connections can be determined by squaring the number of locations and multiplying it with the number of products ($n^2 * k$). Since it is not pursued for one company to collaborate with all of the included participants, the definition of the maximum amount will be for a company to cooperate with one other company

($n * 1 * k$). Since it is still possible for companies to cooperate with more than one other company, this relative value of the total number of connections and possible connections can exceed 100%. Table 5.6 shows that the relative value for this is decreasing with an increasing number of potential locations. Even though the relative number of participating companies and collaborations decreases with an increase of locations, the percentage of waste avoided due to collaboration tends to increase.

Set of data	Total open Open vs. Total number			Total connections of total possible in the network			% of waste avoided		
Scenario 100-2	70.0	100	70%	221	200	110%	5685.05	44500.41	13%
Scenario 100-4	65.0	100	33%	396	400	99%	26862.98	93651.77	29%
Scenario 100-6	69.0	100	23%	647	600	108%	19612.63	139379.70	14%
Scenario 100-8	59.0	100	15%	712	800	89%	39362.89	183021.90	22%
Scenario 100-10	74.0	100	15%	1153	1000	115%	39065.56	236321.71	17%

Table 5.7: Content-related results five cases with a different number of products

Similar to the previously described five cases, the relative number of participants out of all potential participants in the optimized eco-industrial network decreases with an increase of products. A reason for this could be that more companies can receive different types of flow material and thus fewer locations are required to avoid waste. It is interesting to observe that the total number of connection is not diminishing with an increase of material types considered in the network.

A weak tendency shows between the relative value for number of connections between locations and the avoided waste. The table shows that the higher the relative number of connections between locations in the network is, the less waste comes out of the system. This can be rationally explained by the fact that once a location is participating in the network, it emits all the output flows. The more companies there are to receive the output flow, the less waste is emitted by the system eventually.

Performance related findings. While applying the IONA approach to the randomly generated data, information about the program processing and solution process has been collected. From this information, the impact of the properties of the set of input data, e.g. number of locations and number of products, on the computer program can be assessed. For this purpose, properties of the mathematical program, such as number of variables and constraints, are provided as well as running times and iterations required. Table 5.8 and 5.9 show the information collected during the tests for the five cases with a variation of the number of locations and products respectively.

Set of data	Number of variables	Number of binaries	Number of constraints	Total Runtime	Solver time	Pro-cessing time	Simplex iterations	Non-zeros
Scenario 100-2	20500	300	800	4.195	1.564	2.631	3668	60466
Scenario 200-2	81000	600	1600	222.78	211.648	11.134	229534	240917
Scenario 300-2	181500	900	2400	234.048	211.582	22.466	160256	541365
Scenario 400-2	322000	1200	3200	491.900	438.378	53.522	89929	961857
Scenario 500-2	502500	1500	40000	320.570	254.246	66.325	12674	1502331

Table 5.8: Performance related information collected during the IONA (part 1)

Set of data	Number of variables	Number of binaries	Number of constraints	Total Runtime	Solver time	Pro-cessing time	Simplex iterations	Non-zeros
Scenario 100-2	20500	300	800	4.195	1.564	2.631	3668	60466
Scenario 100-4	40700	300	1200	6.872	2.102	4.770	2519	120817
Scenario 100-6	60900	300	1600	17.073	9.606	7.467	5957	181202
Scenario 100-8	81100	300	2000	153.222	143.751	9.471	266282	241549
Scenario 100-10	101300	300	2400	325.560	313.459	12.101	428312	301927

Table 5.9: Performance related information collected during the IONA (part 2)

The table shows the number of variables, constraints, runtime, iterations, and non-zero parameters of each of the ten conducted test cases. The number of variables for increasing number of locations grows exponentially while the number of variables with an increase of products increases linearly. The number of constraints grows linearly for both cases. The exact number of variables can be calculated as follows:

$$I * I * K + I * K + 3 * I = I^2 * K + I * (K + 3) \tag{5.1}$$

Equation (5.1) shows the mathematical proof for exponential growth of the model with an increase in the number of locations I. The number of decision variables related to the material type appears with no higher exponent than one and does thus not contribute to an exponential growth of the model. The same mathematical proof can be given for the growth of the set of constraints with an increase of locations or material types:

$$3 * I + 2 * K * I + I = I * (4 + 2K) \tag{5.2}$$

Formula (5.2) shows that the cardinality of the set of locations as well as material types do not have an exponential impact on the model size.

Besides the size of the mathematical model, the runtime is an important performance measure and aspect to assess the model. Total runtime consists of two elements, the time required by the solver to solve the mathematical model and the processing time for the program to process parameter and array. The total runtime is thus the sum of solver time and processing time. Tables 5.8 and 5.9 show the runtimes grow exponentially in both variation of locations and variation of material types. However, the processing time shows a lower increase rate than the solution time. Furthermore, a strict increase of the solution time with an increase of locations or material types cannot always be observed. Some problems require a much longer solution time (such as scenario 400-2) while others are solved quicker than expected (scenario 500-2). The processing time and the number of simplex iterations increase strictly with an increasing complexity of the problem. However, the number of simplex iteration does not correlate with the solver time. While the solving time can be limited by a number of iterations or a time constraint, the processing time is limited by the available memory space. On the test machine with 1GB memory, cases with 1000 locations and higher and two products cannot be proceeded due to a lack of memory.

Conducting the simplex algorithm usually contains many zero-coefficients in the model. The higher the number of zeros is, the more calculation can be skipped due to the property of zero to equal zero after multiplication with any real number. Thus, a high number of non-zero coefficients indicates that a high capacity for calculations is required. The non-zeros grow exponentially for the first five cases and linearly for the second five cases investigated and illustrated in Table 5.8 and 5.9 respectively.

This subsection seeks to explain the results of applying the generated data to the computer program. Interpretations of the outcomes of the two case studies conducted in Section 5.1 and 5.2 and general findings on the IONA approach are described and derived in Section 5.3.

5.3 Discussion of the concept

The outcomes of the case studies conducted in the previous sections of this chapter study the previously developed IONA approach and apply it to sets of practical relevant data. In order to summarize general findings of the experiments conducted with the IONA and emphasize the scope of application, this section discusses the concept. Followed by general findings for both the mathematical model and the computer program in Subsection 5.3.1, Subsection 5.3.2 derives strengths and weaknesses of this approach. Subsection 5.3.3 closes with an assessment of the approach using the evaluation framework developed in Chapter 3.

5.3.1 General findings

This subsection distinguishes general findings regarding the mathematical model on one side and the algorithm and its computer implementation embedding the mathematical model on the other side.

Mathematical model. The mixed-integer linear model is based on the main idea of a multi-commodity network and the facility location problem. It is a promising approach due to its flexibility regarding additional constraints, different measures of variables and parameters, and diversity of flow types. Findings do not necessarily need to lead to an eco-industrial network but can also support the establishment and investigation of bilateral or multilateral industrial symbiosis relationships between companies. With the main objective of promoting a tool for developing and promoting industrial ecology, this mathematical model can be applied to many cases.

> *The core of decision making in the field of industrial ecology is found to be highly related to strategic location decision problems.*

A main disadvantage of many multi-objective optimization methods is that the suggested solution algorithms are only applicable for a specific problem and are very inflexible and difficult to adapt to other problems. Since this model is based on a linear goal programming approach, it can be easily adapted for different problems around the field of industrial ecology. When distances are small enough, the resulting networks are eco-industrial parks. Data of existing as well as planned locations can be included.

Extensions for recycling rates and other limitations or requirements can easily be introduced as an additional set of constraint(s). Since a monetized value for accounting factors in the objective function is unnecessary, other economic, environmental, and social targets can be included. For instance, instead of using the CSR index for every company as a social measure, any other numerical information representing a social aspect can be included. The number of jobs provided in an area could serve as a replacement for the CSR index. However, it is necessary to assess all potentially participating companies through the same measure.

Without applying the step of negotiation, the mathematical model can be used for both the improvement of existing systems as well as the creation of new eco-industrial parks and networks. The objective function is structured in a way that achievements of a goal can be overachieved or never achieved depending on the provided target values. The optimization results are highly sensitive to the target values. It follows the rule that a less utopian target value is more sensitive to the respective goal dimension. Maximizing flows in this network could be an alternative objective to be pursued with this model.

The study of arbitrary examples shows that with an increase of social objectives, the networks become smaller. Since the economic objective seeks to reduce transaction cost, the minimum cost considered separately would result from no exchange activity. It is thus crucial to the network that a general interest for at least two out of the three objectives, i.e. economic, environmental, and social, is available and improvement desired by the decision makers. The model can further account for different scenarios regarding the flow types. Flows can be sold to the market when prices are negative, or disposed to the market when prices are positive values. In some cases, emissions still do not cost any money, especially in the United States. Artificial disposal market prices may be introduced for the purpose of optimization.

Assumptions for the model are described in Subsection 4.3.1. Some assumptions are more intuitive than others. Assuming completely deterministic circumstances is an example for a critical assumption. The model is based on the idea that transaction costs can be reduced within a permanently established network in contrast to the costs and prices offered at the market. It has not been investigated in literature whether or not this is the case. However, it is accurate since a higher forecast reliability leads to a reduction of costs for both sender and receiver of a transaction.

Optimization provides the best results of all solutions. There is a chance that the real world data may vary from the initially provided data. In these cases, the optimal solution provided by the program can actually be a decision with negative consequences for all network partners. Small changes in data can have large impacts on the results.

The network resulting from the optimization can contain locations that send out material, locations that receive material and locations that do both. Industrial ecology and industrial symbiosis require companies that mutually exchange materials. However, in a real world problem, it may be desirable to include large companies that either send or receive manufacturing or recycling companies' materials. This allows a larger amount of waste materials and byproducts to flow through the network and additionally reduces the transaction cost (see drivers of developing an EIP in Section 2.2.4).

Economy of scale is an essential aspect of an eco-industrial park or network. Modeling approaches are suggested in Subsection 4.3.5. Further, El-Haggar (2007) and Tudor et al. (2007) support this finding and state successful examples of eco industrial parks and networks which show one main, leading company. The goal programming approach combined with achievement functions allows the simultaneous optimization of many goals with measured in different units and magnitudes. However, this has not been implemented for the different material types. While some material types with a huge greenhouse potential only occur in small amounts (milligrams), others occur in large amounts (metric tons). All materials are thus accounted on the same basis. This leads to neglecting smaller amounts. Many approaches face the problem of different impacts of emissions on the environment. One possibility is to measure, normalize, and standardize the impact of a certain amount to a reference material. This has been done with plenty of greenhouse gases in relationship to carbon dioxide (Wiedmann and Minx 2008). The model also seeks to reduce distances as a part of the environmental objective. An example for why this is necessary can be provided by recent examples showing that from the economic perspective the recycling of certain materials is actually profitable when shipped abroad and imported as recycled material. During this process, many tons of greenhouse relevant gases are emitted, which does not lead to sustainable recycling approaches. To avoid this phenomenon, the distances should be as minimal as possible.

Computer program. In addition to the mathematical model developed to support decisions embedded into the negotiation algorithm, the algorithm itself and the computer program show some general characteristics to be discussed.

An important aspect of this approach is that it provides optimal decisions for participants of the resulting network without publishing all the information. Most of the information is hidden in the model and will not be accessible to any of the potential decision makers. This property makes it more likely for companies to provide internal information. The tool can further be used to plan fictional networks or already existing locations, or even a mix of both philosophies. Location decisions can thus be supported.

The developed IONA approach promotes multi-objective multi-participant decision making without publishing internal data, making it more likely for companies to participate in an EIP project.

It is crucial for a successful approach of interactive multi-objective optimization to provide a graphical user interface in order to support the decision making process (Miettinen 1999). Providing a graphic user interface can also lead to biased behavior of the decision makers. In this implementation, the decision maker decides the weights of objective dimensions in a subsequent process, choosing first the economic weight, then the environmental weight, and finally social weight. This may lead to the fact that the social dimension is only set as a result of the previous two dimensions. The user may prioritize preferences depending on the GUI layout. Being aware of this biased behavior, the target value for the social objective is set to an achievable value in order to make the optimization sensitive to this goal even if it is not considered to be highly relevant.

A solution to this biased behavior is a method where the user chooses all three dimensions simultaneously. This can be technically implemented by a triangle selector instead of a slider element as depicted in Figure 5.5.

source: author

Figure 5.5: Representing relative relevance of objective dimensions as a triangle

However, this programming intensive triangular relationship requires further review.

Some general patterns were found while investigating the runtime of the optimization. The more objective dimensions taken into consideration (weights greater than zero), the longer the solution process. The introduction of social targets especially led to an increase of the runtime. The processing time is a significant factor.

Another critical assumption for the IONA approach is that companies can receive and send only a determined amount of different types of flows and that these are independent to each other. This is not always given in real world problems. The production of many waste materials or byproducts can be coupled. Further, it has not been taken into consideration that companies can run their activities at different levels. The determination of the optimum could also relate to every waste producing activity at an activity level independent of the respective plants.

The solver’s output shows that a current best value close to the final best solution is often found after just a fraction of the total number of iterations and in a short runtime. An approach could thus be to interrupt the solution process after a certain amount of time and take the current solution as a non-optimal solution. The problem with this proceeding is that it is difficult to determine how good the solution is, and the result after a time-based or iteration-based interruption can be non-optimal and often bad.

General Characteristics. The threshold for companies to join an eco-industrial park is very high. Despite minor economic benefits, companies cannot, or only with much effort, assess long term benefits of such projects. In fact, the largest benefits occur for the environment and local communities. It is thus crucial to the concept to lower the entry barrier as much as possible.

> *A central and independent EIP authority or network management accounting for all planning efforts and a low risk for participants due to a minimum of internal information to be shared by companies has a significant positive influence on the practical establishment of industrial ecology.*

5.3.2 Strengths and weaknesses

This subsection summarizes main strengths and weaknesses of the IONA approach. Some of the outstanding characteristics and development potentials of this approach have already been mentioned in the previous subsection. All strengths and weaknesses are collectively illustrated in Figure 5.6.

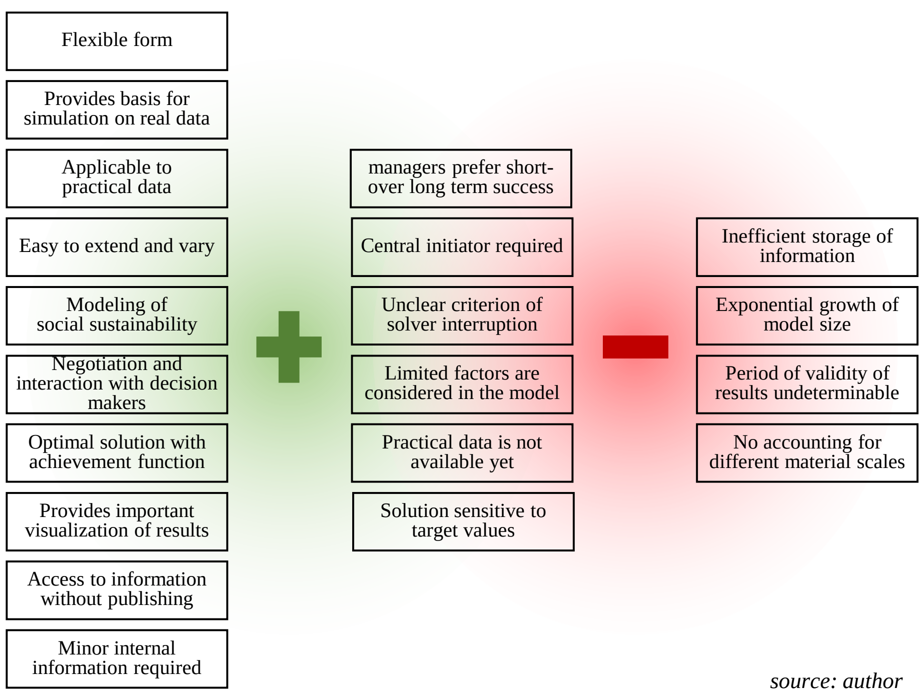

Figure 5.6: Strengths and weaknesses of IONA

Some strengths lead to advantages of this approach in contrary to other approaches investigated in Chapter 3. Some properties can be strengths and weaknesses of this approach depending on the point of view. Some aspects leave space to further develop.

The flexible form of the algorithm allows the application of this methodology too many different scenarios. Manufacturing, recycling, and service companies can simultaneously be considered along with other eco-industrial parks.

The subject types considered to flow through the network are not limited to materials but can represent intangible subjects such as energy or even information. A standardized unit should be decided. The difference between an eco-industrial park and an eco-industrial network is only expressed by the geographic proximity of locations. If distances are short, the result will be an eco-industrial park. In this situation, it is more likely that planned locations are considered rather than existing locations.

After optimizing, a criterion for selecting participating companies could be that only companies sharing more than x different flow types are part of the new eco-industrial network. The algorithm requires a central initializing subject such as an EIN authority or management. This leads to a good centralized decision including much information. In contrast, such an initiator always requires additional expenses, which make it even more difficult to economically justify the introduction of industrial ecology. An independent and central initiator further allows implementation of this approach without publishing individual company information. The initiator will collect all the information from different companies and accomplish an optimization. The other participating companies will not receive any information about individual company data. Information is hidden in the model and not explicitly accessible. If the exact data cannot be determined for a network, the random data generator can be set up with the respective parameters or an existing network can be investigated. Applying the randomly generated data or data about an existing network to the computer program with different weights, changes within the network, depending on different relevance of the three dimensions of sustainable development, can be investigated. The behavior of network partners can thus be simulated by means of this program.

A major critique of an optimization approach in general is the reliability of the solution when input data varies. The MILP in this study is not dynamic and thus very sensitive to changing input data. The long-term validity of the solution is questionable. The approach further contains many decision variables, which lead to a rather inefficient algorithm. The required CSR index is complex and costly. However, once determined, the CSR index as a measure for participating companies is a solid indicator for sustainable development as well as economic success in the long run. The concept further allows the exchange of the CSR index with another measure for a location-individual performance indicator with minor changes of the model. However, most managers in decision-making positions still have interest in short term success.

In order to set up a useful and applicable model, some information such as customer loyalty, are not included. Furthermore, the actual statement of a percentage of relevance of an objective dimension is not clearly defined. Once weighted as a relevant factor in the model, the impact highly depends on the target value provided for a model. The concept of storage is inefficient due to many zeros in auxiliary arrays. Besides inefficiency, the approach of optimization has a general disadvantage. If the input data lacks certainty, no forecast about the accuracy of the results can be made. The optimal solution can result in a decision inefficient exchange flows. While studying the two provided case studies in Section 5.1 and 5.2 the large number of occurring zeroes in the arrays were a conspicuous for inefficient structures.

5.3.3 Evaluation of IONA

Using the evaluation framework developed in Chapter 3, the Interactive Optimized Negotiation Algorithm developed in Chapter 4 is evaluated in this subsection.

IONA provides an approach for the consideration of all three dimensions of sustainable development simultaneously in an optimization. The decision maker determines the relative or absolute relevance of each objective dimension. Optimizing a network of many locations and many tangible and intangible flows as part of a negotiation algorithm allows the EIP authority, as well as every potential participant, to influence the optimal solution.

Further, additional constraints can easily be added in order to represent legal or public concerns, such as recycling rates or minimal and maximum local output. Many stakeholders are taken into consideration for every decision made regarding the potential network. While negotiating, companies can conduct an interactive sensitivity analysis and see the variation of their situation due to a change of input/output behavior. Thus, a level of uncertainty can be studied before applying the optimal solution determined by the program.

With a minimal amount of internal data, new eco-industrial parks and networks can be set up using this approach. Planned and existing facilities can be taken into consideration. Already existing links in the network can be included in the optimization as additional constraints. The IONA thus allows to develop entirely new eco-industrial parks and networks, or even industrial symbiosis relationships. It further allows to consider current system properties and thus to improve existing industrial ecology.

The evaluation framework is completely fulfilled by the proposed IONA approach.

Summary of chapter 5. Chapter 5 describes the application of the computer program, including the previously developed algorithm and embedded mathematical model, to specific case data. These result in two major outcomes:

The first outcome due to the application of a simple two-product case is the proof of concept. This case study shows that the IONA can be applied to data adapted from a recycling network. The optimization with different preferences on goals and individual negotiation steps guide through decision-making for EIP establishment.

The second outcome is a comprehensive test on the properties and capabilities of the computer program. Arbitrary case data for up to 500 locations and up to 10 different flow types have been investigated. Even though higher solution times were found with more locations and flow types, the tests were limited by the memory of the machine.

Discussing the approach, it was found that the model could be applied under flexible circumstances. Planned and existing locations like manufacturing, service, recycling companies, or even EIPs can be considered in this model, optimizing numerous tangible and intangible flows. Based on a linear problem, additional constraints can easily be introduced in order to consider stakeholder limitations. A minimal amount of data is required to study the network behavior without publishing private data.

The approach developed (Chapter 4) and validated (Chapter 5) meets all requirements and purposes for modeling in industrial ecology (Chapter 3). It can help to set up an eco-industrial park, an eco-industrial network, or simply industrial symbiosis relationships between companies. The following Chapter 6 summarizes and concludes main outcomes of this work and provides recommendations for further research.

6 CONCLUSION AND RECOMMENDATIONS

This chapter provides an overview of the main outcomes and benefits resulting from this thesis and discusses recommendation for future research and industry.

Summary. As a consequence of major investigations on limited natural resources coupled with a growing population on earth, the United Nations World Commission on Environment and Development promotes the urge for sustainable development. A "development that meets the need of the present without compromising the ability of future generations to meet their own needs" (Brundtland 1987, p. 398). Many concepts, such as design for environment, cleaner production, industrial ecology, and circular economy, have been theoretically elaborated and practically applied to today's industry.

Suggesting industrial systems work as nature does and waste and byproducts of one company could be the input of another, Frosch and Gallopoulos (1989) define the term industrial ecology. Matching the view of the initially quoted German philosopher Immanuel Kant about nature's means, industrial ecology is a promising approach for further research and mathematical investigation. This concept introduces the closed-loop approach of material and energy flows and seeks to leverage synergies based on the example of natural symbiosis. A practical approach that applies these ideas is an eco-industrial park. With the goal of simultaneously increasing economic, environmental, and social performance, these corporate networks promote sustainable development. However, industrial practice still lacks implementations of this concept.

The methodology of mathematical and computational modeling supports Kant's opinion regarding the significance of mathematical foundation in research. Modeling has proven to be a powerful tool for decision support in different fields of science. In order to analyze, improve, and create industrial ecology on a corporate level, this thesis seeks to research mathematical modeling and simulation based on two guiding questions.

The first chapter provides a comprehensive description of the background and problem statement, emphasizing the main focus of research. The first of two question focuses on requirements for a modeling approach, a resulting evaluation of existing approaches, and an identification of potential gaps in research. Based on these findings, the second question of the thesis focuses on the feasibility and realization of an advanced modeling approach, to bridge the researched gap.

In order to provide a common understanding of main terms, concepts, and methods referred to in this work, the second chapter summarizes the required theoretical foundation. It describes the increasing importance of sustainable development in the three dimensions economy, environment, and society, illustrated by the triple bottom line model. After introducing the aforementioned concepts of industrial ecology and industrial symbiosis, the application of an eco-industrial park is defined as *"a community of manufacturing and service businesses located together on a common property. Member businesses seek enhanced environmental, economic, and social performance through collaboration in managing environmental and resource issues (...)." (Lowe 2001).* Broadening this practical approach, an eco-industrial network is defined as *"networks of EIPs at national or global levels" (Roberts 2004).*

The main example for an existing eco-industrial park is in Kalundborg, Denmark. Learning from working examples like Kalundborg, it was found that those parks can establish through three different ways, i.e. due to fortunate circumstances over time, promoted by an institution, or through centralized planning as a green field project. The presence of a large firm acting as a magnet for other businesses and an existing level of trust between the participants are two out of many drivers of the successful establishment. Following up on investigations of the subject matter, the methodology of mathematical and computational modeling is introduced to support decisions in the field of IE. The warehouse location problem, multi-commodity flow networks, and multi-objective optimization considering the decision maker's preference are described.

The third chapter investigates requirements of modeling industrial ecology. Besides the consideration of all three dimensions of sustainable development in the objective function, the integration of many stakeholder interests is a main requirement for a model. Multiple tangible and intangible flows in a corporate collaborative network and the capability to support the negotiation process are significant properties of suitable approaches for the underlying problem. A usable computer model generating a unique optimal solution for decisions regarding the improvement and creation of industrial ecology can meet the requirements. The evaluation of existing models shows that an advanced approach in order to bridge the current research gap, must consider mathematical modeling of social performance in addition to economic and environmental targets. A model for creating new EIPs and EINs is the most desirable. A classification and criteria for evaluation of existing and future models are provided.

As one of the main accomplishments of this thesis, the fourth chapter describes the development of the Interactive Optimized Negotiation Algorithm (IONA) for creating new eco-industrial parks. Embedding a multi-commodity warehouse location model into a negotiation algorithm and implementing this into a computer program helps to create entirely new eco-industrial networks and closes the investigated gap of research. The development of the mathematical and computational model, including major assumptions and specifications, are described in this chapter.

Since the main problem of today's sustainable development is found to be the implementation of theoretical concepts in practice, the fifth chapter provides a comprehensive proof of concept and an investigation on both model and computer program. Capabilities, flexibility, and performance are tested based on two case studies. The results of these case studies show that the program supports the negotiation process providing optimal network decisions at any time. The mathematical model is easy to extend with further information and generates results even with a minimum amount of data to be shared by potentially participating companies. Individual and bilateral relationships between companies can be investigated by means of the additional functionality of the computer model. This leads to an even wider range of application.

The algorithm shows a lack of efficiency during the solution process of larger cases. However, IONA meets all of the aforementioned requirements for modeling industrial ecology and provides the flexible application to different scales of corporative networks and measures defining the performance regarding goal dimensions.

Conclusion. This thesis provides two main outcomes in order to push the boundaries of state-of-the-art modeling for industrial ecology in the field of sustainable development.

Current approaches proposed in the literature for modeling industrial ecology have been developed for individual cases and lack generalization and flexibility. A classification for modeling approaches in the field of IE has yet to be suggested. The first outcome is thus, a classification of existing approaches based on general valid requirements for the purposes of modeling industrial ecology. In order to answer the first fundamental question Q1 in this thesis, a set of general requirements for IE models is established and existing approaches are evaluated. No approach was found that meets all requirements.

> *A1: The gap is defined by an advanced modeling approach for creating new eco-industrial parks or networks under a consideration of social performance in addition to economic and environmental goals.*

While one of the first approaches for creating industrial symbiosis is based on a mathematical model recently proposed by Gu et al. (2013), Romero and Ruiz (2014) propose a simulation of company networks that seek to develop industrial symbiosis. However, it has been found that none of these approaches pursue the consideration of social performance, which is a main goal of sustainable development. Neither an optimization model nor a simulation considered separately are satisfying approaches.

> *A2: As the first approach explicitly accounting for social performance of an industrial system, the Interactive Optimized Negotiation Algorithm overcomes many weaknesses of current models.*

This approach is the second main outcome of this thesis and shows that the second fundamental question Q2 can be approved. It embeds an optimization model seeking to support optimal decision-making in a complex process with concurrent stakeholders under non-hierarchal circumstances. Emphasizing the applicability to practice and lowering the threshold for companies to participate in EIPs or EINs, the approach requires a minimum of internal information. IONA proves that insight can be gained with minor information. While the analysis of existing EIPs and EINs has been studied by many publications, this thesis proposes an algorithm for creating entirely new eco-industrial parks and networks. Even if a complete network cannot be setup, an accurate investigation of potential relationships can be a profound result. In those cases, the developed decision support tool can provide a starting point for promoting the promising concept of industrial ecology. The networks investigated can be a set of existing and planned facilities and other participants. Moreover, many existing approaches only consider single material flows mostly restricted to utilities, e.g. waste water. This approach provides capabilities of considering the share of utilities, waste material, byproducts, components, and even information. An economy of sharing is a further idea, allowing companies to leverage even more synergies from sharing materials, sites, workforce, and knowledge. Another main advantage of this approach is its flexibility and general validity. Many current approaches are developed for a specific case and can thus not be efficiently used under different circumstances.

It is crucial to this approach and the concept of industrial ecology that participating companies and the respective decision makers express a general interest in obtaining environmental and social performance in addition to economic goals. Studies show that especially small and medium-sized companies are highly interested in environmental and social concerns (Wulf et al. 2011, Hansen 2004). Activities by global institutions and global corporate decision makers towards sustainable development are necessary.

The main deficit of today's effort toward sustainable development appears in implementing theoretical ideas to practical systems. As soon companies share their information for the sake of achieving performance with less waste outputs and not only socially bearable but also responsible corporate activities, the need for eco-industrial parks will increase significantly. Companies and communities can synergistically reduce transaction cost, benefit of economies of scale, and create jobs with benefits for workers even for their private life, e.g. energy prices. Mathematical and computational models will have a major role in supporting the establishment of new collaborations. The classification of existing models and IONA promote this development towards "*our common future*". As a consequence, this idea does not stay a theoretical concept but supports and encourages decision makers of today and tomorrow.

Recommendations. Emphasizing the flexible application to various practical case data, both the mathematical model and the computer program have been tested for feasibility and capabilities. However, the actual asset of the IONA approach must be proven by actual case studies. The aluminum industry is an example of an industry with high concerns for sustainable development and significant byproduct intensity. The collection of practical data sets must be the next step in order to promote this approach. Furthermore, tests in this thesis were conducted on an average machine. Reductions of runtime are expected when using a different computer with more memory and additional processor cores. The flexible structure of the mathematical model allows the study of a solution’s deviation when different objectives are introduced and constraints are added. The achievement-objective functions even allow the introduction of different measures than those proposed in this work. Besides CSR, the numerical values for hiring and firing costs as well as certain employee rates should be considered in the future (see O’Connor and Spangenberg 2008 and Hutchins et al. 2008).

As a main critique of the proposed approach, the sensitivity of results to uncertainty should be investigated further. The development of a heuristic in contrast to an optimization model could be used for a comprehensive assessment of the results calculated by this model and the impact of data deviation.

During the process of testing, the program was also found to be suitable for additional purposes. Used as a tool for simulating corporate networks, existing cases can be investigated depending on their alignment toward different dimensions of sustainability. The change of collaborative networks facing challenges of increasing importance of environmental or social goals can be investigated by means of this program.

Cleaner production, sustainable consumption, design for environment, and circular economy are just some of many examples for additional promising concepts besides industrial ecology. Combined with the suggested potential research to be done on the advanced approach proposed in this thesis, the implementation of industrial ecology in practice regarding all three dimensions of sustainable development with an emphasize on social performance can and should be pursued in all future industrial activities.

A.1: Solver outputs for the simple structure two-product case

```
# WEIGHT_VECTOR = (100,0,0)

Optimize a model with 30 rows, 102 columns and 239 nonzeros
Presolve removed 24 rows and 81 columns
Presolve time: 0.01s
Presolved: 24 rows, 27 columns, 72 nonzeros

Loaded MIP start with objective 1
Variable types: 3 continuous, 24 integer (24 binary)
Root relaxation: objective 9.816038e-01, 12 iterations, 0.00 seconds

    Nodes    |    Current Node    |     Objective Bounds      |     Work
 Expl Unexpl |  Obj  Depth IntInf | Incumbent    BestBd   Gap | It/Node Time
*    0     0               0       0.9816038    0.98160  0.00%     -    0s

Explored 0 nodes (12 simplex iterations) in 0.04 seconds
Thread count was 1 (of 1 available processors)
Optimal solution found (tolerance 1.00e-04)
Best objective 9.816037735849e-01, best bound 9.816037735849e-01, gap 0.0%

TOTAL SCORE: 0.98
SOLUTION:
Plant Company A closed!
Warehouse Company A closed!
Plant Recycling company closed!
Warehouse Recycling company open
  Emitts no waste of type 0
  Emitts no waste of type 1
Plant Company C closed!
Warehouse Company C open
  Emitts 500 units of waste type 0
  Emitts no waste of type 1
Plant Company D closed!
Warehouse Company D open
  Emitts no waste of type 0
  Emitts 900 units of waste type 1
Plant Eco-industrial park B closed!
Warehouse Eco-industrial park B closed!
Plant Eco-industrial park C closed!
Warehouse Eco-industrial park C closed!

Open_receiver = [0.0, 1.0, 1.0, 1.0, 0.0, 0.0]
Open_receiver = [0.0, 1.0, 1.0, 1.0, 0.0, 0.0]
Open_receiver = [0.0, 1.0, 1.0, 1.0, 0.0, 0.0]

X[i][j][k]=[
[[0.0, 0.0], [0.0, 0.0], [0.0, 0.0], [0.0, 0.0], [0.0, 0.0], [0.0, 0.0]],
[[0.0, 0.0], [0.0, 500.0], [0.0, 0.0], [0.0, 0.0], [0.0, 0.0], [0.0, 0.0]],
[[0.0, 0.0], [0.0, 0.0], [0.0, 800.0], [0.0, 0.0], [0.0, 0.0], [0.0, 0.0]],
[[0.0, 0.0], [0.0, 0.0], [0.0, 0.0], [100.0, 0.0], [0.0, 0.0], [0.0, 0.0]],
[[0.0, 0.0], [0.0, 0.0], [0.0, 0.0], [0.0, 0.0], [0.0, 0.0], [0.0, 0.0]],
[[0.0, 0.0], [0.0, 0.0], [0.0, 0.0], [0.0, 0.0], [0.0, 0.0], [0.0, 0.0]]]

Z[i][k]=[[ [1200, 850], [0, 0], [500, 0], [0, 900], [300, 100], [5000, 3000]]
```

```
# WEIGHT_VECTOR = (80,20,0)

Optimize a model with 30 rows, 102 columns and 239 nonzeros
Presolve removed 19 rows and 77 columns
Presolve time: 0.00s
Presolved: 29 rows, 31 columns, 88 nonzeros

Loaded MIP start with objective 1
Variable types: 7 continuous, 24 integer (24 binary)
Root relaxation: objective 9.610296e-01, 16 iterations, 0.00 seconds

    Nodes    |    Current Node    |     Objective Bounds      |     Work
 Expl Unexpl |  Obj  Depth IntInf | Incumbent    BestBd   Gap | It/Node Time
*    0     0               0       0.9610296    0.96103  0.00%     -    0s

Explored 0 nodes (22 simplex iterations) in 0.05 seconds
Thread count was 1 (of 1 available processors)
Optimal solution found (tolerance 1.00e-04)
Best objective 9.610295986076e-01, best bound 9.610295986076e-01, gap 0.0%

TOTAL SCORE: 0.96
SOLUTION:
Plant Company A closed!
Warehouse Company A closed!
Plant Recycling company open
  Take 500 units of product 1 from warehouse Recycling company
  Take 300 units of product 0 from warehouse Eco-industrial park B
Warehouse Recycling company open
  Emitts no waste of type 0
  Emitts no waste of type 1
…
Plant Eco-industrial park C closed!
Warehouse Eco-industrial park C open
  Emitts 4980 units of waste type 0
  Emitts 3000 units of waste type 1

Open_receiver = [0.0, 1.0, 1.0, 1.0, 0.0, 0.0]
Open_sender = [0.0, 1.0, 1.0, 1.0, 1.0, 1.0]
Open_location = [0.0, 1.0, 1.0, 1.0, 1.0, 1.0]

X[i][j][k]=[
[[0.0, 0.0], [0.0, 0.0], [0.0, 0.0], [0.0, 0.0], [0.0, 0.0], [0.0, 0.0]],
[[0.0, 0.0], [0.0, 500.0], [0.0, 0.0], [0.0, 0.0], [0.0, 0.0], [0.0, 0.0]],
[[0.0, 0.0], [0.0, 0.0], [0.0, 800.0], [0.0, 0.0], [0.0, 0.0], [0.0, 0.0]],
[[0.0, 0.0], [0.0, 0.0], [0.0, 0.0], [100.0, 0.0], [0.0, 0.0], [0.0, 0.0]],
[[0.0, 0.0], [300.0, 0.0], [0.0, 0.0], [0.0, 0.0], [0.0, 0.0], [0.0, 0.0]],
[[0.0, 0.0], [0.0, 0.0], [0.0, 0.0], [20.0, 0.0], [0.0, 0.0], [0.0, 0.0]]]

Z[i][k]=[[1200, 850], [0, 0], [500, 0], [0, 900], [0, 100],[4980, 3000]]
```

```
# WEIGHT_VECTOR = (30,70,0)

Optimize a model with 30 rows, 102 columns and 239 nonzeros
Model has 6 quadratic constraints
Presolve removed 11 rows and 57 columns
Presolve time: 0.00s
Presolved: 37 rows, 51 columns, 157 nonzeros

Loaded MIP start with objective 1
Variable types: 27 continuous, 24 integer (24 binary)
Root relaxation: objective 7.714461e-01, 21 iterations, 0.00 seconds

    Nodes    |    Current Node    |     Objective Bounds      |     Work
 Expl Unexpl |  Obj  Depth IntInf | Incumbent    BestBd   Gap | It/Node Time

*    0     0               0       0.7714461    0.77145  0.00%     -    0s

Explored 0 nodes (26 simplex iterations) in 0.06 seconds
Thread count was 1 (of 1 available processors)
Optimal solution found (tolerance 1.00e-04)
Best objective 7.714460580840e-01, best bound 7.714460580840e-01, gap 0.0%

TOTAL COSTS: 0.77
SOLUTION:
Plant Company A closed!
Warehouse Company A open
  Emitts no waste of type 0
  Emitts no waste of type 1
Plant Recycling company open
  Take 1200 units of product 0 from warehouse Company A
  Take 500 units of product 1 from warehouse Recycling company
  Take 500 units of product 0 from warehouse Company C
…
Plant Eco-industrial park C closed!
Warehouse Eco-industrial park C open
  Emitts 4580 units of waste type 0
  Emitts 3000 units of waste type 1

Open_receiver = [0.0, 1.0, 1.0, 1.0, 1.0, 0.0]
Open_sender = [1.0, 1.0, 1.0, 1.0, 1.0, 1.0]
Open_location = [1.0, 1.0, 1.0, 1.0, 1.0, 1.0]

X[i][j][k]=[
[[0.0, 0.0], [1200.0, 0.0], [0.0, 850.0], [0.0, 0.0], [0.0, 0.0], [0.0, 0.0]],
[[0.0, 0.0], [0.0, 500.0], [0.0, 0.0], [0.0, 0.0], [0.0, 0.0], [0.0, 0.0]],
[[0.0, 0.0], [500.0, 0.0], [0.0, 800.0], [0.0, 0.0], [0.0, 0.0], [0.0, 0.0]],
[[0.0, 0.0], [0.0, 0.0], [0.0, 350.0], [100.0, 0.0], [0.0, 0.0], [0.0, 0.0]],
[[0.0, 0.0], [0.0, 100.0], [0.0, 0.0], [0.0, 0.0], [300.0, 0.0], [0.0, 0.0]],
[[0.0, 0.0], [300.0, 0.0], [0.0, 0.0], [20.0, 0.0], [100.0, 0.0], [0.0, 0.0]]]

Z[i][k]=[[0, 0], [0, 0], [0, 0], [0, 550], [0, 0], [4580, 3000]]
```

```
# WEIGHT_VECTOR = (30,60,10)

Optimize a model with 30 rows, 102 columns and 239 nonzeros
Presolve removed 11 rows and 57 columns
Presolve time: 0.01s
Presolved: 37 rows, 51 columns, 157 nonzeros
Loaded MIP start with objective 0.9
Variable types: 27 continuous, 24 integer (24 binary)
Root relaxation: objective 6.928756e-01, 21 iterations, 0.00 seconds

    Nodes    |    Current Node    |     Objective Bounds      |     Work
 Expl Unexpl |  Obj  Depth IntInf | Incumbent    BestBd   Gap | It/Node Time
     0     0    0.69288    0    3    0.90000    0.69288  23.0%     -    0s
H    0     0                       0.7288375    0.69288  4.93%     -    0s
H    0     0                       0.7003802    0.69288  1.07%     -    0s

Explored 0 nodes (29 simplex iterations) in 0.06 seconds
Thread count was 1 (of 1 available processors)
Optimal solution found (tolerance 1.00e-04)
Best objective 7.003801838768e-01, best bound 7.003801838768e-01, gap 0.0%

TOTAL SCORE: 0.7
SOLUTION:
Plant Company A closed!
Warehouse Company A open
  Emitts no waste of type 0
  Emitts no waste of type 1
Plant Recycling company open
  Take 1200 units of product 0 from warehouse Company A
  Take 500 units of product 1 from warehouse Recycling company
  Take 480 units of product 0 from warehouse Company C
  Take 300 units of product 0 from warehouse Eco-industrial park B
  Take 100 units of product 1 from warehouse Eco-industrial park B
Warehouse Recycling company closed!
…
Plant Eco-industrial park B open
Warehouse Eco-industrial park B open
  Emitts no waste of type 0
  Emitts no waste of type 1
Plant Eco-industrial park C closed!
Warehouse Eco-industrial park C closed!

Open_receiver = [0.0, 1.0, 1.0, 1.0, 1.0, 0.0]
Open_sender = [1.0, 1.0, 1.0, 1.0, 1.0, 0.0]
Open_location = [1.0, 1.0, 1.0, 1.0, 1.0, 0.0]

X[i][j][k]=[
[[0.0, 0.0], [1200.0, 0.0], [0.0, 850.0], [0.0, 0.0], [0.0, 0.0], [0.0, 0.0]],
[[0.0, 0.0], [0.0, 500.0], [0.0, 0.0], [0.0, 0.0], [0.0, 0.0], [0.0, 0.0]],
[[0.0, 0.0], [480.0, 0.0], [0.0, 800.0], [20.0, 0.0], [0.0, 0.0], [0.0, 0.0]],
[[0.0, 0.0], [0.0, 0.0], [0.0, 350.0], [100.0, 0.0], [0.0, 0.0], [0.0, 0.0]],
[[0.0, 0.0], [300.0, 100.0], [0.0, 0.0], [0.0, 0.0], [0.0, 0.0], [0.0, 0.0]],
[[0.0, 0.0], [0.0, 0.0], [0.0, 0.0], [0.0, 0.0], [0.0, 0.0], [0.0, 0.0]]]

Z[i][k]=[[0, 0], [0, 0], [0, 0], [0, 550], [0, 0], [5000, 3000]]
```

```
# WEIGHT_VECTOR = (30,60,10) | Negotiation: max. capa recycling company 1600

Optimize a model with 33 rows, 102 columns and 242 nonzeros
Presolve removed 14 rows and 60 columns
Presolve time: 0.00s
Presolved: 35 rows, 47 columns, 143 nonzeros

MIP start did not produce a feasible solution
MIP start violates constraint open_negotiation1 by 1.00
Variable types: 27 continuous, 20 integer (20 binary)
Found heuristic solution: objective 0.7959075
Root relaxation: objective 7.012621e-01, 22 iterations, 0.00 seconds

    Nodes    |    Current Node    |     Objective Bounds      |     Work
 Expl Unexpl |  Obj  Depth IntInf | Incumbent    BestBd   Gap | It/Node Time
     0     0    0.70126    0    3    0.79591    0.70126  11.9%     -    0s
H    0     0                       0.7840822    0.70126  10.6%     -    0s
     0     0    0.70144    0    3    0.78408    0.70144  10.5%     -    0s
     0     0    0.70144    0    3    0.78408    0.70144  10.5%     -    0s
     0     0    0.70161    0    3    0.78408    0.70161  10.5%     -    0s
H    0     0                       0.7017158    0.70161  0.02%     -    0s
     0     0     cutoff    0         0.70172    0.70172  0.00%     -    0s

Cutting planes:
  Implied bound: 2
  Flow cover: 2

Explored 0 nodes (30 simplex iterations) in 0.07 seconds
Thread count was 1 (of 1 available processors)
Optimal solution found (tolerance 1.00e-04)
Best objective 7.017158061054e-01, best bound 7.017158061053e-01, gap 0.0%

TOTAL SCORE: 0.7
SOLUTION:
Plant Company A closed!
Warehouse Company A open
  Emitts no waste of type 0
  Emitts no waste of type 1
Plant Recycling company open
  Take 1200 units of product 0 from warehouse Company A
...

Open_receiver = [0.0, 1.0, 1.0, 1.0, 1.0, 0.0]
Open_sender = [1.0, 1.0, 1.0, 1.0, 1.0, 0.0]
Open_location = [1.0, 1.0, 1.0, 1.0, 1.0, 0.0]

X[i][j][k]=[
[[0.0, 0.0], [1200.0, 0.0], [0.0, 850.0], [0.0, 0.0], [0.0, 0.0], [0.0, 0.0]],
[[0.0, 0.0], [0.0, 500.0], [0.0, 0.0], [0.0, 0.0], [0.0, 0.0], [0.0, 0.0]],
[[0.0, 0.0], [400.0, 0.0], [0.0, 800.0], [20.0, 0.0], [80.0, 0.0], [0.0, 0.0]],
[[0.0, 0.0], [0.0, 0.0], [0.0, 350.0], [100.0, 0.0], [0.0, 0.0], [0.0, 0.0]],
[[0.0, 0.0], [0.0, 100.0], [0.0, 0.0], [0.0, 0.0], [300.0, 0.0], [0.0, 0.0]],
[[0.0, 0.0], [0.0, 0.0], [0.0, 0.0], [0.0, 0.0], [0.0, 0.0], [0.0, 0.0]]]

Z[i][k]=[[0, 0], [0, 0], [0, 0], [0, 550], [0, 0], [5000, 3000]]
```

A.2: Abstract of code for the random data generator

```
#---------------------------------------------------------------------------#
# Creation of eco-industrial parks and networks
# Biased random data generation
#
# (c) by Fabian Schulze
# Last update: 08/01/2014
#---------------------------------------------------------------------------#

#--- Import ----------------------------------------------------------------#
import math
import string
import random
import numpy

#--- Initializations and Definitions ---------------------------------------#
random.seed = 16
locations = int(input("Number of locations:"))
produkte=int(input("Number of products:"))

#--- Initializations -------------------------------------------------------#
par_coord_x = []
…

#--- Functions -------------------------------------------------------------#
def distance(lat1,long1,lat2,long2):
    earth_radius = 3959 #6371 #6367.4447
    dlat = math.radians(lat2-lat1)
    dlong = math.radians(long2-long1)
    lat1 = math.radians(lat1)
    lat2 = math.radians(lat2)
    a = math.sin(dlat/2) * math.sin(dlat/2) + math.sin(dlong/2) *
math.sin(dlong/2) * math.cos(lat1) * math.cos(lat2)
    c = 2 * math.atan2(math.sqrt(a), math.sqrt(1-a))
    return earth_radius*c

#--- Import city information -----------------------------------------------#
f = open("worldcitiespop.txt")
citylist = []
dist=[]
zahl = 0

for line in f:
    if line[:2] == "us" and string.split(line,",")[4] <> "" and
float(string.split(line,",")[4]) > 10000 and string.split(line,",")[3] <> "HI"
and string.split(line,",")[3] <> "PR" and string.split(line,",")[3] <> "AK":
        if string.split(line,",")[1] == "fairbanks":
            print(line)
        zahl += 1
        line = line.replace("\n", "")
        citylist.append(string.split(line,","))
        citylist[-1][4] = float(citylist[-1][4])
        citylist[-1][5] = float(citylist[-1][5])
        citylist[-1][6] = float(citylist[-1][6])
f.close()

#--- Generate biased data --------------------------------------------------#
step=int(len(citylist)/float(locations))
…
```

```
#--- Generate biased data ------------------------------------------------------#
step=int(len(citylist)/float(locations))

for k in range(produkte):
    par_price_market.append(random.randrange(5,9))
    par_trans_cost.append(random.randrange(3,8)*0.01*10)

for i in range(len(citylist)):
    if enu < locations:
        par_coord_x.append(float(citylist[i*step][5]))
        par_coord_y.append(float(citylist[i*step][6]))
        par_coord_name.append(citylist[i*step][1])
        par_csrs.append(random.randrange(50,90))
        par_price_network.append([])
        par_flowin.append([])
        par_flowout.append([])
        for k in range(produkte):
            par_price_network[enu].append(random.randrange(3,6))
            tempval=random.randrange(0,100)*citylist[i*step][4]*0.01*0.01 # x% *
1% of population
            if tempval > 40:
                par_flowin[enu].append(round(tempval,3))
            else:
                par_flowin[enu].append(0)
            tempval=random.randrange(0,100)*citylist[i*step][4]*0.01*0.01 # x% *
1% of population
            if tempval > 40:
                par_flowout[enu].append(round(tempval,3))
            else:
                par_flowout[enu].append(0)
    enu += 1

for i in range(len(par_coord_x)):
    dist.append([])
    for j in range(len(par_coord_x)):
        dist[i].append(distance(par_coord_x[i], par_coord_y[i], par_coord_x[j],
par_coord_y[j]))

for i in range(len(par_coord_x)):
    for j in range(len(par_coord_x)):
        if tmp < distance(par_coord_x[i], par_coord_y[i], par_coord_x[j],
par_coord_y[j]):
            tmp = distance(par_coord_x[i], par_coord_y[i], par_coord_x[j],
par_coord_y[j])
            cities= [i,j]

gen_x_coord = par_coord_x
…
#--- Write data file -----------------------------------------------------------#
f = open('data_scenario_'+str(locations)+'-'+str(produkte)+'.txt','w')
f.write(writer1[:-1]+"\n")
…

#--- Write protocol file -------------------------------------------------------#
f = open('data_scenario_'+str(locations)+'-'+str(produkte)+'_log.txt','w')
f.write("--- General info ----------------------------------------"+"\n")
f.write("locations: "+str(locations)+"\n")
f.write("products: "+str(produkte)+"\n")
f.write(""+"\n")
f.write("--- Location info ---------------------------------------"+"\n")
f.write("Distance: Agv. | minimum | maximum: "+str(round(numpy.mean(dist),3))+"
| "+str(round(numpy.min(dist),3))+" | "+str(round(numpy.max(dist),3))+"\n")
…
```

A.3: Example output protocol of the random data generator

```
--- General info ----------------------------------------

locations: 100
products: 4

--- Location info ---------------------------------------

Distance: Agv. | minimum | maximum: 1123.687 | 0.0 | 2762.764

     from kendall to anacortes (2762.76 miles)

Avg. CSR index: 69.32


Avg. input | total input: 200.9475075 | 80379.003

     product 0: 224.8108 | 22481.08

     product 1: 213.15037 | 21315.037

     product 2: 163.65181 | 16365.181

     product 3: 202.17705 | 20217.705


Avg. output | total output: 234.1294125 | 93651.765

     product 0: 219.29085 | 21929.085

     product 1: 249.03145 | 24903.145

     product 2: 244.26017 | 24426.017

     product 3: 223.93518 | 22393.518


--- Product info ----------------------------------------

Avg. prices | Market price: 3.9625 | 5.75

     product 0: 4.01 | 5

     product 1: 4.02 | 5

     product 2: 3.98 | 6

     product 3: 3.84 | 7
```

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