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Production Process Design Using Multi-Criteria Analysis



universitätsverlag karlsruhe

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meinem Vater

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Karlsruhe, im November 2006 Martin Treitz

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Chapter 1

Introduction

The need to increase efficiency, improve environmental performance, comply with legislation and simultaneously preserve social responsibility are some of the key challenges to be faced by industry today and in the future. These challenges stem from both the low costs of labour and less constrained local production in emerging countries and the rapid development in consumer demand and questions concerning environmental and safety standards in industrialised countries [Charpentier, 2005]. In addition, globalisation has connected markets through lower trade barriers and e-commerce and because the operating environment has changed, new approaches need to be developed to meet the challenges. This results in an increased drive for process optimisation to reduce both energy and material loss in the production process and to provide non-polluting, defect-free and recyclable products and by-products.

1.1 Decision Support for Process Design

Optimisation is an ongoing task in the chemical process industry. Since the operating range of mass and energy flows within a process is directly determined by the process design, it is consequently necessary to understand which process design characteristics are the main drivers of its impact in order to improve the performance of a process. Thus, the parameters for the optimisation must be connected to the process design stage. The power of process design tools lies in the modelling of the relationship between the underlying chemical and physical principles of unit operations and the knowledge of which combinations lead to beneficial designs [Barnicki and Siirola, 2004].

1.1.1 Process Design and Technique Assessment

The aim of production process design is the identification and creation of innovative process designs by combining mathematical and chemical engineering optimisation approaches. Therefore, the quantification of effects and the systematic generation of design alternatives are necessary to support the decisions in the design process for finding the best utilisation of a stream. The term process design is used here in a very broad sense and refers to chemical plant design, industrial construction and technology management (cf. Figure 1.1).

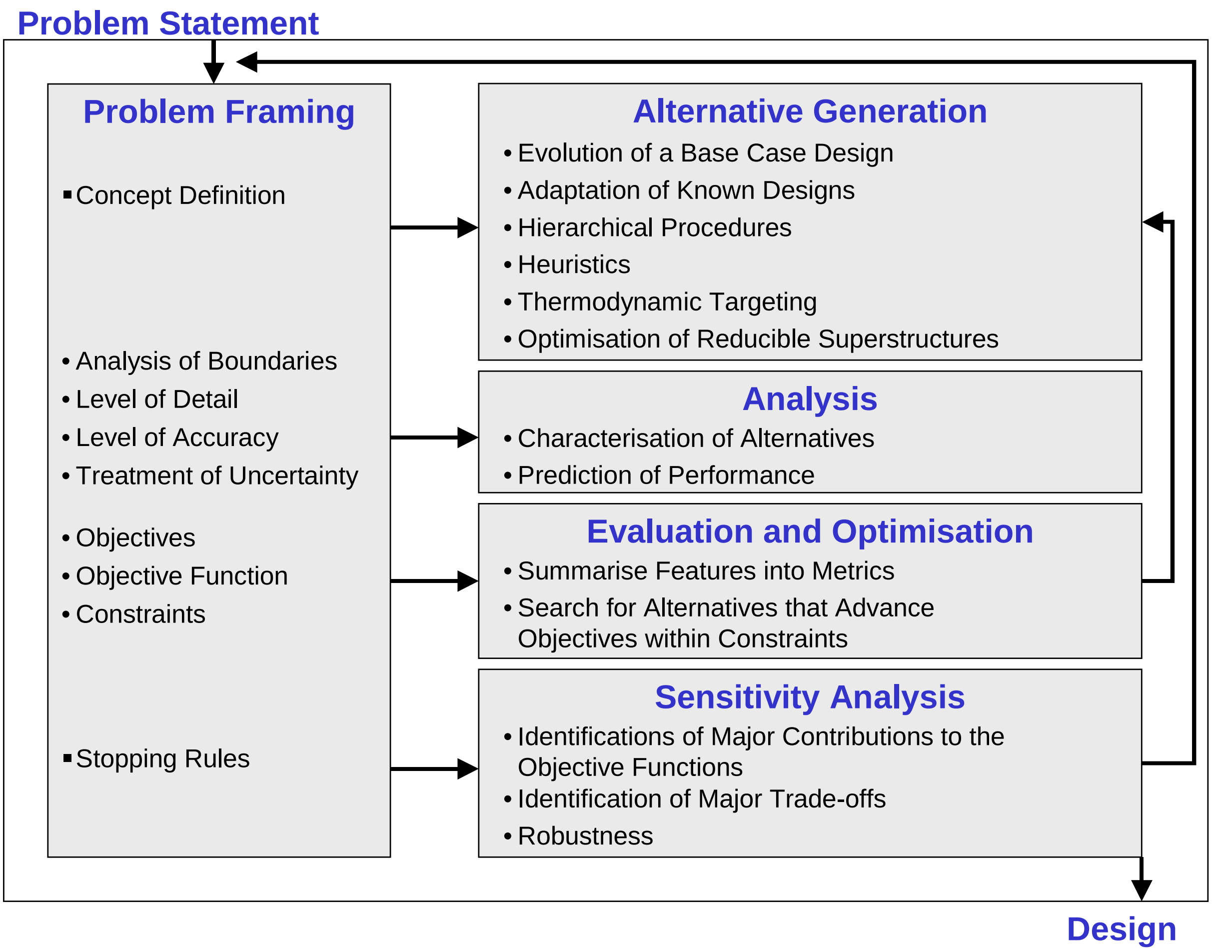

Figure 1.1: The Design Process [Cano-Ruiz and McRae, 1998]

In Europe the use of the *Best Available Techniques (BAT)* approach [Rentz et al., 1999a, 2003; Jansen, 2004] is an essential element in designing environmental legislation as for example is required by the *Directive on Integrated Pollution Prevention and Control* (IPPC 96/61/EG) [EC 96/61]. In particular, the implementation of BAT should reduce waste generation and increase the efficiency of energy consumption. In this context, *Integrated Technique Assessment* [Geldermann, 1999, 2006a] can be applied to determine the BAT considering impacts to all environmental media (air, water, land) and energy consumption in a cross-media evaluation of all implemented and emerging techniques in relevant industrial sectors [Geldermann and Rentz, 2001].

Methodological parallels between production process optimisation and Operations Research have been pointed out by several authors (e.g. [Rentz, 1979]). For example, integrated production planning by linear optimisation for ammonia synthesis takes into account by-products, residues and emission taxes [Penkuhn et al., 1997]. Unit operations, modelled by the process simulation software *Aspen Plus*[1], are also the basis for a Mixed Integer Linear Programming (MILP) of products at the end of their lifetime in the steel industry [Spengler et al., 1997]. Other examples are the combined use of Goal Programming (GP) and the Analytical Hierarchy Process (AHP) for prioritisation of the different goals of process optimisation, which are demonstrated by a case study on the optimisation of three petrochemical plants (ammonia- , refinery- and polypropylene-plant) influenced by social, economic and environmental objectives [Zhou et al., 2000]. In contrast to these "as a whole" optimisation approaches and centralised-view analyses, agent-based approaches focus on decentralised installations within a supply chain [García-Flores and Wang, 2002]. Using simulation and a formalised language between the agents, a batch process for the manufacture and supply of paints and coatings can be modelled and design implications can be identified, which highlight agile structures for a competitive advantage [García-Flores and Wang, 2002]. Consequently, combining process optimisation tools with Operations Research provides the basis for better identifying improvement opportunities. Structuring the preferred combination of approaches for different contexts and system boundaries is the key challenge.

By defining the design frame and the system boundaries, the overall production process design or consideration of a particular subsystem, e.g. reactor, is specified. The expected performance of a process is modelled and simulated by indicators [Cano-Ruiz and McRae, 1998]. The design alternatives are evaluated by a number of different criteria (economic, health, safety, environmental impact, energy consumption, controllability, flexibility, ease of maintenance, etc.) and future evaluation might even include further criteria, such as labour utilisation, risk minimisation and security [Barnicki and Siirola, 2004].

[1] Aspen Plus is a process modelling tool within the Aspen Engineering Suite for steady state simulation, design, performance monitoring, optimisation and business planning for chemicals, specialty chemicals, petrochemicals and metallurgy industries. For further information refer to http://www.aspentech.com/

1.1.2 Multi-Criteria Analysis Approach

Materials are defined by a multitude of different functions and a wide range of properties. When utilising materials for their intended purposes undesired effects also occur, for example incompletely converted raw material, unavoidable by-products, spent catalysts and solvents as well as inherent contaminants in the raw material [Charpentier, 2005]. The risks to humans and the environment by the production, use and disposal of chemicals are addressed in various initiatives, e.g. the *Registration, Evaluation and Authorization of Chemicals* (REACH) in Europe or the *Toxics Substances Control Act* (TSCA) in the United States. There exists a trade-off between information on hazards and information on safer alternatives. Ultimately pollution prevention and cleaner production approaches are generally acknowledged to be superior to pollution control [Koch and Ashford, 2006]. The development of new technologies and process innovation "necessitates an integrated system approach for a multi-scale and multidisciplinary modelling of complex, simultaneous and often coupled momentum, heat and mass transfer phenomena and processes taking place at different time scales (10^{-15} to 10^{8} s) and length scales (10^{-8} to 10^{4} m) encountered in industrial practices" [Charpentier, 2005].

Promoted by various initiatives, sustainability strategies (not limiting the quality of life or options available for future generations [WCED]) are being applied increasingly throughout Europe, with the aim of raising efficiency and preventing environmental damage amongst broader sustainability goals. Closed loop approaches for the whole supply chain, *Life Cycle Assessment* (LCA) criteria for products and connected processes [Hunkeler et al., 2003] and techno-economic assessment methods are used to improve performance [Geldermann et al., 2000a; Rentz et al., 2003]. However, these approaches are still maturing in industrialising countries, where evolving financial institutions do not value the extra environmental and social benefits that cleaner production processes provide. Consequently, an applicable and practical approach to improve production efficiency is needed that considers both the technical requirements of the production processes and the impacts caused. There are various approaches aimed at the improvement of production processes at the plant and company level, the inter-enterprise level and even the global level. For example, the research field of *Industrial Ecology* endeavours to study "flows of materials and energy in industrial and consumer activities and effects of these flows on the environment and the influences of economic, political, regulatory, and social factors of the flows, and the transformation of resources" [White, 1994]. Hence, Industrial Ecology considers different scopes of application on the firm, inter-enterprise and global level, thereby incorporating various methodological approaches (cf. Figure 1.2).

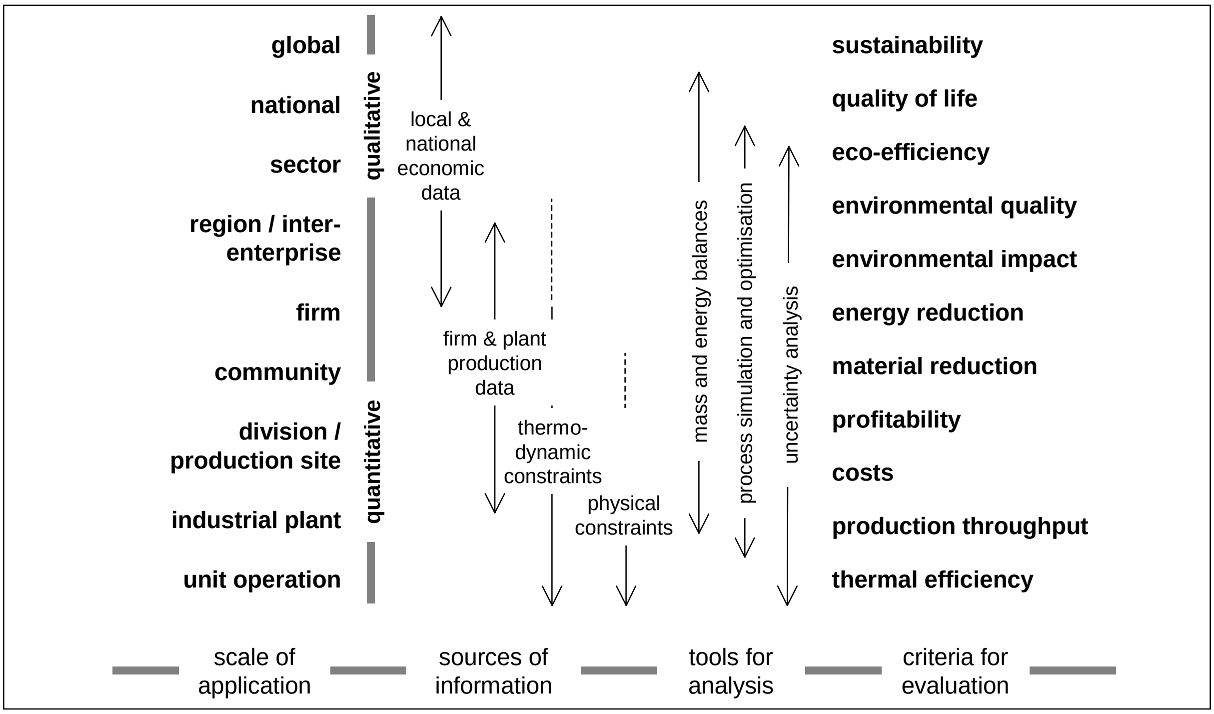

Figure 1.2: Conceptual Framework for the Process Analysis Approach, adapted from [Diwekar and Small, 2001]

Beyond *Industrial Ecology* [Graedel and Allenby, 2003] various other approaches exist for incorporating different levels of firm, process, or product assessment, such as *Cleaner Production* [UNEP, 1994], *Eco-Efficiency* [Fussler, 1999; Lehni, 2000; Saling et al., 2002; Geldermann et al., 2007a], the *Zero-Emission* concept [Suzuki, 2000], *supply chain management* based concepts (*Green Supply Chain Management* [Sarkis, 2003], *Environmental Supply Chain Management* [Nagel, 2000] and *Integrated Chain Management* [Seuring, 2004b]). Due to varying definitions, the relationship and overlap between approaches are often unclear [see e.g. Seuring, 2004a]. These approaches may be based on different objectives and levels (product, process, company, inter-company or regional level), and might differ in the application of various methods, but they share the common challenge of applying methods for identifying practically applicable solutions: "Sustainable development is widely accepted as a guiding principle in business. Still, this principle needs to be transformed into business practices" [Seuring, 2004b].

Technological progress provides new opportunities to improve resource efficiency in industrial production, for example combustion could be eventually replaced by fuel cell technology or the potential of bio-processing of renewable resources must be exploited [Grossmann, 2004]. Since the portfolio of available unit operations continuously changes through innovation, re-evaluating of processes is essential. The techno-economic assessment of different production process options (new process design or modifications to existing installations) depends to a great extent on the input materials and their properties as well as the specific technical application. Different sources of information and different available methodologies exist depending on the scale of the application. Moreover, different criteria prevail depending on the research target. Broad scheme, such as sustainability on a global level, break down to more detailed criteria such as thermal efficiency on the level of unit operations. The diverse evaluation criteria on the various scales of application comprise different attributes with partially conflicting objectives, which necessitate a multi-criteria decision analysis and sensitivity analysis. The required sensitivity analysis, however, must consider not only data uncertainties, such as estimated costs, unknown temperatures or tolerance towards changes in material quality, for the robustness of the operation of a process and ultimately the selection decision, but also the preferential uncertainty of the decision maker involved.

1.1.3 Special Conditions in Industrialising Countries

Taking into account the challenge to improve resource efficiency, the regional and global energy and material markets will be affected by growing economies and industrialising countries and vice versa. Thus, the world development report of 2003 *"Sustainable Development in a Dynamic World"* [Worldbank, 2002] calls for a dynamic growth in income and productivity for industrialising countries in accordance with a sustainable development. The considerable economic growth in industrialising countries in the last decades, however, has generated increasing environmental pollution. Thus, the success or failure of a resource efficient development will impact on the world's economy. Due to the rapid growth of emerging economies and their increasing demand for resources, it is essential to include these countries and their special conditions in the development of new strategies for sustainable development. Especially approaches suitable for *Small and Medium Sized Enterprises* (SME) are required, since significant changes in supply chain structures (e.g. due to market dynamics) especially challenge SME, which are the backbone of various emerging countries (cf. Chapter 4).

Supply chains are no longer a linear arrangement of processes ending at a final consumer, but there is an increasing shift towards recycling and utilisation of by-products in other supply chains. By handling waste streams (e.g. reduction, reuse, remanufacture, recycling and disposal [Sarkis, 2003]) material cycles can be closed within the supply chain network and resource consumption can be reduced. While the reuse of production scrap (mostly cuttings or defective products) is required foremost in the manufacturing industry

[Spengler et al., 2003], chemical process engineering in contrast must consider a multitude of by-products with various material properties. In particular the conversion of harmful substances into useful products is a traditional field for mass and energy flow management and process engineering in chemical supply chains. Integrated analysis of different process systems can provide valuable insight into, and also identify improvements in the financial and environmental performance of industrial global supply chain systems.

Industrialising countries face different financial, environmental and industrial conditions compared to Europe, Japan or North America. For example, financing is a key barrier to investment for SME in cleaner production facilities [UNEP, 2003; Ciccozzi et al., 2003] since financial institutions do not value the extra environmental and social benefits. Consequently, due to missing know-how, access to technologies and higher interest rates, SME face not only higher transaction costs compared to larger companies, but applying for funding for integrated resource improvement is difficult. Furthermore, disparity of the economic development and the scarcity of some resources in relation to the population presents a challenge to the environmental policy of many emerging countries. In addition to traditional environmental problems (such as for example deforestation, erosion, and water shortage) the generation of emissions, wastewater, solid waste, or noise contributes to the pollution of air, water and soil.

One major problem is air pollution from man-made sources, due to the increased use of fossil fuels (e.g. nitrogen oxides (NO_x) emissions), manufacturing processes and the use of chemicals, posing a risk to both human health and the environment. Reducing air pollution is a complex task. Whereas pollution reduction measures of pollutants like NO_x and SO_2 in large industrial installations have been implemented comparably well via technology transfer, the pollution reduction of *Volatile Organic Compounds (VOC)* is more problematic. Emitted VOC are precursors of ozone, which is of major concern in both urban and rural areas. Some studies indicate that for example in China the harvest of soybean crops is reduced by 10% or more and spring wheat production by 20% and 3% respectively, in comparison with the potential production [ECON, 2002]. Overall, more than 5.3 million hectares of land are estimated to be affected by air pollution in China with ozone pollution likely to increase in China in the years to come, due to several factors including growing numbers of motor vehicles and SME [ECON, 2002]. In Chile for example the capital region of Santiago is especially affected by air pollution and has been declared a saturated zone in terms of ozone and several other contaminants. Thus, a decontamination plan must be executed for the region, and environmental impact assessments are obligatory for all industrial, urban or real estate projects.

Besides air quality, the aim to provide public access to freshwater and water quality standards are of great importance to industrialising countries [UNEP, 2004]. Most industrialising countries need to improve their water resource management. Considerable health effects must be considered, but also significant effects to the structure of industrial applications are observed. Insufficient wastewater regulations based on a central authority vs. a demand-oriented management can be observed [UNEP, 2004]. Furthermore, in China for example, inequalities in water supply between western vs. the coastal and eastern regions lead to different water perception [ECON, 2002].

A third major concern is energy consumption. Taking into account the rising energy demand of industrialising countries, major improvements in efficiency and the incorporation of renewable energy sources are necessary. Furthermore, due to the highly regulated power supply in numerous countries the energy prices are commonly state-controlled. As a result, in most cases energy prices are below market prices and thus do not encourage energy saving measures.

Besides general differences between Europe and emerging countries, geographical conditions and differences in infrastructure can determine unequal development within these countries. For example in China a disproportionate level of progress exists in the different regions. As it is true for the natural water and mineral resources, the economic development of the eastern and coastal provinces also outplays the underdeveloped western regions and Inner Mongolia. Therefore, the 10^{th} five-year plan (2001-2005) contains 225 projects furthering development in these regions with tax advantages, technological innovations and development of infrastructure [Staiger et al., 2003]. Comparable to the general situation of Latin America, Chile is characterised by a structural dualism. More than 98 % of the companies are small businesses. The SME account for less than 25 % of the total sales in the non-agricultural sector, but offer more than 80 % of the employment [Troncoso, 2000]. In addition other structural deficits stem from the distribution of the industrial activity in the different sectors as for example 80 % of the exports are based on natural resources [Giurco, 2005]. Therefore, not only is the exploitation of the natural resources a problem, but also the small ratio of value added (e.g. copper, pulp industry, fruits, wine, fish). Furthermore, the lack of skilled human resources affects the productivity of the SME in all sectors in Chile.

1.2 Objective of the Thesis

Intra- and inter-company networks, namely production networks, industry parks, procurement networks, have gained increased importance in developed and industrialising countries. Synergies and improved access to resources and financial markets are seen as a competitive advantage. By seeking to optimise both the material and energy flows and the utilisation of by-products, ecological and economic benefits are gained [Tietze-Stöckinger, 2005; Frank, 2003]. By reusing waste of industrial sites as a valuable input within the production network, material cycles can be closed and resource efficiency can be improved. Also aspects of reducing the consumption of natural resources (e.g. water, oil, etc.) and the reduction of environmental impacts by lowering emissions must be considered while regarding techno-economic aspects.

Therefore, the objective of this thesis is to develop a model for production process design combining approaches from chemical engineering and Operations Research using integrated multi-criteria decision support. These aspects will be addressed in six consecutive chapters within this thesis, reflecting the different objectives of this work:

Chapter 2 explains the *pinch analysis* as a process design method for integrating processes and closing material cycles. The basic idea behind the thermal pinch analysis is a systematic approach to the minimisation of lost energy in order to come as close as possible to a reversible system. First, the main features of the *thermal pinch analysis* approach (cf. Section 2.1) are presented and second, the *water pinch analysis* (cf. Section 2.2) is described as an extension of the heat exchange problem to a mass exchange problem addressing minimal fresh water consumption in a production network. Third, the *solvents pinch analysis* (cf. Section 2.3) is presented as a method to assess the recovery of organic solvents via condensation in a production network. Economic parameters are included in all approaches to address the trade-off between savings of operating costs and investment. Finally, the advantages and limitations of the various approaches are discussed. The combination of the different pinch analysis approaches for intra- and inter-company production networks into one integrated model is to be developed: *Multi Objective Pinch Analysis (MOPA)* provides the framework for pinch analysis combined with a subsequent multi-criteria evaluation.

Chapter 3 presents two different approaches to address the problem to integrate the different targets determined by pinch analyses in one solution to evaluate the overall resource efficiency. The aim is the assessment of a techno-economic production process improvement based on resource efficiency. A general introduction addresses the problem of comparing different technical options (cf. Section 3.1). Missing preferential parameters are identified as key information to resolve incomparabilities between the different technical options. A metric is described to roughly assess techniques using a distance measure and weighting factors between the criteria considered (cf. Section 3.2). The application of the multi-criteria approach PROMETHEE is presented to resolve the incomparabilities between alternatives by preferential information between the criteria (weighting factors) and within criteria (preference functions) (cf. Section 3.3). A unique combination of sensitivity analyses for preferential as well as data uncertainty for PROMETHEE is applied.

Chapter 4 presents results for multi-criteria decision support for production process design. The optimisation and assessment methodology is demonstrated by a case study. First, based on a company in the bicycle production industry target values for the discussion of savings potentials in the context of several process design options are discussed. The case study shows the application of the various pinch analysis modules and a subsequent multi-criteria assessment for the coating section of the bicycle production. Second, the application of the methodology to an inter-company production network is discussed and implications for the optimisation of the production planning are shown.

The case study is the main focus of this research and demonstrates the features of the preceding chapters. Special focus is set on the application of the methodology to SME.

Chapter 5 compiles the main facets of the methodology developed in this thesis and shows the major contributions of this work. This is followed by an in-depth discussion of the model, which contrasts the advantages and limitations. The Multi Objective Pinch Analysis combines technical, economic and ecological aspects with a multi-criteria analysis incorporating an uncertainty analysis. This makes the assessment of the different targets operational. In addition, aspects for further research are highlighted.

Chapter 6 summarises the important findings and limitations of the developed multi-criteria decision support model for production process design and points out aspects for future research.

Chapter 2

Integrated Process Design Based on the Pinch Analysis Approach

The problem of synthesising chemical process networks attracted much attention in the 1970s (surveys are for example provided in [Furman and Sahinidis, 2002; Linnhoff, 1993]). Especially for heat recovery, amongst others, branch and bound techniques [Lee et al., 1970], heuristics, such as matching the hot stream of the highest supply temperature with the cold stream of the highest target temperature [Ponton and Donaldson, 1974], and multi-criteria algorithms (attempting to optimise total heat transfer area, energy recovery and total costs) [Nishida et al., 1977] were discussed. Rather than concentrating on the network topology, focus can also be put on the feasibility, for example controllability, start-up procedures, safety constraints, and the flexibility of the system [Hohmann, 1971; Ram et al., 1975; Alexander et al., 2000]. By focussing on the flexibility, theoretical minimal consumption targets are identified and then the design of the network is simplified by the trade-off between those and complexity, operability and costs of additional unit operations.

The integration of processes is performed predominantly by simulation, i.e. by automatically generating design variants and selecting the best one. Hereby, simulation based approaches can explicitly consider incomplete, uncertain data, such as material properties, thermodynamic data and kinetics of partial processes [Mosberger, 2005]. Through the interpretation of the problem from a thermodynamic rather than from a combinatorial point of view, the field of *process integration* [Linnhoff and Flower, 1978; Linnhoff and Hindmarsh, 1983; Douglas, 1988; El-Halwagi, 1997; Dunn and Bush, 2001] in engineering design was established. It can be described as a "system-oriented, thermodynamics-based, and integrated approach to the analysis, synthesis, and retrofit of process plants that examines an entire process in order to develop ways of integrating materials and energy that minimise both costs and waste production" [Mann and Liu, 1999]. Three key principles describe the process integration methodology towards more efficient production systems [Mann and Liu, 1999]:

- "Treat the entire manufacturing process as a single integrated system of interconnected processing units and use process, utility, and waste streams for both analysis and design.
- Apply process engineering principles (e.g. thermodynamics, mass and energy balances) to key process steps in order to establish a priori attainable performance targets on the use of materials and energy and the generation of emissions and wastes.
- Finalise the details of the process design in order to realise the established performance targets."

Heat integration (cf. Chapter 2.1) is one branch of process integration and it "provides a fundamental understanding of energy utilisation within the process and employs this understanding in identifying energy targets and optimising heat recovery and energy-utility systems. ... Of particular importance are the thermal pinch techniques that can be used to identify minimum heating and cooling utility requirements for a process" [El-Halwagi, 1997]. Today, the *thermal pinch analysis* is a well established and mature design methodology in chemical engineering.

A second branch of process integration is *mass integration*. Here, the basic question is to establish a fundamental understanding of the flow of mass within the process and to employ this holistic understanding in identifying performance targets and optimising the generation and routing of types of material throughout the process [El-Halwagi, 1997]. The *water pinch analysis* (cf. Chapter 2.2) represents a specific case of mass integration. It is based on the principle of a mass transfer from a contaminant source (i.e. contaminant rich process stream) to a contaminant lean water stream. The design of processes for recovering VOC from a gaseous waste stream can be formulated via mass integration, such as with adsorption or absorption, but also as a condensation problem [Dunn and El-Halwagi, 1994]. Since the recovery of solvents can be achieved via thermal condensation, the problem can be stated as a heat transfer problem and consequently be addressed by a so-called *solvents pinch analysis* (cf. Chapter 2.3).

Aim of this thesis is the implementation of a generic methodology incorporating the different pinch analyses to assess the overall savings potential. By a module-wise implementation of the different pinch analysis approaches the results of the different modules can be integrated and transferred to the multi-criteria evaluation (cf. Chapter 3). Nevertheless, by addressing a specific problem the module-wise implementation provides the flexibility for a substitution of one module with another software[2].

2.1 Thermal Pinch Analysis

The assessment and optimisation of process systems with an exergo-economic approach has a long tradition in the process industry [Tsatsaronis et al., 1990]. The focus thereby is on a formalised integrated approach considering energy and mass flows of an entire system instead of investigating the degree of efficiency of single energy-conversion processes, such as heat exchangers, independently [Linnhoff et al., 1979; Umeda et al., 1979; Linnhoff and Turner, 1981; Linnhoff, 2004]. In chemical processes heat is utilised for the operation of reactors and the subsequent thermal separation of the reaction products. The basic idea behind energy pinch analysis is a systematic approach to the minimisation of lost energy in order to come as close as possible to a reversible system. In its first step the pinch analysis yields the best possible heat recovery. Further recovery can only be achieved by changing the conditions or structures of the investigated system, for example flow rates, pressures or routing of flows [Parthasarathy and El-Halwagi, 2000].

In the following the very basic concepts and ideas of the pinch analysis are described. For a more detailed description and additional aspects the relevant literature is recommended [see e.g. Linnhoff and Flower, 1978; Umeda et al., 1979; Linnhoff and Hindmarsh, 1983; Linnhoff, 1998; Peters et al., 2003; Radgen, 1996; Linnhoff and Sahdev, 2005].

[2] e.g. the *Centre for Process Integration (CPI)* within the School of Chemical Engineering and Analytical Science of *The University of Manchester* (www.ceas.manchester.ac.uk/research/researchcentres/centreforprocessintegration), *Aspentech* (www.aspentech.com) and *Linnhoff March* as a division of KBC Process Technology Ltd (www.linnhoffmarch.com) offer specialised software for specific problems, such as for example the simulation and optimisation of distillation columns, multiphase chemical reactor networks, refinery networks, or multiple feed streams in a water pinch analysis.

Table 2.1: Nomenclature for the Thermal Pinch Analysis

Variable	**Unit**	**Name**
T	$[K]$	temperature
ΔT_{min}	$[K]$	minimum temperature gradient (driving force)
STP	$[-]$	standard temperature and pressure with $T_{STP} = 0\,°\text{C} = 273.15\,K$ and $p_{STP} = 101325\,Pa = 101325\,N/m^2$
R	$[J/mol \cdot K]$	ideal gas constant, $R = 8.314472$
n_x	$[mol]$	amount of substance
V	$[m^3]$	volume
V_M	$[m^3/mol]$	molar volume
V_{STP}	$[m^3/mol]$	molar volume of an ideal gas under standard conditions for temperature and pressure, $V_{STP} = 22.414\ m^3/kmol$
L	$[-]$	number of temperature intervals, $L \in \mathbb{N}$
C	$[-]$	number of cold process and cold utility streams
s	$[-]$	number of cold utility streams
$C - s$	$[-]$	number of cold process streams
H	$[-]$	number of hot process and hot utility streams
t	$[-]$	number of hot utility streams
$H - t$	$[-]$	number of hot process streams
c_{ik}	$[-]$	cold process stream i in temperature interval k, $k \in \{1, 2, \ldots, L\}$
h_{jl}	$[-]$	hot process stream j in temperature interval l, $l \in \{1, 2, \ldots, L\}$
a_{ik}	$[kJ/h]$	enthalpy flow in interval k of cold stream i
b_{jl}	$[kJ/h]$	enthalpy flow in interval l of hot stream j
$q_{ik,jl}$	$[kJ/h]$	thermal energy transferred from source h_{jl} to heat sink c_{ik}
$C_{ik,jl}$	$[€/kJ]$	costs of transferring a single unit of $q_{ik,jl}$
r_{STP}	$[m^3/h\,(STP)]$	flow rate under STP
ΔT_{ln}	$[K]$	logarithmic mean temperature difference (LMTD)
A	$[m^2]$	heat transfer area
α_{ij}	$[kW/m^2 \cdot K]$	heat transfer coefficient
c_p	$[kJ/kmol \cdot K]$	specific heat capacity
n	$[-]$	factor for economies of scale
κ_{proc}	$[€/m^2]$	specific costs for heat exchanger surface area for a match of two process streams

Table 2.1: Nomenclature for the Thermal Pinch Analysis (cont.)

Variable	Unit	Name
$\kappa_{util,s,t}$	$[€/m^2]$	specific costs for heat exchanger surface area for a match of cold utility s with hot process streams $[1, H-t]$ or of hot utility t with cold process streams $[1, C-s]$
w	$[-]$	component w of a process stream ($w = (1, 2, \ldots, W)$, W as number of components ($W \in \mathbb{N}$))
χ_w	$[-]$	mole fraction of component w
σ_{util}	$[€/kJ]$	price of utility *util*

2.1.1 Principles of the Pinch Analysis

The starting point of the pinch analysis lies in the objective of achieving optimal energy utilisation in a process by interconnecting material flows requiring heating (cold flows) with those requiring cooling (hot flows) and therefore was originally orientated exclusively at minimising additional energy utilities. The pinch analysis requires the combination of hot and cold process streams to composite curves and the description of the respective *enthalpy-temperature* (ΔH, T) relationships (cf. Figure 2.1). Additionally, a minimum temperature gradient ΔT_{min} must be set representing the driving force of the heat transfer (cf. Table 2.1).

The result of the pinch analysis is the energy savings potential for the considered set of processes and represents the target for the subsequent design process. Furthermore, information about the amount of heat exchange required between the appropriate streams is obtained, minimising the use of hot and cold utilities. Depending on the chosen design constraints, which reflect technical and chemical requirements, the actual savings are determined resulting in an economically feasible solution.

2.1.1.1 Concept of Composite Curves and Determination of Target Values

The basic idea behind the pinch analysis becomes apparent in the concept of the cold and hot *composite curves*. The individual cold and hot flows are divided into temperature intervals whose limits are chosen so that one interval boundary lies on every entry and exit temperature. In each temperature interval the individual cold and hot heat flows of that interval are added and displayed together as straight lines in the (ΔH, T) diagram (cf. Figure 2.1).

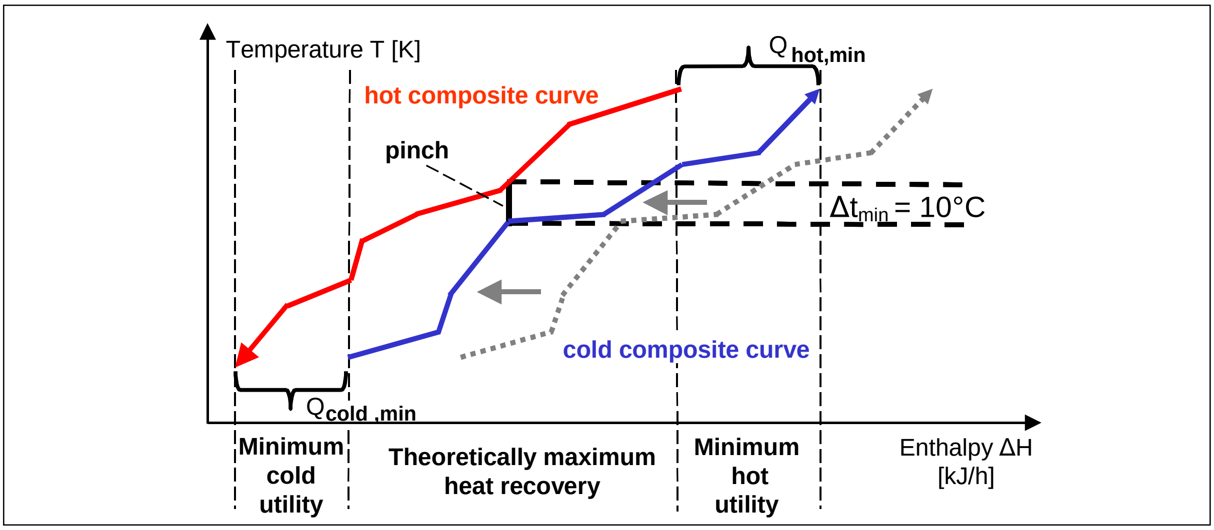

Figure 2.1: Hot and Cold Composite Curve [Linnhoff, 2004]

Since only changes of enthalpy are relevant, the curves can be moved horizontally in the diagram. Figure 2.1 shows a set of hypothetical streams. Together they represent the entire heat balance of the system. The points of a change in the slope in one of the composite curves indicate the start or the end of one flow or the onset of a phase change [Peters et al., 2003]. In order to ensure a heat transfer between cold and hot flows, the combined curves of the hot material flows must lie over those of the cold flows in all points, and thus are moved horizontally until this condition is met. The constraint set by ΔT_{min} is defined as the minimal temperature difference between the flows. Then the pinch point, where the distance between the hot and cold curves is minimal, denotes the possible optimal internal heat transfer between the hot and cold flows. By decreasing ΔT_{min} the composite curves can be shifted closer together, whereby the gradient must be larger than zero to enable a heat transfer ($\Delta T_{min} > 0$). $Q^*_{Hot,min}$ is the minimal amount of hot utility demanded for heating which cannot be covered by utilising the hot flows, whereas $Q^*_{Cold,min}$ represents the amount of heat which must be dissipated by external coolers.

The process streams on the right side of the (ΔH, T)-diagram above the pinch temperature require heating (these streams constitute the *heat sink*), whereas the process streams below the pinch temperature would need cooling (these streams are referred to as the *heat source*). More heating than $Q^*_{Hot,min}$ would lead to additional cooling and increase $Q^*_{Cold,min}$ at the end of the temperature intervals. This would be an indication of suboptimal energy use or mismatched energy demand.

A surplus of heat below the pinch point cannot be balanced with heat demand above the pinch, since energy would then need to be transferred against the temperature gradient. Incorporating these insights three basic rules valid for any pinch problem can be identified [see e.g. Peters et al., 2003; Radgen, 1996; Dunn and Bush, 2001; Linnhoff et al., 1979; Linnhoff and Turner, 1981]:

- no heat dissipation above the pinch,
- no heat supply below the pinch,
- no heat transport across the pinch.

The matching of hot and cold process streams can be done graphically by plotting the composite curves or by using optimisation algorithms (cf. Section 2.1.2).

2.1.1.2 Determination of Enthalpy Values

If the inlet temperature T_{in} and outlet temperature T_{out}, the mean specific heat capacity c_m and the amount G of a specific flow is known, the enthalpy value ΔH of that stream can be determined [Gregorig, 1973]:

$$\Delta H = c_m \cdot G\left(T_{out} - T_{in}\right) \text{ with } c_m = \frac{1}{T_{out} - T_{in}} \int_{t=T_{in}}^{T_{out}} c_p \, dt \tag{2.1}$$

However, in practice each process stream is characterised by a multitude of different material properties. In this case the process stream is not only characterised by inlet and outlet temperature T_{in} and T_{out} in K, but also by the flow rate r of the entire stream and the properties of its components w, such as the concentration as the mole fractions χ_w and the coefficients for the polynominal approximation of the specific heat capacity (phase specific) (A^g, B^g, C^g, D^g, E^g kJ/molK). For example the enthalpy value can then be determined by Equation 2.2 under *standard temperature and pressure (STP)* for a gaseous stream. Hereby, the standard molar volume of an ideal gas can be determined as $V_{STP} = 22.414 \text{ m}^3/\text{kmol}$ using the ideal gas law $(p \cdot V = n_x \cdot R \cdot T)$.

$$\Delta H = \frac{r}{V_{STP}} \cdot \sum_{w=1}^{W} \left(\chi_w \cdot \int_{t=T_{in}}^{T_{out}} \left(A_w^g + B_w^g \cdot t + C_w^g \cdot t^2 + D_w^g \cdot t^3 + E_w^g \cdot t^4 \right) dt \right) \tag{2.2}$$

The integrals are calculated by linear approximation of the sum of the integrals (*numeric integration*) using the midpoint rule [Schwarz, 1997]. An explicit solution is not possible since a primitive (function) cannot be defined for some integrals. For questions concerning the process, analysis focussing on the enthalpy values can be determined through numerical integration of Equation 2.2 with 0.1 K steps. In case of processes where a specific temperature must be maintained, i.e. $T_{in} = T_{out}$, the released or absorbed heat must be modelled differently or the enthalpy requirement must be given explicitly.

2.1.1.3 Concept of the Grand Composite Curve for Multiple Utilities

In a first step the pinch analysis determines the theoretical minimal heating and cooling requirements ($Q^*_{Hot,min}$ and $Q^*_{Cold,min}$) by using composite curves. However, it does not give information about the temperature levels at which the various utilities are used. As a pure thermodynamic analysis it assumes that there is enough utility at the maximal/minimal heating/cooling temperature level, but in most processes the utilities are used at different temperatures and different pressures. Table 2.2 shows some typical values.

Table 2.2: Typical Temperatures and Pressures for Utilities

Utility	**Temperature [K]**	**Pressure [bar]**
high pressure steam	703.15	26
middle pressure steam	523.15	15
low pressure steam	423.15	3
water	293.15	–
sole water	273.15	–
mechanical cooling I	253.15	–
mechanical cooling II	233.15	–
liquid nitrogen	193.15	–

In order to minimise overall costs, the costs of utility consumption must be considered. "The general objective is to maximise the use of the cheaper utility levels and minimise the use of the expensive utility levels" [Linnhoff, 1998]. Hence, if possible, low pressure steam is preferred to high pressure steam and conversely cooling water is preferred to mechanical cooling whenever possible. The concept of the *grand composite curve* enables this analysis by employing a heat profile. The grand composite curve shows the enthalpy demand above the pinch and the enthalpy supply below the pinch at each temperature level [Linnhoff, 2004]. It is the difference between the hot composite curve reduced by

$\frac{1}{2}\Delta T_{min}$ and the cold composite curve increased by $\frac{1}{2}\Delta T_{min}$. Consequently, the heat profile touches the ordinate at the pinch temperature (cf. Figure 2.2).

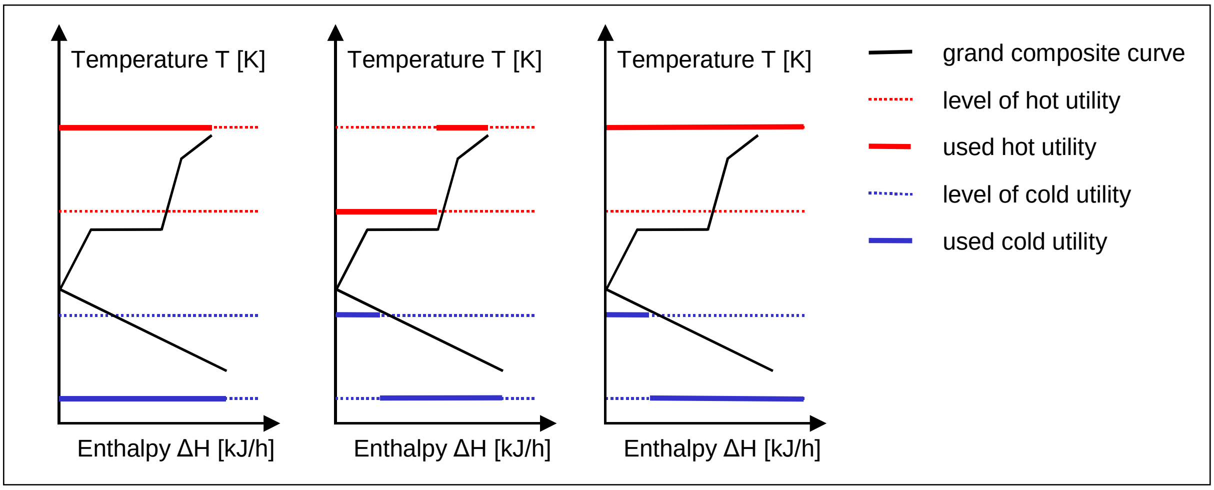

Figure 2.2: Heat Profiles by the Grand Composite Curve (adapted from [Linnhoff, 2004])

Figure 2.2 (left diagram) shows schematically the heat profile of a system. The maximal distance of the heat profile above the pinch marks the minimal heating requirement $Q^*_{Hot,min}$ and the maximal distance below the pinch marks the minimal cooling $Q^*_{Cold,min}$. These are identical to the minimal requirements in the analysis of the composite curves. The temperature levels of the available heating and cooling utilities are added as dotted lines in Figure 2.2. The actual utility used is marked as a bold line covering the utilities at each level.

The maximal use of low pressure instead of high pressure steam or cooling water instead of mechanical cooling can be calculated by the difference of the grand composite curve to the ordinate at the given temperature level (cf. dotted, horizontal line in the middle diagram in Figure 2.2). These points are called "utility pinch points". Depending on the costs for each utility and the specific costs for the heat exchanger it can be more economic to use more than the required minimal heating or cooling (cf. right diagram in Figure 2.2). By utilising the gradient higher than ΔT_{min} a smaller transfer area is needed in case of using heat exchanger, which could outbalance the costs of the additional utilities in contrast to the maximal integration.

2.1.2 Application of the Transportation Algorithm

The problems addressed by the pinch analysis can be solved graphically or analytically. By linearising the hot and cold flows a transformation of the pinch problem into an automated solving routine, as a transportation problem from Operations Research where efficient algorithms exist for solving the *minimal energy input*-optimisation problem, can be demonstrated [Cerda et al., 1983]. Questions concerning the aspects of this section have been addressed in [Treitz et al., 2004a; Geldermann et al., 2006b].

In order to solve the pinch analysis problem with a linear optimisation approach, the objective function of the general minimisation equation of the classical transportation problem is extended. The original parameter c_{ij} indicates the costs per unit transported material from production site i to customer j and x_{ij} denotes the transported quantity. In an analogous manner, the extended objective function as the minimum utility problem can be stated as follows [Cerda et al., 1983]:

$$\min_{q_{ik,jl}} \sum_{i=1}^{C} \sum_{k=1}^{L} \sum_{j=1}^{H} \sum_{l=1}^{L} C_{ik,jl} \cdot q_{ik,jl} \qquad (2.3)$$

The variable $q_{ik,jl}$ (heat transferred) corresponds to x_{ij} (material transported) [Geldermann et al., 2006b]. The transport prices c_{ij} per unit transported material are translated to the parameter $C_{ik,jl}$, which defines the costs associated with an possible heat exchange. In order to solve the transport algorithm with a linear optimisation algorithm it is transformed with a truncated incidence matrix into a standard linear programming problem [Neumann and Morlock, 1993]. In this way the transport algorithm can be solved with the *OptimisationToolbox* of *MATLAB*™ . In general, two types of analysis are possible: *(1)* a *thermodynamic approach* and *(2)* an *economic approach*. For both of these, if the temperature of the cold composite curve is already warmer than the temperature of the hot composite curve (i.e. $l > k$) a heat exchange against the temperature gradient is impossible and $C_{ik,jl}$ is allocated for a numeric determination with a large (infinitely high) value M (cf. Equation 2.4 and Equation 2.7).

2.1.2.1 Thermodynamic Approach

In the *thermodynamic approach* the possible heat exchanges between process flow combinations are allocated zero costs, whereas the fulfilment of heating or cooling duty by utility consumption are allocated costs of one [Cerda et al., 1983]. For the thermodynamic approach only one hot utility and only one cold utility are considered, i.e. $s = 1$ and $t = 1$, since a distinction between different available utilities is not necessary.

$$C_{ik,jl} = \begin{cases} 0 & \text{for } i \text{ and } j \text{ are both process streams and match is allowed, i.e. } k \leq l \\ 0 & \text{for } i \text{ and } j \text{ are both utility streams, i.e. } (i = C, j = H, s = 1, t = 1) \\ 1 & \text{only } i \text{ or } j \text{ is a utility stream} \\ M & \text{otherwise, where } M \text{ is a very large (infinite) number} \end{cases} \tag{2.4}$$

2.1.2.2 Economic Approach

In the *economic approach* the cost coefficients are specified in more detail. The driving cost factor is the heat exchange area A of the considered heat exchanger[3], which depends on the heat quantity to be exchanged ΔQ, the mean logarithmic temperature gradient ΔT_{ln} and the overall heat transfer coefficient α (cf. Equation 2.5) [Gregorig, 1973]:

$$A = \frac{\Delta Q}{\alpha \cdot \Delta T_{ln}} \tag{2.5}$$

Whereas the temperature difference ΔT is sufficient for a differential surface element dA of A, integration requires the calculation of a mean temperature difference ΔT_{ln} (cf. Equation 2.6) as a mean for ΔT since the temperature gradient is not constant within the heat exchanger[4] [Eastop and McConkey, 1969]:

$$\Delta T_{ln} = \frac{\Delta T_1 - \Delta T_2}{ln \frac{\Delta T_1}{\Delta T_2}} \tag{2.6}$$

For example Figure 2.3 shows the temperature profile in a concurrent and a countercurrent heat exchanger and the schematic run of the temperature curves. In case $\Delta T_1 = \Delta T_2$ then ΔT_{ln} is defined as $\Delta T_1 = \Delta T_2 = \Delta T_{ln}$.

[3] Depending on the geometry of the heat exchanger the surface area A depends on further variables as for example for a tube and shell heat exchanger the surface area A depends in addition on the length l, the diameter d, the number of tubes, etc. [Gregorig, 1973]. In the following Equation 2.5 is used as an estimate for A.

[4] The definition of Equation 2.6 depends on the geometry of the heat exchanger and specific correction factors can be defined for the different heat exchangers as for example tube and shell heat exchanger [Gregorig, 1973]. In the following Equation 2.6 is used as an estimate for the mean temperature difference.

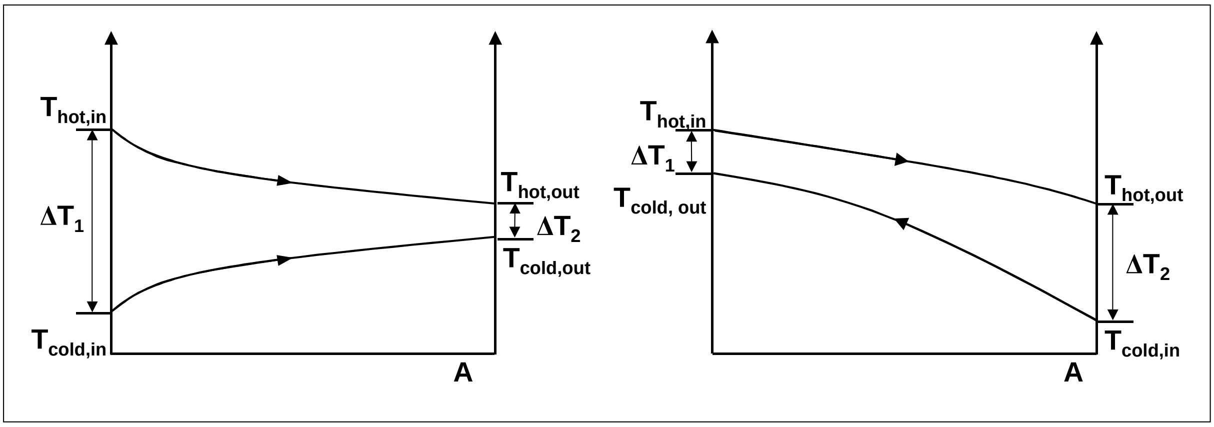

Figure 2.3: Profile of the Temperature Gradient within a Concurrent (left) and Countercurrent (right) Heat Exchanger [Eastop and McConkey, 1969]

Therefore, the cost coefficients $C_{ik,jl}$ for the economic approach can be formulated as shown in Equation 2.7:

$$C_{ik,jl} = \begin{cases} f_{proc}(A^n \cdot \kappa_{proc}) & \text{for } i \text{ and } j \text{ are both process streams and match is allowed, i.e. } k \leq l \\ 0 & \text{for } i \text{ and } j \text{ are both utility streams, i.e. } (i = C, j = H, s = 1, t = 1) \\ f_{util}((A^n \cdot \kappa_{util,i,j}) + \sigma_{util}) & \text{only } i \text{ or } j \text{ is a utility stream} \\ M & \text{otherwise, where } M \text{ is a very large (infinite) number} \end{cases} \quad (2.7)$$

The specific costs are referred to per unit heat transferred, i.e. $\Delta Q = 1\,\text{kJ/h}$. In the case of integration, i.e. a heat exchange between two process streams, the costs[5] depend on the heat exchange area A and the specific costs [€/m^2] for the heat exchanger κ_{proc}. In the case of heat transfer between a process stream and a utility, individual specific costs $\kappa_{util,i,j}$ [€/m^2] are assumed and the price of the utility σ_{util} [€/kJ] is considered. Since the actual quantity of heat transferred is not known in advance of the optimisation, an iterative, for example simulation based approach, would generate more exact cost parameters using the factor n of the economies of scale[6]. Nevertheless, the relative cost structure can be estimated sufficiently.

[5] In addition further costs are generated as for example the costs for the pump energy. These costs are neglected in the following.

[6] In general 0.6 is a good approximation for n and consequently n is also called the six-tenth factor. In case of heat exchangers depending on the geometry, material etc., more specific values for n can be determined (e.g. 0.82 for a plate heat exchanger).

2.1.2.3 Constraints

Equation 2.8 states that the heat required by cold stream i in interval k must be transferred from any hot stream. In the same manner, Equation 2.9 states that the cooling of hot stream j in interval l must come from any cold stream. The transferred heat $q_{ik,jl}$ must be nonnegative ($q_{ik,jl} \geq 0 \,\forall\, i, k, j, l$), which ensures that there is no heat moving from a cold stream to a hot stream.

$$\begin{aligned} &\sum_{j=1}^{H} \sum_{l=1}^{L} q_{ik,jl} = a_{ik} \\ &i = 1, 2, ..., C \\ &k = 1, 2, ..., L \end{aligned} \tag{2.8}$$

$$\begin{aligned} &\sum_{i=1}^{C} \sum_{k=1}^{L} q_{ik,jl} = b_{jl} \\ &j = 1, 2, ..., H \\ &l = 1, 2, ..., L \end{aligned} \tag{2.9}$$

$$a_{C-s+1,1} \geq \sum_{j=1}^{H-1} \sum_{l=1}^{L} b_{jl} \quad \forall\, s \tag{2.10}$$

$$b_{H-t+1,L} \geq \sum_{i=1}^{C-1} \sum_{k=1}^{L} a_{ik} \quad \forall\, t \tag{2.11}$$

Furthermore, there is the assumption that there is enough cooling (cf. Equation 2.10) and enough heating capacity (cf. Equation 2.11) of each of the utility streams to satisfy all cooling and heating requirements. Moreover, the problem stated assumes a given minimum ΔT_{min} driving force, implicitly given by the required heat a_{ik} and the available heat b_{jl} per interval k and l respectively.

In addition, constraints can be chosen in such a way that certain energy flow combinations are excluded, for example due to excessive distances between sources and sinks. For an in-depth description of the application of the transport algorithm to the pinch point analysis see [Cerda et al., 1983].

2.1.2.4 Determination of the Pinch Points

The pinch point denotes the optimal internal heat transfer between the hot and cold flows [Linnhoff and Flower, 1978]. In order to numerically calculate the position of the pinch points on the composite curves two approaches are possible based either on the tableau of the transportation problem [Cerda et al., 1983] or on heat balances of the individual temperature intervals [Linnhoff and Flower, 1978]. Using the heat balances of the composite streams the pinch points can be identified efficiently.

With the linear approximation of all process streams within each temperature interval, the composite curves are a combination of straight lines aggregated from the different streams in the intervals k and l for all cold streams i and all hot streams j. It can be shown that only corner points (points where at least one of the composite curves changes its slope) and end points can be potential pinch points [Cerda et al., 1983]. These are the boundaries of the different intervals k and l of L. In a preceding step a set of viable pinch points can be identified thus reducing the size of the initial problem significantly [Cerda et al., 1983]. Since only points with a change in the slope of either one of the composite curves can be candidate pinch points, intervals without any change in slope of both of the composite curves can be merged. This distinction is even more precise because points on the cold composite curve are only candidates if the slope becomes flatter at this point, whereas points on the hot composite curve are only candidates if the slope is steeper above the point [Cerda et al., 1983].

Energy balances are determined for each temperature interval $T_k = [T_{in,k}, T_{out,k}]$ of the composite curves of heat demand I_k ($I_k = \sum_{i=1}^{C-s} a_{ik}$) and heat supply O_k ($O_k = \sum_{j=1}^{H-t} b_{jk}$) starting at the highest temperature. A positive balance thus implies a heat demand in temperature interval T_k. Basic thermodynamics states that heat transfer can take place only from higher to lower temperatures. This means that a resulting heat supply balance from higher temperature intervals can be passed on to lower temperature intervals (i.e. there is a heat flow between the temperature intervals). Consequently, a heat oversupply can be passed on whereas a shortage must be filled by utilities. The assumption in this case is that it is irrelevant whether the utility supply takes place in every temperature interval individually or the total heat demand is supplied to the temperature interval with the highest temperature and is then distributed through the temperature intervals by a heat flow [Linnhoff and Flower, 1978]. Thus, the maximal aggregated heat demand of the heat balances must be supplied to the system. In this case the heat flow between the intervals balances generated heat demand. The pinch point lies in the temperature interval in which the remaining supplied heat is completely consumed. At this point no heat flow exists between the temperature intervals above and the temperature intervals below.

2.1.3 Discussion of the Thermal Pinch Analysis

The fact that an optimum is sought with respect to heat recovery rather than costs in the *thermodynamic approach* might at first appear to be a disadvantage. However, since the overall costs are dominated to a large extent by the costs of energy, all different networks which feature maximum heat recovery are suitable as starting networks for the design [Linnhoff and Flower, 1978].

Numerous papers exist proposing modifications to the classical pinch analysis in order to cover unique processes not considered in the simple model. Special attention must be paid to processes where the composition of the stream changes, for example separation processes, mixing points, direct heating, etc. Furthermore, discontinuous composite curves can be modelled [Lakshmanan and Fraga, 2002]. In general the methodology assumes that at least one cold and one hot process stream within the temperature range exist. If this is not the case it is possible to acquire multiple pinch points and then determine lower and upper bounds on ΔT_{min} in order to determine the thermodynamic optimum [Lakshmanan and Fraga, 2002].

2.1.3.1 Application of the Thermal Pinch Analysis to Batch Processes

The classical pinch analysis approach only considers continuous processes and assumes the parameters to be time independent. In batch processes, however, not only temperature levels determine which processes can be combined, but also the changing availability over time addressed in *time average models*, *time event models* and *time slice models* [Obeng and Ashton, 1988; Linnhoff, 1993], where an analysis is done for each time interval and excess heat can be transferred not only from hot to cold streams, but also from earlier to later time intervals. Thus, as for any process integration analysis the modelling of batch process requires data about mass- and energy flows. However, for the determination of target values for batch processes further information is required concerning the time aspect of the operations. Three different approaches can be identified for the modelling of batch processes [Ashton, 1992]:

- **Time Average Models**: The heating and cooling requirements of the batch processes are "averaged" with respect to defined time intervals and the analysis is carried out analogous to the thermal pinch analysis of continuous process streams.
- **Time Event Models**: The scheduling of the operations is the base for the analysis using Gantt Charts by determining a critical path through the different heating and

cooling requirements and their specific time schedule. Focus of the analysis is the de-bottling of peak times of the system.

- **Time Slice Models**: Similar to the temperature intervals in the classical thermal pinch analysis, in time slice models starting and finishing points of all operations are ascertained a specific time interval. For each time interval the heating and cooling requirements are balanced. Nevertheless, excess heat of one time interval can be transferred to the next time interval constituting a heat source. By this preceeding a cascade of heat sources and sinks can be constructed.

Nevertheless, the models consider an intermediate heat integration as favoured over heat storage and later integration by constructing the batch cascade. In this context the type of energy with respect to storage and convertibility must be considered. An approach based primarily on a time analysis and to a lesser degree on temperature is also possible. By analysing the scheduling of the different processes an optimisation of the heat integration is targeted by re-scheduling the processes in order to reduce storage and peak loads of the utilities [Wang and Smith, 1995].

2.1.3.2 Translation of the Thermal Pinch Analysis to Production Planning

A modification to the modelling of the thermal requirements of batch process streams is an analysis of intra- and inter-company production networks on the basis of product streams. The *time-material production* relationship can be used for a pinch analysis approach for aggregate production planning [Singhvi and Shenoy, 2002; Singhvi et al., 2004]. One demand composite curve and one production composite curve can be constructed on a time average basis similar to batch processes (cf. Figure 2.4).

In this context aggregated production planning is defined as the identification of an overall level of production for an individual company or production network. The focus of the analysis is the evaluation of seasonal changes on the demand side, such as the demand of ice-cream or bicycles over a period of one year, and its effect on the level of production during the period considered.

Ideas from the analysis by the classical thermal pinch analysis can be used to find a robust production strategy: For example first, the translation of the minimal temperature difference ΔT_{min} as the gradient or driving force of the system into the minimal inventory level ΔI_{min}, or second, ideas from the optimisation of the scheduling of batch processes in time slice or time event models to the modelling of demand and supply relationships.

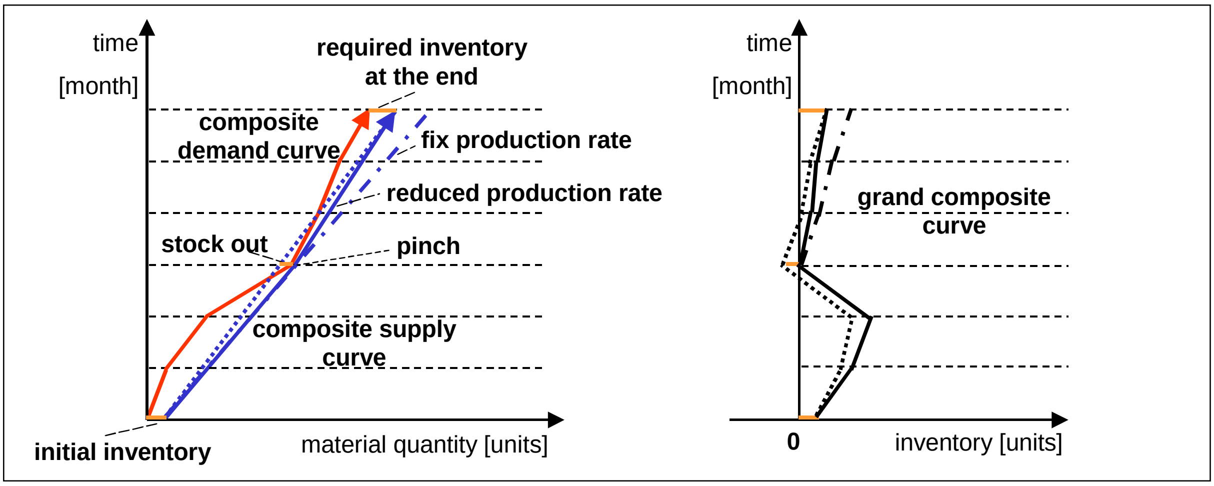

Figure 2.4: Production Planning [Singhvi and Shenoy, 2002]

2.1.3.3 Applicability of the Pinch Analysis Approach

In general the pinch analysis determines the composite curves and thus the theoretical minimal energy requirements for a fixed process layout and given process and material balances. If these parameters are altered a new iteration is necessary. However, the pinch analysis can be used to estimate if a modification is likely to be beneficial. As a general rule, however, for optimised process design the so-called *plus-minus principle (± principle)* [Linnhoff, 1998] is based on the concept that no heat transfer across the pinch point exists and states:

- reducing hot utility targets by
  - increasing hot stream duty above the pinch temperature
  - decreasing cold stream duty above the pinch temperature
- reducing cold utility targets by
  - decreasing hot stream duty below the pinch temperature
  - increasing cold stream duty below the pinch temperature

By applying the ± principle the proposed process modification can be evaluated and an approximation can be made about whether it will be beneficial or detrimental to the overall heat balance. The pinch analysis is used to evaluate a given design with respect to its heat balances and utility consumption.

The flexibility of the design is of importance too. If the layout of a standard design can be evaluated and its flexibility assessed, then modifications can be carried out using heat integration and the flexibility of the subsequent design can be compared to the original one [Alexander et al., 2000]. Consequently, layout planning is not only driven by a trade-off between equipment (such as heat exchanger) and operating costs (energy utility costs), but also by the feasibility, such as for example controllability, starting-up procedures, safety constraints, etc., and flexibility of the system.

2.2 Water Pinch Analysis

Although the pinch analysis was originally developed for the minimisation of energy consumption by effectively combining hot and cold streams, its principles can also be employed for water consumption and other auxiliary materials. The goal is always to reuse heat, water and auxiliary materials as efficiently as possible, while adhering to the requirements of the process steps. Analogous to the application of the thermal pinch analysis approach, the water pinch analysis can be used to calculate the target values based on either minimum fresh water consumption or minimum wastewater generation that maximise water reuse in a network of various water streams. Just as in the energy pinch analysis this approach focuses on the network of process streams instead of single process units: In this case reducing the demand for water by using the outlet water of one process unit to realise its own water requirements or that of other unit operations. The opposite approach would be to modify single processes or process units to reduce the overall water demand, such as using air-cooled instead of water-cooled condensers or improved blowdown rates.

The first pinch analysis based approach focussing entirely on water minimisation was a graphical methodology targeted at minimal fresh water and wastewater flow rates through the analysis of the *concentration vs. the mass load* of the different process streams [Wang and Smith, 1994]. This approach is based on a mass exchange problem between a set of contaminant rich process streams and a set of contaminant lean process streams [El-Halwagi and Manousiouthakis, 1989] and because "the amount of water required is a function of the quality of the water provided" [Polley and Polley, 2000] it is an approach based on water quality (cf. Section 2.2.1). Since unit operations with an unchanging mass load of the water stream, for example a cooling operation, can only be mapped with difficulty by the concentration vs. mass load approach different approaches were developed and coexist. The analysis on *concentration vs. flow rate* diagrams takes the water quantity (i.e. fixed flow rates) as the general basis to identify the water savings potential [Dhole et al., 1996; Polley and Polley, 2000; Sorin and Bédard, 1999; Linnhoff, 2004] (cf. Section 2.2.2.1). Further modifications used a simulation based approach considering various mixing possibilities of water source streams [Hallale, 2002]. Furthermore, a conceptually different approach used stream mapping diagrams (composition vs. flow rate) or condition mapping diagrams, for example *Chemical Oxygen Demand (COD)* vs. flow rate, focussing on identifying different recycling possibilities of single streams rather than constructing composite curves [Dunn and Bush, 2001] (cf. Section 2.2.2.2).

Table 2.3: Nomenclature for the Water Pinch Analysis

Variable	**Unit**	**Name**
c	$[ppm]$	concentration
ΔC_{min}	$[ppm]$	minimum concentration difference (driving force)
C_{reg}	$[ppm]$	concentration where regeneration starts
C_0	$[ppm]$	outlet concentration of the regeneration process
C_{pinch}	$[ppm]$	pinch concentration
R	[-]	regeneration
R_{const}	[ppm]	constant regeneration performance
$\Delta\dot{m}$	$[kg/h]$	mass transfer requirements
F_{WS}	$[m^3/h]$	feedstream of the fresh water supply
κ_{WS}	$[€/m^3]$	specific costs for fresh water supply
κ_{reg}	$[€/m^3]$	specific costs for regeneration
κ_{WW}	$[€/m^3]$	specific costs for wastewater discharge

The fundamental difference between the thermal pinch analysis and the water pinch analysis lies in the definition of the quality of a stream [Linnhoff, 2004]. The quality parameter in a heat integration analysis is the temperature. In a water pinch analysis the water quality is characterised by various parameters, for example COD, pH, suspended solids (SS) or the conductance of the water. If more than one quality parameter of the water streams is of significance to the processes they must be taken into account for the optimisation. Such "key contaminants" are defined as "any property that prevents the direct reuse of a wastewater stream" [Tainsh and Rudman, 1999]. In fact an analysis for each key contaminant has to be executed and a design must be developed iteratively. Given that graphical approaches are generally quite complex for multi-parameter cases or distributed wastewater treatment systems, the use of mathematical methods is more appropriate. A comprehensive overview of the theoretical principals, the different methodological approaches and industrial applications is provided by [Mann and Liu, 1999].

2.2.1 Approach based on Water Quality

The water pinch analysis approach based on water quality assumes a water network with several operations using water, which have individual inlet and outlet thresholds for a certain contaminant [Wang and Smith, 1994]. It requires no fundamental change to the process network layout during the analysis, which would necessitate a new start. The aim of the analysis is the determination of minimal water flow rates. It is a quality-based approach since the driving force of the analysis is the mass load that must be transferred from the process unit by the process water, for example measured in kg/h, which means that it is basically a contamination transfer problem from process streams to water streams. In order to achieve a reduction in the water consumption three generic strategies are used [Wang and Smith, 1994]:

- **Reuse**: consumption of wastewater in other unit operations either directly or blended with other wastewater or freshwater flows (cf. Section 2.2.1.1);
- **Regeneration Reuse**: consumption of wastewater in other operations (without re-entering the previous process again) after partial treatment and possible mixing with other wastewater or freshwater flows (cf. Section 2.2.1.2);
- **Regeneration Recycling**: consumption in all operations (including re-entering the previous process again) after partial treatment and possible mixing with other wastewater or freshwater flows (cf. Section 2.2.1.3).

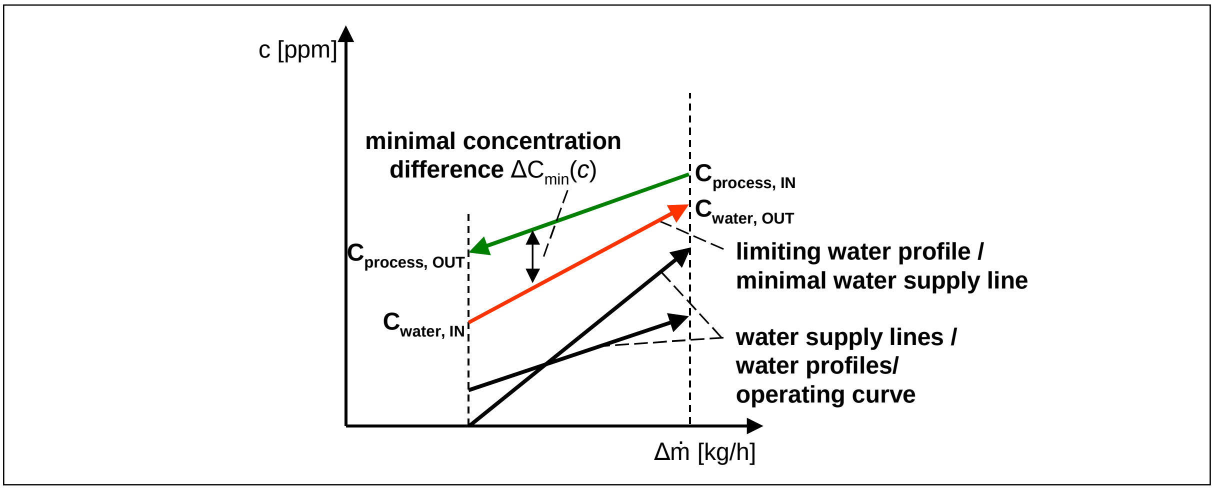

Figure 2.5: Representation of Water Using Processes [Wang and Smith, 1994]

The mass transfer requirements $\Delta\dot{m}$ and the inlet and outlet concentrations of a specific contaminant composition are the key indicators of the analysis. A linear behaviour is assumed for the transfer which is a good approximation for diluted streams, for example water used for washing [Henßen, 2004], and the driving force is the minimal concentration difference ΔC_{min}. The mass transfer requirements $\Delta\dot{m}$ of a process unit are specified and in combination with the concentration requirements they determine the minimal potential water flow rate, the so-called *limiting water profile* (cf. Figure 2.5). Different operating curves, i.e. water profiles or water supply lines, can be used in the process, but the limiting water profile is based on the highest possible inlet concentration and therefore maximises the reuse possibilities.

The maximal inlet and outlet concentrations of each process unit depend for example on the *(1)* required minimal mass transfer driving force ΔC_{min}, *(2)* maximal solubility, *(3)* precipitation avoidance, *(4)* fouling of equipment, *(5)* corrosion limitations, *(6)* minimal flow rate that prevents the settling of solid particles [Wang and Smith, 1994].

2.2.1.1 Case 1: Reuse

In the case of reuse the limiting water profiles of all operations are compiled in one concentration vs. mass load diagram (cf. Figure 2.6). Inlet and outlet concentrations of the different operations define concentration intervals. Overlapping concentrations are combined to a *limiting composite curve* (also *concentration composite curve*) taking into account all mass loads of the different operations of the respective concentration interval. The minimal freshwater supply is calculated by determining the steepest water supply line below the limiting composite curve. Assuming that the contaminant concentration of the freshwater at the inlet is zero, the water supply curve begins at the origin. The point where the water supply curve touches the limiting water profile is the pinch point. Since the mass transfer driving force is considered in the maximum inlet and outlet concentration, the driving force is not zero at the pinch point even if the water supply curve touches the limiting water profile.

The slope of the limiting water profile describes the worst water quality acceptable, and the water supply line defines the actual water flow rate in the system: A steeper straight line corresponds to a higher accumulation of the contaminant in the water which means the same mass load is collected by a smaller flow rate. Hence, the steepest possible water supply curve minimises the required flow rate and the optimisation potential can be determined by the difference in the slopes. The difference between the operating water supply line and the limiting water profile illustrates the water savings potential (cf. Figure

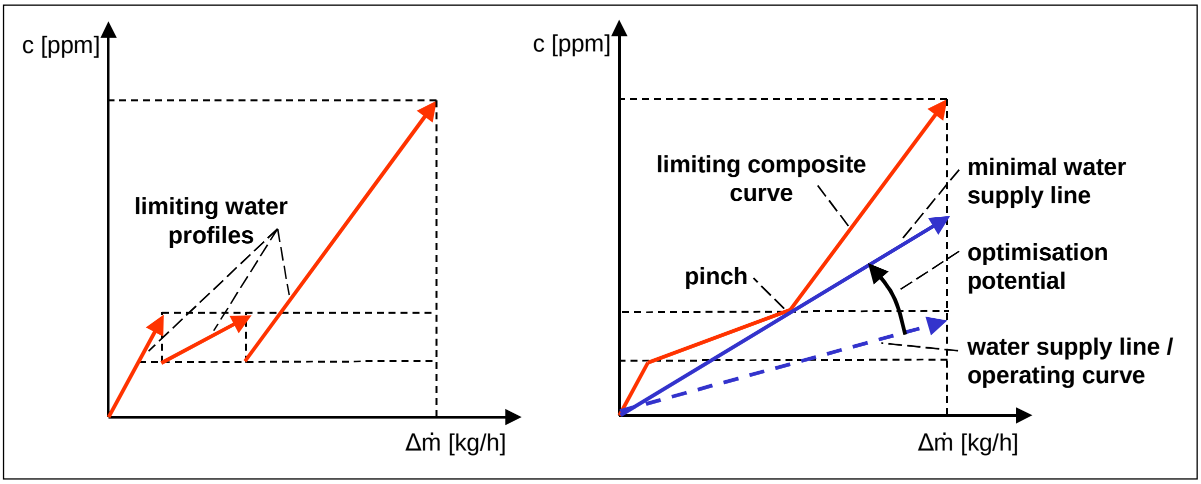

Figure 2.6: Match of Limiting Composite Curve and Water Supply Line [Wang and Smith, 1994]

2.6). However, a steeper line corresponds to a lower fresh water flow rate, but since the total mass load is fixed, this leads to higher contaminant outlet concentrations.

Practical problems often require the consideration of several contaminants or parameters. If it is not possible to aggregate multiple contaminants to a single parameter, such as Chemical Oxygen Demand - COD, an iterative process must be applied by shifting the inlet and outlet concentrations of each process in order to find the overall pinch in the system. The basic assumption in this approach is an underlying correlation between the mass transfer of the different contaminants, for example a proportional mass transfer of all contaminants to one reference contaminant.

2.2.1.2 Case 2: Regeneration Reuse

Furthermore, the concept of regeneration and reuse takes into account that wastewater regeneration lowers the concentration of the contaminants and consequently allows further reuse options and a reduction in fresh water demand. Using individual or combined preliminary and primary wastewater treatment operations, for example grates, filtration, settling tanks, or biological treatment operations, such as fixed bed reactor, aeration tank, the concentration of certain contaminants can be reduced. Consequently, the water can be used in processes for which the concentration was too high before regeneration. In the case of several wastewater treatment operations, all operations are combined to a single one characterised by a certain degradation rate R_{const} or outlet concentration C_0. In the analysis the same flow rate before and after the regeneration is assumed: visualised by the same slope of the water supply curve before and after regeneration (cf. Figure 2.7).

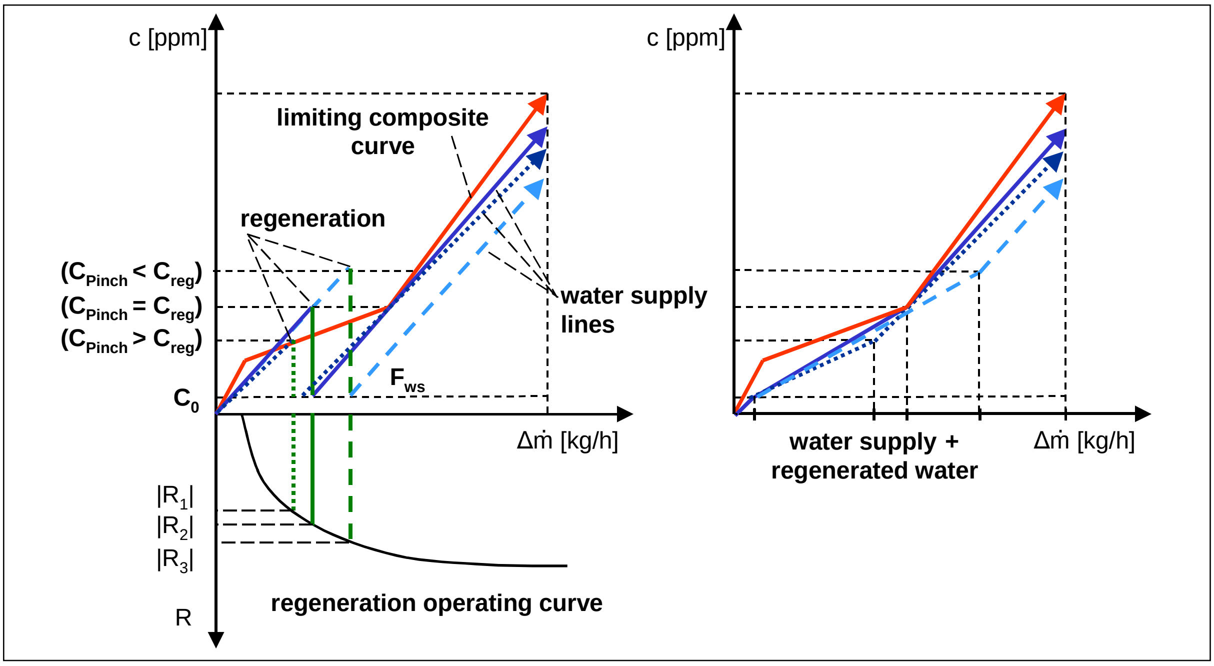

Figure 2.7: Regeneration of Water with Fixed Outlet Concentration of the Regeneration [Wang and Smith, 1994; Henßen, 2004]

In case of a constant outlet concentration, the concentration of the contaminant in the wastewater is reduced to C_0 as soon as the regeneration concentration C_{reg} is reached. Between C_0 and C_{reg} the water supply curves are combined to a single composite water supply curve. C_{reg} should be chosen in such a way that the composite water supply curve is as close as possible to, and below the limiting composite curve. Assuming a constant outlet concentration C_0 different performances of regeneration R can be determined for different C_{reg} (cf. Figure 2.7). It can be shown that it is optimal if C_{reg} is equal to the concentration at the pinch point C_{pinch} [Wang and Smith, 1994]. A lower regeneration concentration would stand for a larger difference between the composite curves and hence would require a higher flow rate. A higher regeneration concentration would still minimise the flow rate, but would require an unnecessary effort (cf. Section 2.2.1.4).

2.2.1.3 Case 3: Regeneration Recycling

In the case of regeneration operations including the possibility of recycling of water even higher reductions in the water consumption can be achieved. The processes below C_0 must be fed by freshwater supply since this concentration level cannot be achieved by the regeneration process. Hence, if a circulation of the process water is possible, the flow rate is determined by the slope of the limiting composite curve below the concentration C_0 (cf.

Figure 2.8). In this case the water flow rate after regeneration is increased by the closed loop water and the slope after regeneration shows the amount of regenerated water.

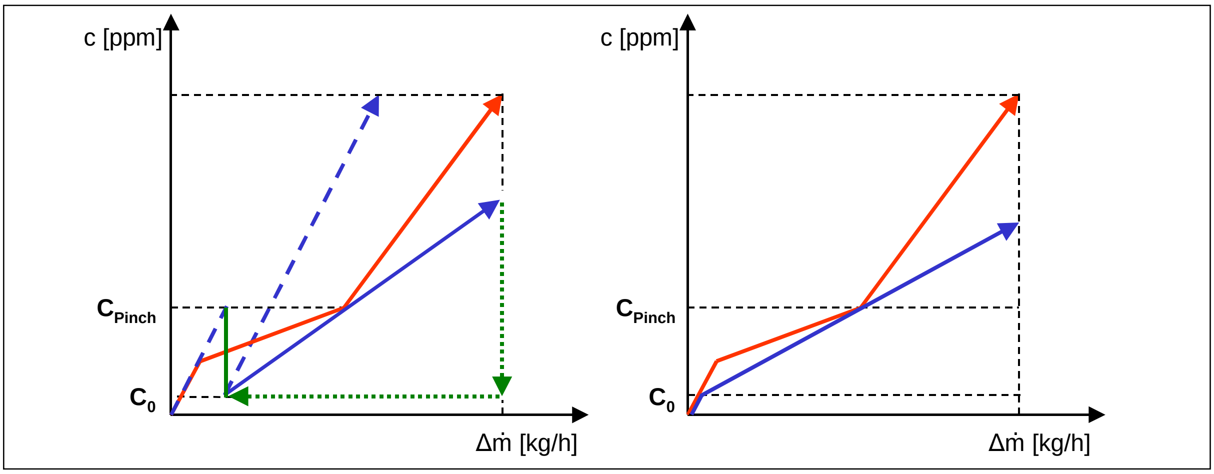

Figure 2.8: Recycling of Regenerated Water [Wang and Smith, 1994]

In the event no recycling of water would be used, but regeneration only, a constant flow rate before and after regeneration, illustrated as the blue dotted curve to the left in Figure 2.8, would result. However, the limiting composite curve would be crossed. In order to prevent this, the additional demand for water must be covered using recycling water.

2.2.1.4 Economic Considerations

Economic considerations have been introduced to the water pinch analysis based on water quality [El-Halwagi, 1997; Henßen, 2004]. In this thesis the trade-off between the costs of regeneration and fresh water supply is modelled by the cost coefficients κ_{WS} for the specific costs for fresh water supply and κ_{reg} for the specific costs for regeneration in €/m^3. As shown in the thermal pinch analysis (cf. Section 2.1.1.3) the flow rate of the fresh water supply can vary from the minimal flow rate because of economic reasons. Furthermore, the discharge of water can be penalised by a wastewater charge κ_{WW}

The consideration of multiple feedstreams for fresh water supply and multiple contaminants with economic considerations can be achieved by an iterative approach [Henßen, 2004]

2.2.2 Approaches based on Water Quantity and Mapping

Different approaches for the optimisation of water networks evolved from criticism of limitations of the quality based approach. The major limitation of the quality based approach stems from the central role of mass transport [Dhole et al., 1996]:

- The mass transfer model is only suitable for fundamental operations of mass transport on the water stream, such as cleaning. Reactors, boilers or cooling towers with negligible mass transfer, where the flow rate is of crucial importance, cannot be modelled sufficiently as mass transfer operations.
- Operations consisting of several water streams containing different contamination levels can only be modelled poorly.
- Flow changes within a certain plant component, such as evaporation in a cooling tower, are difficult to take into account.

Therefore, approaches focussing on the quantity of water demand and supply of the single processes (cf. Section 2.2.2.1) and on identification of correct mixing and recycling possibilities (cf. Section 2.2.2.2) exist.

2.2.2.1 Approach based on Water Quantity

In the approach based on water quantity each sink is characterised by its water demand and the maximum allowable inlet contaminant concentration, and each source by its water supply and respective contaminant outlet concentration. In the case of a single quality parameter the streams can be plotted in the *purity vs. concentration profile* (cf. Figure 2.9). In contrast to the quality based approach the water quality of the streams is constant. The maximum concentration of inlet and outlet concentration is shown and consequently each stream can be expressed by a horizontal line. The length illustrates the flow rate of each stream for a given (or allowable) concentration.

All sources together (red line) and all sinks (blue line) constitute stepped composite curves (cf. Figure 2.9). The composite curves can be shifted horizontally, since the streams are independent of the absolute mass load requirement. The sink composite curve can thus be moved from the right towards the source composite curve until they touch. The point at which they contact is termed the pinch, analogous to the thermal pinch analysis. Sinks located beneath the source curve can reuse the water from the sources above, since the source streams have the necessary quality. Uncovered sinks located to the right of the

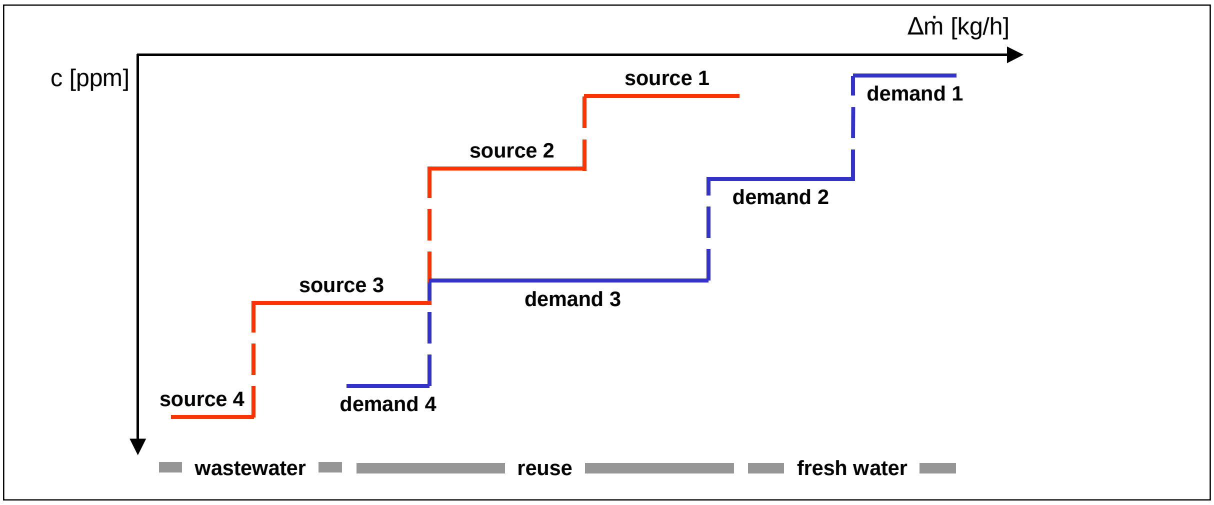

Figure 2.9: Water Composite Curves [Dhole et al., 1996]

potential reusable water area need fresh water, while those to the left produce wastewater, which means that a portion of the source streams of poor quality have no corresponding sink.

The pinch divides the streams into two subsystems of water deficit and water oversupply. As in the case of the thermal pinch analysis the optimal water transfer is governed by three rules [Linnhoff and Hindmarsh, 1983]:

- Water cannot be transferred across the pinch. Transfer from sources below the pinch to sinks above the pinch is impossible due to the contaminant concentration. If, on the contrary, water from sources above the pinch is passed to sinks below the pinch, a deficit of previously available source water above occurs, which must be compensated by additional fresh water. More water is now available below, however, it can only be discharged as wastewater since all the sinks are already completely supplied by the sources. Transport across the pinch would thus lead to more fresh water and wastewater;

- Wastewater cannot occur above the pinch since in this area of water deficit all source streams can be reused for the sinks;

- Below the pinch no fresh water can be employed because this area is characterised by a water oversupply and the water demand from all the sinks is satisfied by the source streams.

Constructing the composite curves on the basis of the source streams does not consider any changes in the source stream composition. Hence, mixing of source streams changes the shape of the source composite curve and consequently the targets (cf. Figure 2.10). In this sense the proposed methodology based on water quantity does not calculate the complete potential for reuse, but rather a too small savings potential. Therefore, the methodology does not determine the overall target detached from any network design.

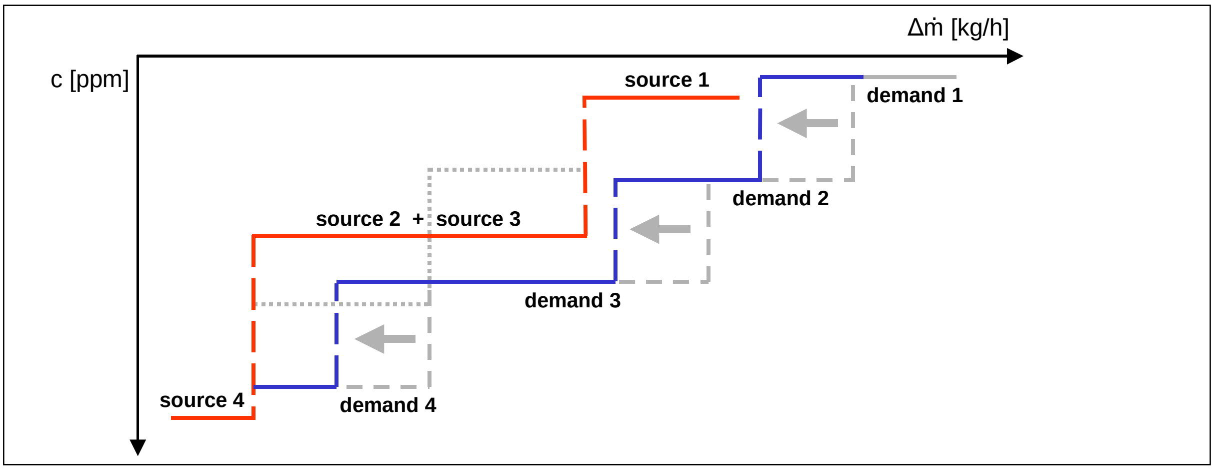

Figure 2.10: Mixing Modifies the Shape of the Source Composite Curve [Dhole et al., 1996]

Consequently, the approach was extended using systematically the key principle: "Fresh water use is minimised when the contaminant uptake of water demand is maximised" [Polley and Polley, 2000]. This means that if source streams cannot be used directly they are mixed with each other and where necessary with fresh water until they are able to meet the demand of the water using process with the highest requirements both in terms of quantity and in terms of quality. Source and sink streams are used in ascending concentration order [Polley and Polley, 2000].

This approach is visualised in Figure 2.11: In a first step the demand of stream "demand 1" is satisfied because it has the strictest water requirements. Since the quality of "source 1" does not meet the requirements of "demand 1" it is diluted with fresh water. The residual of source stream 1 is mixed with source streams 2 until it just meets the water quality requirements of "demand 2". The remaining quantity is filled with fresh water.

According to the general procedure the required quantity is determined and in case of a disequilibrium a shortage is balanced by fresh water. In case of an excess supply the water quality is concentrated with other source streams of higher contaminant concentration until it just meets the demand requirements. Applying this principle guarantees a

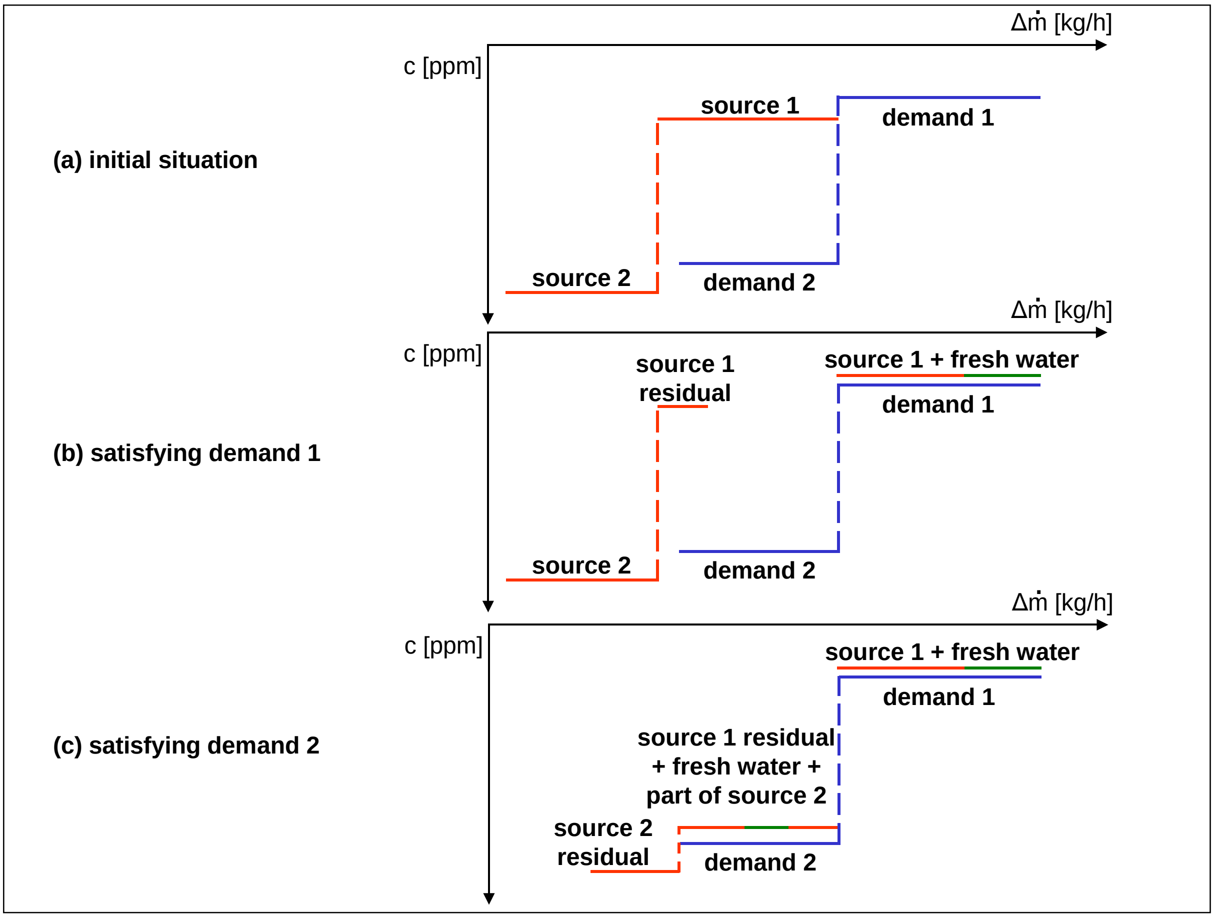

Figure 2.11: Conceptual Example of Mixing of Source Streams with Fresh Water [Polley and Polley, 2000]

minimum fresh water supply. Instead of allowing a higher concentration difference as a driving force in the process the source streams are mixed to maximise reuse possibilities. This approach might lead to a combination of various source streams and a very complex network. Hence, a simplification of the network is necessary after the analysis increasing the fresh water demand again. A general disadvantage of this approach is that only reuse of water is considered and no regeneration or recycling processes are modelled. In order to identify reasonable recycling alternatives an approach based on stream mapping diagrams (cf. Section 2.2.2.2) can be used to identify a well selected source composite curve.

2.2.2.2 Approach based on Stream Mapping

In general, the same data set (*concentration vs. mass load* of the individual water streams) is used in the approach based on stream mapping to identify recycling options in a given water flow network. However, rather than constructing composite curves the outlet concentrations of the different sources are compared to the required inlet concentrations of the various sinks (cf. Figure 2.12). In this sense the approach based on stream mapping is not a water pinch analysis. Rather than systematically analysing the given process streams, different recycling possibilities can be identified by stream conditions.

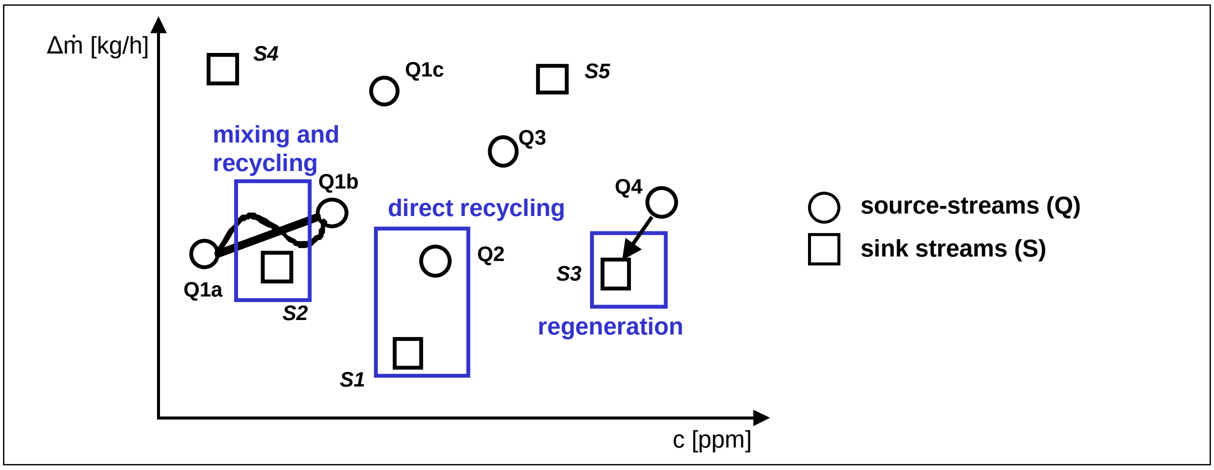

Figure 2.12: Stream Mapping Diagram [Dunn and Bush, 2001]

By plotting existing or required flow rates of the source and sink streams against existing or required parameters different connection options arise. Three generic possibilities to identify connection options through the network exist [Dunn and Bush, 2001]: *(1) direct recycling* (including splitting up of sources, e. g. Q_1 into Q_{1a},Q_{1b},Q_{1c}), *(2) mixing* of water streams and *(3) regeneration* opportunities, i. e. the source stream is regenerated to reduce the composition to an acceptable level for reuse. The general procedure begins with sinks requiring fresh water (contaminant concentration equals zero), which must be satisfied. Next the requirements of all other sinks are met by reusing the regenerated water of the process itself or by mixing it with fresh water or streams containing lower contaminant concentrations. However, by this procedure not an overall savings potential can be identified and higher gradients for reusing water are not considered. Nevertheless, the strength of this approach lies in the analysis of a complete process network illustrating the streams in the stream mapping diagram and selecting appropriate streams to be mixed.

2.2.3 Discussion of the Water Pinch Analysis

Each of the presented water pinch methodologies has its own inherent advantages and shortcomings. But the accepted and numerous applications of the water pinch approaches found in a variety of industry sectors show their impact on industrial wastewater management, for example in the pulp and paper industry [Koufos and Retsina, 2001], breweries [Linnhoff, 2004], citrus plants [Thevendiraraj et al., 2003] or beat sugar plants [Vaccari et al., 2005].

One significant advantage of the approach based on water quality is that wastewater streams of varying contaminant level can be mixed and an overall target can be determined. By characterising fresh water and wastewater streams with specific costs and associating costs to regeneration processes an economic assessment is possible.

The central role of mass transport limits this approach to fundamental operations of mass transport, such as cleaning as a quality controlled operation, and other operations with negligible mass transfer, where the flow rate is of crucial importance, cannot be modelled adequately, such as reactors, boilers or cooling towers as quantity controlled operations. Furthermore, the application of the methodology to multi-parameter cases is quite complex even for small numbers of streams and the correlated transfer is not always valid.

The approach based on water quantity can adequately present water using processes without mass transport and the optimal combination of sources and sinks can be modelled as a linear optimisation problem. However, this simple combination of streams is also the major drawback to the approach: The mixing of multiple source streams is not considered or if explicitly permitted leads to a multitude of counterproductive mixing solutions. Consequently, purity - concentration profiles only portray a certain interpretation of the total process [Hallale, 2002]. The results of the optimisation therefore need not be equivalent to the actual optimum, because a suitable mixing of the source streams can shift the pinch point and thus lead to an improved reuse of the water. The same is true for the approach based on stream mapping. The major advantage of that approach is the identification of correct mixing and recycling possibilities.

Considering the various aspects only a case specific application of the different approaches or their combination appears reasonable to identify meaningful target values.

2.3 Solvents Pinch Analysis

Besides pure heat integration in the classical pinch analysis and mass integration, as for example in the water pinch analysis, another application of the pinch analysis is for solvents or multi-component solvents. The recovery of organic solvents (Volatile Organic Compounds (VOC)) of a gaseous waste stream can be translated into a heat exchange problem because the solvents can be separated from the waste gas via thermal condensation [Dunn and El-Halwagi, 1994; Parthasarathy and El-Halwagi, 2000]. The reduction of VOC in gaseous waste via mass integration, for example adsorption and absorption, is not considered in this section [see e.g. El-Halwagi, 1997, for more details on this].

Table 2.4: Nomenclature for the Solvents Pinch Analysis

Variable	**Unit**	**Name**
T	$[K]$	temperature
T_{End}	$[K]$	end point temperature of condensation
$T_{LowerEnd}$	$[K]$	lower bound of temperature range of condensation
$T_{UpperEnd}$	$[K]$	upper bound of temperature range of condensation
T^S	$[K]$	supply (inlet) temperature of gaseous waste stream
T^C	$[K]$	dew temperature of VOC
ΔT_{min}	$[K]$	minimum temperature gradient (driving force)
ΔT_{ln}	$[K]$	logarithmic mean temperature difference (LMTD)
h	$[kJ/kmol \cdot K]$	specific enthalpy of gaseous stream
r_{STP}	$[m^3/h\,(STP)]$	flow rate under standard temperature and pressure (STP)
A	$[m^2]$	heat transfer area
α	$[kW/m^2 \cdot K]$	heat transfer coefficient
$c_{p,L}$	$[kJ/kmol \cdot K]$	specific heat capacity of the VOC liquid
$c_{p,V}$	$[kJ/kmol \cdot K]$	specific heat capacity of the VOC vapour
$c_{p,g}$	$[kJ/kmol \cdot K]$	specific heat capacity of the VOC-free gas
κ^D	$[€/m^2]$	specific costs for heat exchanger surface area for dehumidification
κ^C	$[€/m^2]$	specific costs for heat exchanger surface area for condensation
κ^I	$[€/m^2]$	specific costs for heat exchanger surface area for integration

Table 2.4: Nomenclature for the Solvents Pinch Analysis (cont.)

Variable	**Unit**	**Name**
w	$[-]$	component w of the gaseous stream ($w = (1, 2, \ldots, W)$, W as number of components ($W \in \mathbb{N}$)
χ_w	$[-]$	mole fraction of component w
χ^s	$[kmol\ VOC/\ kmol\ VOC\ free\ gas]$	supply composition of gaseous waste stream
χ^t	$[kmol\ VOC/\ kmol\ VOC\ free\ gas]$	target composition of gaseous waste stream
λ	$[kJ/kmol]$	latent heat of condensation
σ_{util}	$[€/kJ]$	price of utility *util*

By using phase diagrams the targeted solvents concentration can be described by the temperatures of the gaseous waste stream [Geldermann et al., 2004]. Thus, the required temperature intervals for applying the pinch analysis can be obtained. When using multi-stage condensation for VOC recovery the waste gas can be pre-cooled by the cold cleaned gas stream. This approach of incorporating the cleaned gas stream can also be applied when other emission reduction measures are used, such as thermal incinerators [Geldermann et al., 2006b]. The application of the solvents pinch analysis and the subsequent integrated design are used to find the most cost-effective solution. Consequently, the quantity of solvents to be recovered can be determined [Parthasarathy and El-Halwagi, 2000]. The total costs in the case of VOC are a combination of those for purchased solvents and those for condensation. The recovered solvents can be reused in the same process or they can even be sold, for example for cleaning applications, depending on the option finally selected. The properties of the employed solvents (VOC) determine the temperature intervals used in the pinch analysis. Since a complete condensation of the VOC is theoretically possible ($\chi^t = 0$), the objective is to find a feasible economic solution through a techno-economic assessment of available techniques.

2.3.1 Principles of the Condensation System

Fundamentally, the analysis is based on *temperature - concentration relationships* (cf. Figure 2.13) depending on the temperature-sensitive *saturation pressure curves* of the single or multi-component VOC considered in a gaseous waste stream [Schollenberger and Treitz, 2005]. By describing the concentration of VOC in the waste gas as dependent variable of the waste gas temperature, the mass transfer problem is converted into a heat transfer problem. Consequently, each recovery target χ^t, i.e. VOC concentration in the gaseous stream, can be translated into a required endpoint temperature T_{End} of the condensation [Richburg and El-Halwagi, 1995].

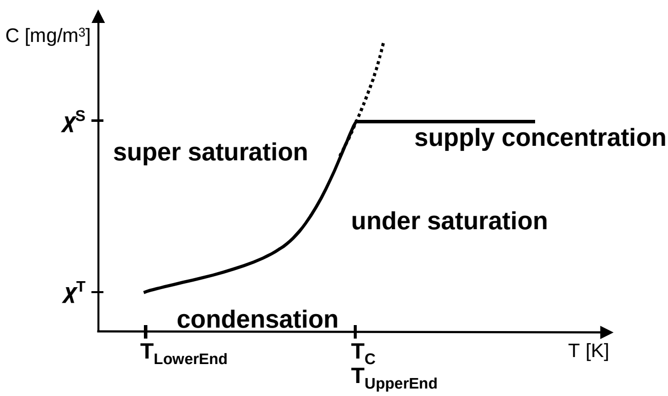

Figure 2.13: Schematic Representation of a Saturation-Pressure Curve within the Operating Range of the VOC-Condensation System

In the special case of one single organic solvent, the temperature of condensation T^C, i.e. the dew point, of the solvent depends on its partial pressure $p_{pp}^{VOC}(T)$. In the case of a multi-component VOC or a mixture of gases, the temperature of condensation T_j^C of one component, i.e. the j^{th} solvent, depends on the partial pressure of the component $p_{pp}^{j}(T)$. By cooling down the gaseous waste stream the concentration of VOC in a dilute system is constant, i.e. $\chi_{VOC}(T) = \chi_{VOC}^{s}$ for $T > T^C$, until the condensation starts at T^C where the partial pressure equals the vapour pressure of VOC, i.e. $p_{pp}^{VOC}(T^C) = p_{vp}^{VOC}(T^C)$, and saturation is reached. In this case the concentration of VOC $\chi_{VOC}(T)$ approximately equals the fraction of the partial pressure to the total pressure of the gaseous waste for $T \leq T^C$ (cf. Equation 2.12) [Richburg and El-Halwagi, 1995]:

$$\chi_{VOC}(T) = \frac{p_{pp}^{VOC}(T)}{p^{total} - p_{pp}^{VOC}(T)} \approx \frac{p_{pp}^{VOC}(T)}{p^{total}} \text{ since } p_{pp}^{VOC}(T_{End}) << p^{total} \tag{2.12}$$

Using the equation of the saturation pressure curve (cf. Equation 2.12) the target concentration χ^t can be determined by the end point temperature of condensation T_{End} (cf. Equation 2.13) [Richburg and El-Halwagi, 1995]:

$$\chi^t_{VOC} = \frac{p^{VOC}_{pp}(T_{End})}{p^{total}} \tag{2.13}$$

In general, a condensation system consists of at least two units (cf. Figure 2.14 [Dunn and El-Halwagi, 1994]). The first step is a dehumidification unit for eliminating the moisture in the waste gas. This step is necessary in order to prevent icing of the system during further refrigeration and it is usually operated at around 278 K (5 °C). A recuperator utilises the cold gaseous stream of the condensation system accompanied by additional cooling utilities. The heat transfer between the process streams or the utilities is modelled by the process stream specific heat-transfer coefficients. The second step consists of the condensation unit. The dehumidified waste gas is cooled further in order to condense the VOC. Depending on the objective (fulfilment of a concentration threshold of VOC in the gaseous stream vs. pure cost efficient operation of the condensation system) very low temperatures may be necessary. For the additional cooling of the waste gas in the lowest temperature range either mechanical cooling or a cryogenic cooling agent is used, such as liquid nitrogen (N_{2_l}), the quantity of which can be derived from its specific heat-transfer coefficient α.

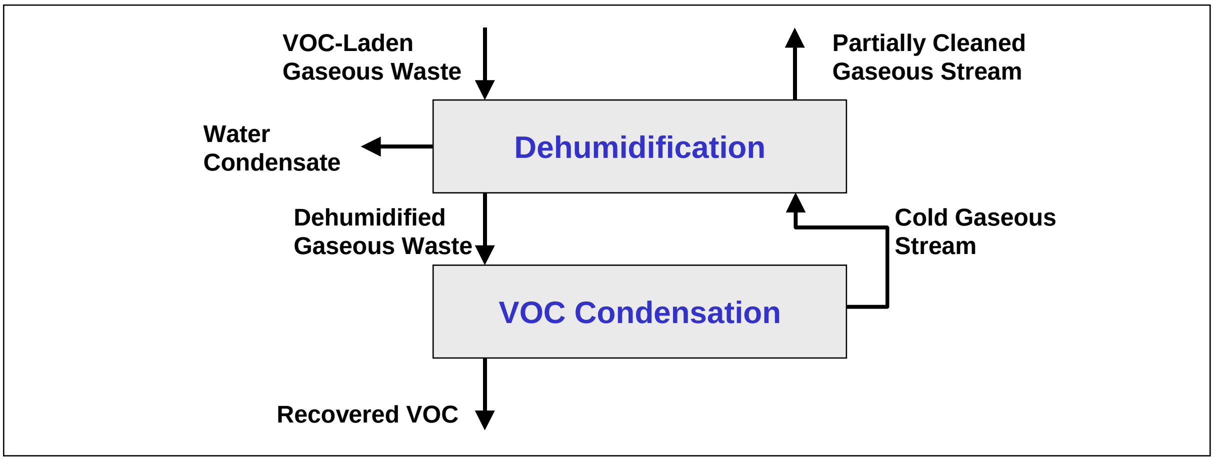

Figure 2.14: Schematic Representation of a VOC-Condensation System [Dunn and El-Halwagi, 1994]

The operating temperature range depends on the supply temperature of the VOC-laden gaseous waste stream (e.g. 20 °C (293 K) as the upper boundary (where the starting point of condensation depends on the VOC concentration in the gaseous waste stream) (cf. $T_{UpperEnd}$ in Figure 2.13) and on the maximum of the system dependent temperatures (freezing point of the coolant, minimal machine-dependent system temperature, freezing point of solvent, etc.) as the lower boundary (cf. $T_{LowerEnd}$ in Figure 2.13)). In practise de-icing procedures (continuous vs. breaks) are used to diminish the ice caused by the remaining moisture in the waste gas. These de-icing procedures are not considered in the following. Furthermore, the technical constraints that must be considered in the calculation are the maximum and minimum solvent concentration given by the process itself. For example, in order to allow quick drying and to limit the lasting effects of the solvent on the object, the concentration of the solvents in the air should not exceed a certain value. Additionally, safety requirements must be carefully followed due to the risk of explosion from the solvents [DIN 1539].

The procedure is implemented in a module using $MATLAB^{TM}$ to provide the possibility to include country specific cost parameters and to make the results available to the subsequent multi-criteria analysis. The integrals of the heat balance are solved in $MATLAB^{TM}$ by numeric integration in 0.1 K steps. The same procedure is used in the thermal pinch analysis (cf. Section 2.1.1). The calculation considers the temperature dependent heat capacities $c_{p,V}$ of the waste gas and the gaseous stream after condensation. In addition the specific heat capacity of the VOC-free gas $c_{p,g}$ is taken into account. Furthermore, the heat of condensation λ is taken into account as well as the heat capacity of the condensed liquid solvent $c_{p,L}$ (cf. Equation 2.14) [Richburg and El-Halwagi, 1995]:

$$\Delta H = \int_{t=T^S}^{T} c_{p,g}(t)dt + \int_{t=T^S}^{T} \chi(t) \cdot c_{p,V}(t)dt + [\chi_s - \chi(t)] \cdot \lambda + \int_{t=T^C}^{T} (\chi_s - \chi(t)) \cdot c_{p,L}(t)dt \quad (2.14)$$

In a first step the enthalpy supply and demand of the gas flows are determined for each given temperature step (e.g. 0.1 K). Next, the heat balances within the system are calculated depending on the chosen temperature gradient. Thereafter, imbalances are adjusted by heat integration or through utilities [Richburg and El-Halwagi, 1995]. By modifying the temperature gradient (configuring the heat transfer area) or the end point of condensation (controlling the quantity of recovered solvents) the system performance can be evaluated (cf. Section 2.3.2).

Additionally, a number of assumptions are made:

1. in the case of condensation as an abatement technique it is assumed that the temperature of the end point of the condensation is low enough to fulfil possible legal requirements concerning a threshold of VOC concentration in the gaseous stream;
2. the various gases and liquids are regarded as ideal, i.e. their thermodynamic characteristics do not affect each other;
3. the heat losses are neglected;
4. the condensate of solvents is cooled down to the end point temperature of the condensation, since locking out of the condensate is not considered.

2.3.2 Economic Analysis of the Recovery of VOC

Since a complete condensation of the VOC in the gaseous waste stream is theoretically possible, economic parameters are additionally taken into account in order to identify a cost-efficient solution. The objective of the analysis is to determine the economically reasonable amount of recoverable solvents which can be translated into an endpoint temperature T_{End} of the condensation at which this recovery target is reached. Thus, the optimisation objective is the minimal total annual costs of the plant. In addition to the investment and the operating costs of the condensation system, the developed model also considers possible operating income. If the recovered solvents are re-used in the same process (closed loop recycling) the quantity of recovered solvents is valued with the price for new solvents. In case the solvents are not used within the process, for example due to quality restrictions, the value equals the price for which the solvents can be sold.

The heat-transfer between the gaseous waste and the (partially) cleaned cold gaseous stream is modelled via the heat transfer coefficient α, and the investment is calculated on the basis of heat exchanger surface area dependent values. Parameters such as geometry and material are considered using surface area dependent values and the operating costs of the heat exchanger, such as maintenance and repair is not considered. However, the costs of the cooling agent, due for example to constant loss through evaporation of N_{2_l}, is added to the operating costs. It must be noted, however, that the economic parameters, particularly the ratios between them, are a crucial factor for the result of the calculation.

The integrated and dissipated heat depend on the endpoint temperature of the condensation T_{End}. Hence, the solution is driven by the trade-off between the amount of recovered solvents, i.e. savings for the solvents, on the one hand, and the necessary investment in the heat exchanger and costs for the coolants on the other hand. However, the investment and the amount of coolants for a given recovery target χ^t depend on the temperature gradient ΔT_{min}. For example, a higher temperature gradient allows less heat integration and therefore requires less investment, but necessitates more cooling agents. For each end-point temperature of the condensation within the condensation range and for each ΔT_{min} within an assumed range (e.g. $2\ K$ to $20\ K$) the total annual costs are determined.

2.4 Multi Objective Pinch Analysis (MOPA)

The inherent advantages of the pinch analysis approach can be used for the application and optimisation of various process streams by understanding the important factors regulating a process and approximating meaningful targets. The advantages and limitations of the pinch analysis approaches are discussed (cf. Section 2.4.1) providing the key elements for a subsequent integration and assessment of intra- and inter-company production networks. Finally, the *Multi Objective Pinch Analysis* provides a framework for the integration of the different pinch analysis approaches. It enables the development of a generic model structuring the various input data for the process optimisation via pinch analyses and provides the base for a multi-criteria decision support model to evaluate the different targets determined by pinch analysis (cf. Chapter 3).

2.4.1 Discussion

The feasibility, economic relevance and environmental impact of the processes are key drivers of the decision process concerning the planning or modification of a plant. Consequently, compliance with emission limits, plant safety, maintenance of product quality, and control of start-up and both planned and unplanned shut-downs must be ensured [Mosberger, 2005]. One approach to evaluate preliminary design and process modifications are *flow sheeting* programs which, on the one hand can simulate in detail operating conditions based on construction data, and on the other hand the overall combination of the various unit operations in the process.

A different approach is based on methods of process integration. The evaluation of the process design is based on target values. Just as in the simulation, the evaluation is based on detailed process characteristics and material properties, and if a parameter is not known it must be calculated either based on measurement data, similar reactions or unit operations. With respect to the assessment it is necessary to explicitly acknowledge this uncertainty in the material properties and unknown parameters.

Other aspects not considered here in detail include the construction geometry and construction materials, e.g. corrosion and thermal requirements. These are only considered rudimentarily here - as cost surcharges dependent on operating conditions (pressure, temperature), type of material and size of equipment. Cost estimation in the context of process design, particularly with regard to heat transfer, is based on scaling effects [Peters et al., 2003]. Depending on the specific case other cost aspects are considered, e.g. costs for piping, which include not only the costs for the piping itself, but also for the labour, valves, foundations, etc. An overview of different cost estimation methods is given in [Peters et al., 2003].

The general purpose of the process evaluation based on process specific data, is to find weak points and bottlenecks in the process design. In general, however, there are reasons for not operating near the theoretical minimum (e.g. for heat integration at the thermodynamic minimum) [Vogel, 2005]:

- start-up operations often require start-up heat exchangers,
- energy utilisation only becomes possible as a result of increasing the column pressure and this means higher investment and may result in material problems (decomposition, side reactions),
- problems associated with the formation of deposits during heat transfer.

Similar statements can be made for water or solvent analyses, e.g. the solution obtained with the water pinch must be translated into a feasible process design. Therefore, strategies such as the bypassing of process water can be applied. In addition to the different parameters being considered (single or multi parameter, water regeneration), a distinction between water as a utility (utility water pinch analysis) and water as a substance required in the process itself (process water pinch analysis) must also be made. A simulation-based approach addressing the problem of several aqueous streams relevant for one operation, including water losses, has been developed by [Hallale, 2002].

2.4.2 Inter-Company Application of the Pinch Analysis

Pinch analysis can also be applied in an inter-company approach considering different supply chain or industry park structures. Linking of various production sites by process streams enables a possible connection of processes with differing outcomes, such as for example bicycle coating and spirits production. Thus, the combined activities can, but not necessarily must, come from one supply chain.

For the implementation of the pinch analysis the considered processes must be treated as one system. The procedure for the calculation of the savings potential is the same as in the case of an intra-company problem. The result is used as a target for the process design which then results in a shared use of the utilities necessary for fulfilling the requirements of, for example heating and cooling, and which cannot be satisfied on the basis of the available process streams. Furthermore, by linking process streams from several sites the stream properties can be improved in order to comply with specific technical, chemical or economic requirements. For example, the combination of waste gas streams from process steps emitting organic solvents may lead to an increased volume of the combined process streams. As a consequence, other technical options for waste gas cleaning and/or solvent recovery may become economically feasible, such as for example the installation of a zeolite wheel or activated carbon filter.

In contrast to one wide-stretching company, the inter-company production network provides additional technical and organisational restrictions. Changes in process parameters or input materials affect the whole production network: E.g. new developed paints at the paint producer with a different solvent content influence the investment decision of a waste gas cleaning system at the coating workshop due to the resulting different solvent emission concentrations. Through the analysis of process streams within a supply chain or within an industry park significant improvements may be realised [Wietschel, 2002]. For example a combined wastewater treatment system could have a more stable COD value and hence a more effective and economical process could be implemented. This could be a viable option especially in industrialising countries where obligations from environmental legislation might be of a lower imperative. These examples show that further optimisation potential can be identified using an inter-company approach based on an analysis of the technical applications [Frank, 2003; Tietze-Stöckinger, 2005].

2.4.3 The Concept of Multi Objective Pinch Analysis

In the approaches of the pinch analyses discussed so far, the energy and mass flows were considered separately from each other. Through the parallel reduction of energy consumption, water use and VOC emissions, a multi-criteria process design problem for intra- and inter-company facility planning must be solved in order to implement efficient recycling cascades. Resulting conflicting solutions must be evaluated based on a multi-criteria approach (cf. Chapter 3). This will introduce new possibilities for cleaner technologies and environmental protection by optimally combining process-integrated emission reduction measures and end-of-pipe technologies, while also creating a challenge for further research in the field of multi-criteria decision support.

The concept of the *Multi Objective Pinch Analysis (MOPA)* is introduced in order to clarify the context of the pinch analysis (cf. Section 2.4.3). Thus, the pinch analysis approach is embedded in a framework beginning with a process analysis and ending in a process design.

Multi Objective Pinch Analysis (MOPA) consists of a combination of pinch analyses with different targets (energy consumption, wastewater generation, consumption of solvents, etc.) and a subsequent multi-criteria analysis. MOPA can be illustrated by the seven modules presented in Figure 2.15. Starting with a process analysis of the company, the industry park or the supply chain (depending on the system boundaries), a process model is developed mapping the various process streams and defining the data requirements. In order to calculate optimisation potentials for each selected company two kinds of information are necessary: process related information (process parameters for each identified process step, parameters of auxiliary processes) and data for the characterisation of the company (annual production figures, growth rates, etc.). The values that must be gathered are both of technical and economic nature. The basic concept, especially in case of the process parameters, is to characterise substance flows (mainly solvent, water and energy) by their absolute and their economic value through direct measurement, indirect measurement (calculations based on measurements), data derived from technical data sheets, data from identical processes of another company, and data derived from comparable processes. Information from the supply chain must be included in order to gather consistent data. For example customers who ordered painted plastic parts must be included in order to know the exact production schedule for that day in advance (especially in just in time production). The paint producer must also be included so that an analysis of the specific solvents and their concentrations used in that specific batch can be obtained.

In a second step a technology screening compiles all required information on *Best Available Techniques (BAT)* and emerging technologies in order to describe the process model and different technology options with characteristic figures (cf. module 3 in Figure 2.15). The optimisation module (cf. module 4 in Figure 2.15) is based on the pinch analysis and is solved using for example the transport algorithm from Operations Research. A set of optimal solutions is delivered, which spans the domain of considered technology combinations and peaks at the most current level. In a multi-criteria decision process the

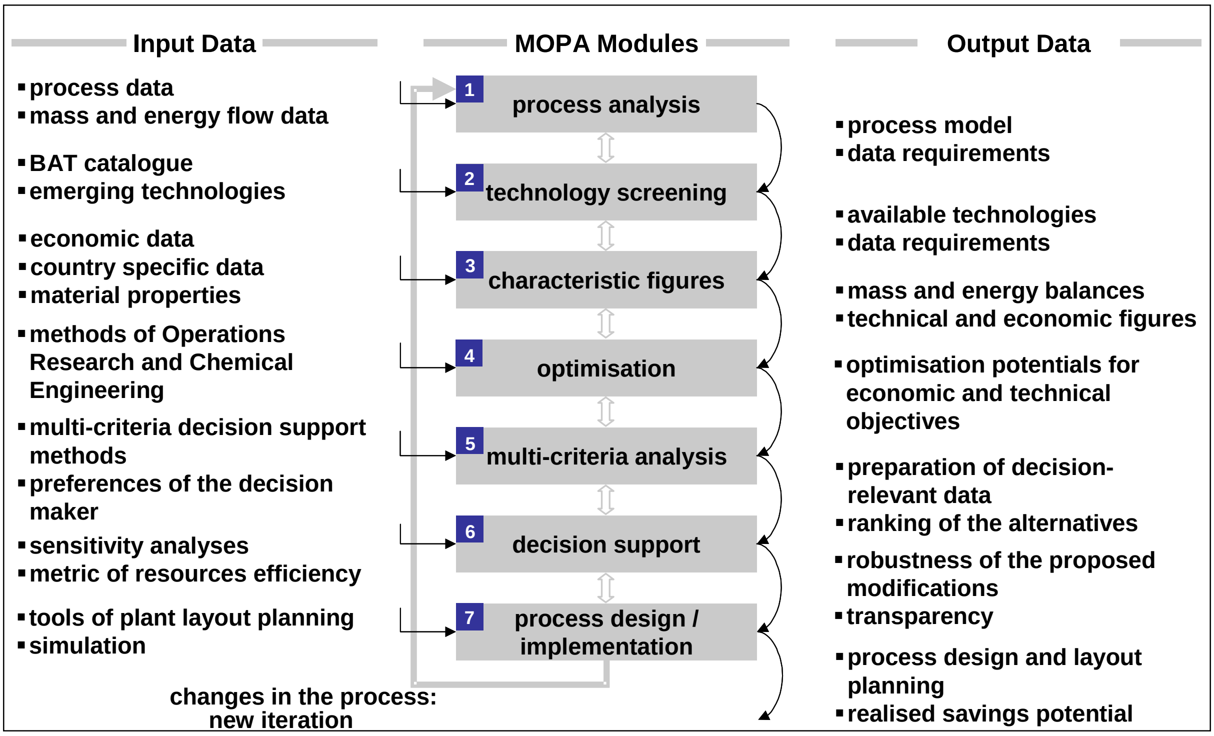

Figure 2.15: Modules of the Multi Objective Pinch Analysis [Treitz et al., 2004b]

preferences, with respect to the different resources, conclusively determine the selection of a set of technologies for consideration (cf. module 5 and 6 in Figure 2.15). Additionally, further criteria such as investment, operating costs, and quality attributes extend the dimension of the given problem [Treitz et al., 2005]. From a techno-economic point of view the set of available technology combinations must be compared and assessed in a multi-criteria analysis (cf. Chapter 3). A metric for resource efficiency or a multi-criteria decision support method can be applied for this purpose. Given the characteristics of the problem (i.e. considering simultaneously quantitative and qualitative data), multi-criteria methods such as PROMETHEE [Brans et al., 1986] or the Multi Attribute Value Theory (MAVT) [Keeney, 1992] are suitable for ranking the different alternatives and to address the problem of modelling preferential information.

The specific technologies implemented in the subsequent process design (cf. module 7 in Figure 2.15) eventually define the savings that can be realised. If there are changes to the process layout (e.g. different temperature intervals, different set of process streams, etc.) in an iterative process the new design can be evaluated by MOPA.

Detailed chemical engineering experience is required in order to model the process streams in the detail required by integration technology for achieving meaningful results. If the process streams are inadequately modelled or oversimplified, only the very obvious results can be obtained. However, using a highly sophisticated level of detail requires complex modelling of the material and time dependencies of the reactions. Therefore, the challenge is to provide an adequate level of modelling. The pinch analysis allows a process evaluation at each stage of the process design phase, from the preliminary design to the fully operational plant, and is a useful tool for decision support where incomplete knowledge about specific details of certain unit operations exists.

Complex models and software tools are available to experts for modelling the process parameters and for analysing the system. Nevertheless, the aim of the pinch analysis is [Kemp, 1991]:

- to give a rapid understanding of the important factors regulating the mass and energy consumption of a process;
- allowing approximate but meaningful mass and energy targets to be set using short-cut calculations;
- pre-optimisation to identify the most promising scheme before embarking on the costly and time-consuming detailed design phase.

The target values obtained by the different pinch analysis approaches can be used for an integrated technique assessment using a multi-criteria approach and enhance the discussion about the resource efficiency of the production network (cf. Chapter 3).

Chapter 3

Using Multi-Criteria Analysis to Evaluate Resource Efficiency

The optimal allocation of resources is a core question in business economics [Koopmans, 1975][7]. Since the various pinch analyses determine the theoretical optimal consumption targets for heat, water and solvents independently from each other, the question must be addressed: which is the optimal allocation for a production system, which has heat, water, energy simultaneously optimised.

The definition of efficiency for an analysis of production systems is the starting point for identifying resource efficient combinations of technologies for specific techniques. In general the *degree of efficiency* is the ratio of desired output to input [Grassmann, 1950]. In the context of thermodynamic processes the input and output parameters are often limited to energy quantities, for example the transferred or converted energy compared to the employed energy, for example in a power station or wind turbine. However, this definition considers only the heat quantity and not the quality, such as temperature, which is relevant for defining its convertibility in for example refrigeration systems (for a discussion see [Grassmann, 1950]). Consequently, if it is not possible to define a single common denominator, such as the heat content or coal equivalent, the definition of the degree of efficiency is highly complex.

Relative efficiency measurement is the starting point of this chapter (cf. Section 3.1). *Data Envelopment Analysis* and *Multi-Criteria Analysis* are discussed as different approaches

[7] In the explanatory statement of the *Nobel Prize Committee* in 1975 for *Leonid Kantorovich* and *Tjalling Koopmans* for their *"contributions to the theory of optimum allocation of resources"*, it is said that the problem of "how available productive resources can be used to the greatest advantage in the production of goods and services" is fundamental to economics [Nobel Prize Comittee, 1975].

to resolve incomparabilities in a technique assessment. Second, a metric is introduced as a multi-criteria assessment tool to illustrate trade-offs and compensation ratios where incomparabilities are investigated by a distance measure and weighting factors (cf. Section 3.2). Third, the outranking approach PROMETHEE is applied for an integrated technique assessment (cf. Section 3.3). Preferential information are modelled by weighting factors and by preference functions based on pairwise comparisons. Because of the subjective assumptions that are unavoidable in decision modelling, sensitivity analyses for value judgements are necessary. New sensitivity analyses for PROMETHEE for preferential and data uncertainties are the major contribution of this chapter.

3.1 Introduction to Efficiency Measurement

The origin of the efficiency definition regarded here is the *activity analyis* [Koopmans, 1951], which also provides an overview of different allocation methods [Koopmans, 1951, 1975]. Leading off from this point in Section 3.1.1 two major interpretations of the definition are discussed considering the *Data Envelopment Analysis (DEA)* and the *Multi-Criteria Analysis (MCA)*. Based on the efficiency definition all non-dominated alternatives are called efficient, which is the origin of all multi-criteria problems [Brans and Mareschal, 2005]. Through special focus on the dominance relation multi-criteria methods seek to reduce incomparabilities by explicitly incorporating preferential information of the decision maker. Hence in Section 3.1.2 and 3.1.3 two different multi-criteria approaches are presented. Firstly, a metric is introduced based on a modified Euclidean norm. As an additive, full-compensatory model, it is a classical multi-criteria method. Secondly, an outranking approach is introduced in order to evaluate different technology combinations, while also taking advantage of sensitivity analyses.

3.1.1 Relative Efficiency of Techniques

The basic idea of the *activity analysis* [Koopmans, 1951] is a static model of the elements *commodity* and *activity*. A decision maker can employ commodities in activities to generate output. The quantity of each commodity is a non-negative coefficient of the activity vector and the pooled activity vectors are the technology matrix. The decision maker tries to optimally combine activities to maximise desired output for the given input. The efficiency definition states that "a possible point in the commodity space is called efficient whenever an increase in one of its coordinates (net output of one good) can be achieved only at the cost of a decrease in some other coordinate (net output of another good)" [Koopmans, 1951]. Consequently, the allocation of resources is efficient if no improvement, i.e. an addition to the output of one or more goods at no cost to the others, is possible. This relative efficiency definition is called *Pareto efficiency* and a possible improvement is referred to as a *Pareto improvement* or *Pareto optimisation* (cf. [Moffat, 1976]). Mathematically, every Pareto efficient point in the commodity space is equally acceptable. Trade-offs and compromises are required by moving from one efficient point to another.

In terms of decision theory, the aim is to identify efficient alternatives. In the following, $\{a_i(\cdot) \,|\, 1 \leq i \leq n,\ n \in \mathbb{N}\}$ denotes the finite set of all alternatives (called A) and $\{g_j(\cdot) \,|\, 1 \leq j \leq k,\ k \in \mathbb{N}\}$ a set of evaluation criteria (called C). Consequently, the basic decision problem is based on the available alternatives and the selected objectives. The objective is to maximise each attribute for a given alternative. The problem is stated as [Brans and Mareschal, 2005]:

$$\max_{a} \{g_1(a), g_2(a), ..., g_j(a), ..., g_k(a) \,|a \in A\} \tag{3.1}$$

Central for the evaluation is the *dominance relation* between the alternatives. If an alternative a_x is better in one criterion g_s than a_y and at least as good in all other criteria as a_y, then a_x dominates a_y. In terms of decision theory, a_x is preferred to a_y based on *preference* relation P (cf. Equation 3.2) [Brans and Mareschal, 2005]:

$$\left\{ \begin{array}{lcl} \forall j & : & g_j(a_x) \geq g_j(a_y) \\ \exists s & : & g_s(a_x) > g_s(a_y) \end{array} \right. \Longleftrightarrow a_x P a_y \tag{3.2}$$

If a_x and a_y are equal concerning all criteria there exists an *indifference* relation I (cf. Equation 3.3) [Brans and Mareschal, 2005]:

$$\forall j : g_j(a_x) = g_j(a_y) \Longleftrightarrow a_x I a_y \tag{3.3}$$

If a_x is better on one criterion g_s and a_y is better on another criterion g_t, it is impossible to decide which alternative is better overall and the relation is an *incomparability* relation R (cf. Equation 3.4) [Brans and Mareschal, 2005]:

$$\left\{ \begin{array}{lcl} \exists s & : & g_s(a_x) > g_s a_y \\ \exists t & : & g_{t(a_x)} < g_t(a_y) \end{array} \right. \Longleftrightarrow a_x R a_y \tag{3.4}$$

Based on dominance relations P, I, and R the relative efficiency definition is stated as (cf. [Koopmans, 1951]):

An alternative $a_{eff} \in A$ is called efficient with regard to the multi-criteria problem 3.1 if no alternative $a' \in A$ exists which dominates a_{eff} based on preference relation P (cf. Equation 3.2).

Two aspects must be pointed out (cf. [Kleine, 2001]):

1. The property of efficiency depends on the problem (cf. Equation 3.1), i.e. the available alternatives A and the selected criteria C. If the considered set of alternatives or criteria change, a previously dominated alternative can be efficient now and vice versa. Consequently, if an alternative is said to be efficient it must be indicated with respect to which set of alternatives A and criteria C.

2. The definition states no reference concerning the comparison of alternatives, i.e. "a_x is more efficient than a_y", since no metric or measure is provided to assess the relative difference between efficient and dominated alternatives.

Therefore, various models refine or use/extend the above mentioned efficiency definition. In the following two major interpretations are discussed: Firstly the *Data Envelopment Analysis (DEA)* as a widespread, macro-economic application, and secondly *Multi-Criteria Analysis (MCA)* as a methodology resolving the incomparabilities of the problem by additional preferential information.

3.1.2 Data Envelopment Analysis (DEA)

The ex-post evaluation of the efficiency and/or inefficiency of many similar organisations (i.e. *Decision Making Units (DMU)* such as hospitals, bank branches, public offices) on the basis of historical data is the focus of the *Data Envelopment Analysis (DEA)* [Charnes et al., 1978; Cooper et al., 2004]. The origin of DEA comes from the evaluation of non-profit organisations since input and output cannot be monetarily valued with market prices and comparison is more difficult. For the purpose of monitoring and control [Belton and Stewart, 1999] one goal is the comparison of *better* and *worse* operational procedures in DMU. In the event that a DMU is identified to be inefficient, a real-valued measure or a degree of inefficiency is calculated.

3.1.2.1 Technology Sets in DEA

The basis for DEA are empirical data of $H \in \mathbb{N}\,(h \in \{1,\dots,H\})$ DMU and a defined operation $(-x,+y)^T$, i.e. production, is characterised by m quantities of negative inputs $-x_h$ and n quantities of positive outputs y_h. All existing modes of production are used to define a set of technologies T^j (cf. Equation 3.5, [Kleine, 2001, 2004]):

$$T^j := \left\{ \begin{pmatrix} -x \\ +y \end{pmatrix} \in R^{n+m} | \begin{pmatrix} -x \\ +y \end{pmatrix} = \sum_{h=1}^{H} \lambda_h \begin{pmatrix} -x_h \\ +y_h \end{pmatrix}; \lambda \in \Lambda^j \right\} \tag{3.5}$$

The set of technologies highly depends on the assumptions concerning the multiplier λ_h, for example assuming non-negative linear combinations the technology set T^{CRS} is defined supposing *constant returns to scale* (cf. Equation 3.5 and Table 3.1). Thus, the technology T^j determines the efficient DMU and the *efficiency frontier* (cf. for CRS the solid line in Figure 3.1). In the case of the *Free Disposal Hull (FDH)* a convex combination of the different production modes is not possible. Using the concept of the FDH the analysis contains numerous incomparabilities and efficient DMU.

Table 3.1: Assumptions for the Multiplier Set Λ [Kleine, 2001]

j	**Name**	**Set Λ^j**
CRS	Constant Returns to Scale	$\Lambda^{CRS} := \left\{\lambda \in \mathbb{R}_+^H\right\}$
DRS	Decreasing Returns to Scale	$\Lambda^{DRS} := \left\{\lambda \in \mathbb{R}_+^H \mid \sum_{h=1}^H \lambda_h \leq 1\right\}$
VRS	Variable Returns to Scale	$\Lambda^{VRS} := \left\{\lambda \in \mathbb{R}_+^H \mid \sum_{h=1}^H \lambda_h = 1\right\}$
FDH	Free Disposal Hull	$\Lambda^{FDH} := \left\{\lambda \in \{0,1\}^H \mid \sum_{h=1}^H \lambda_h = 1\right\}$

3.1.2.2 Efficiency Measurement in DEA

The purpose of the DEA is to compare different production modes. Hence, the efficiency definition is extended by a relative distance measure [Farrell, 1957]. In general it is assumed that the Koopman's efficiency definition is met by this distance measure. However, other measures are discussed, such as the *Russel Measure* [Bardhan et al., 1996] or modifications of the Russel Measure [Pastor et al., 1999; Ruggiero and Bretschneider, 1998]. By determining the efficiency frontier the distance of the inefficient DMU to the frontier can be used as a measure for its inefficiency, for example DMU_2 in Figure 3.1. This step of *envelopment* is the key step in the Data Envelopment Theory. By assuming a certain set of technologies, specific assumptions concerning the production function, the combination of technologies and so forth are made. As illustrated in Figure 3.1, the selection of *efficient* DMU depends on all DMU, the considered inputs/outputs and the defined combinations. Whereas DMU_1 is inefficient assuming CRS or DRS, it is efficient assuming VRS. Only DMU_2 is inefficient considering all possible multipliers λ.

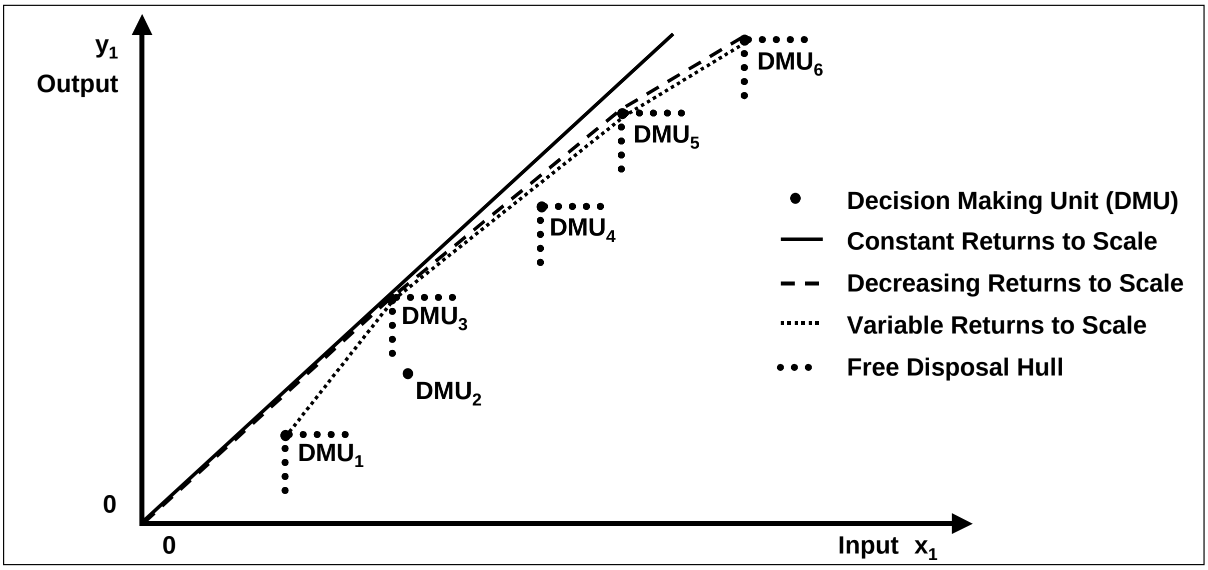

Figure 3.1: Efficieny Frontiers for the Different Technology Sets T^j [Kleine, 2001]

Furthermore, depending on the distance measure, i.e. *norm*, different metrics can be defined to measure the distance to the efficiency frontier [see e.g. Charnes et al., 1978; Kleine, 2001; Cooper et al., 2004; Bertsch et al., 2007, for a selection of different distance norms (e.g. L_1 or L_∞)]. Therefore, a relative assessment of inefficient organisations is possible. By defining a norm the various input/output aspects are aggregated into a scalar measure by implicitly using preferences, i.e. weights or priorities between the different input or output factors.

3.1.2.3 Consideration of Environmental Data in DEA

With respect to DEA, larger quantities of outputs and smaller quantities of inputs are generally desired. Special consideration is required when modelling pollutants. Since a reduction in input quantities or an increase in output quantities automatically improves the input/output combination the model must be extended. For example, the reduction of certain emissions or the increase of recycling input material is an improvement of the resource employment. Consequently, different modelling approaches have been developed to address the environmental parameters. Proposed solutions [see e.g. Dyckhoff and Allen, 2001, for an overview of different methodologies]:

- *Reciprocal* for undesired outputs,
- *Translation* of undesired outputs, i.e. adding a sufficiently large scalar to the additive inverse,
- *Functional Relation*, i.e. the undesired output is modelled through a required increase in unwanted input or a decrease of the desired output,
- *Residue-Ratio*, i.e. ratio of undesired output to total output modelled as an input,
- *Input Modelling*, i.e. modelling of the undesired output as an input parameter.

3.1.2.4 Preferential Information in DEA

In general DEA is based on quantitative data without preferential information to identify solutions out of the set of Pareto efficient solutions. Nevertheless, it is possible to integrate preferential information into DEA [Korhonen, 2002]. By determining a value function the *Value Efficiency Analysis (VEA)* is established and a *Most Preferred Solution (MPS)* can be identified by intersection of the indifference curve of the value function with the efficiency frontier [Korhonen, 2002]. In addition, another approach implicitly uses "most favourable value functions" to perform a self evaluation [Mavrotas and Trifillis, 2006] and to generate a ranking out of the set of Pareto efficient solutions. Moreover, there are increasing applications of DEA for technique assessment or technology selection [see e.g. Sarkis and Weinrach, 2001; Keh and Chu, 2002] creating an overlap to multi-criteria analysis.

3.1.3 Multi Attribute Decision Making (MADM)

In the evaluation of efficiency in *Multi Attribute Decision Making*[8] problems, predominantly efficient alternatives exist according to the definition in Section 3.1.1. Thus, in

[8] The field of *Multi Attribute Decision Making (MADM)* covers the assessment of a finite set of alternatives (discrete solution space) in contrast to *Multi Objective Decision Making (MODM)* focussing on alternatives restricted by constraints (continuous space). Both fields together constitute the research field of *Multi Criteria Decision Making (MCDM)*. Applications of MADM can be divided in *classical approaches*, e.g. *Multi Attribute Value Theory (MAVT)*, *Multi Attribute Utility Theory (MAUT)*, *Analytical Hierarchy Process (AHP)*, etc., and *outranking approaches*, e.g. *PROMETHEE*, *ELECTRE*,

contrast to DEA (*ex-post* evaluation of many similar units for the purpose of monitoring and control) the aim of *Multi Attribute Decision Making* is the *ex-ante* assessment of a few individual options by explicitly considering the subjective preferences of a decision maker for the purpose of decision support and planning (monitoring and control vs. planning and choice [Belton and Stewart, 1999]). In selecting one final solution out of the mathematically equivalent set of Pareto optimal solutions an issue arises, which is not a mathematical question, to be addressed objectively, but a subjective element of the solution. It is the aim of multi-criteria methods to explicitly acknowledge the subjectivity of decision processes.

Concerning the efficiency definition it can be said that it provides only a partial ordering of the alternatives. "No preference is expressed between alternatives A and B if A involves more of one desired commodity, B more of another. We can therefore not expect our model to produce a unique solution of the allocation problem" [Koopmans, 1951]. Thus, multi-criteria methods try to reduce these incomparabilities by incorporating preference models. Preference modelling differs from outranking methods focussing on the magnitude of differences between alternatives to classical methods focussing on relating preferences to objectively measured performance. A wide range of literature about elicitation of value judgements, preference modelling and the ability of the decision maker to provide this information exists [see e.g. Belton and Stewart, 1999; Laux, 2005].

3.1.4 Preference Modelling in Multi-Criteria Analysis

In general, an alternative optimising all criteria simultaneously does not exist. If an alternative is better on one criterion and the other better on a different criterion, it is impossible to decide which alternative is the best without additional information [Brans and Mareschal, 2005]. Again, as discussed in the efficiency definition in Section 3.1.1, all alternatives which are not dominated by another alternative are called *efficient*. Hence, most of the alternatives given in a multi-criteria problem are efficient and incomparable. Consequently, multi-criteria methods require preferential information about relationships between the criteria, i.e. inter-criteria (cf. Section 3.1.4.1), and about each criterion, i.e. intra-criteria (cf. Section 3.1.4.2), to resolve the incomparabilities.

ORESTE, etc.. Computer supported methods are in general referred to as *Decision Support System (DSS)* or *Multiple Criteria Decision Support System (MCDSS)*.

3.1.4.1 Preferential Information between Criteria

The weighting or valuation of different criteria is a subjective element in the assessment of techniques and addresses the relative importance of the different criteria for the decision problem and thus constitutes the preferential information between criteria. The weighting factors have different meanings in different multi-criteria methodologies. In outranking methods the weighting factors represent a kind of a "voting power" [Belton and Stewart, 2002] for each criterion (cf. Section 3.3), rather than trade-offs or compensation ratios as in classical multi-criteria methods such as the proposed metric (cf. Section 3.2). In contrast to the attribute values, where a quantification is possible not only for measurable values, such as operating costs per year, but also for qualitative attributes, such as colour matching quality in the coating industry, which can be characterised by scores, benchmark tests or assigned marks, the weighting is more complex and context specific since no objective value exists to compare it to. Furthermore, behavioural aspects must be taken into account reflecting different perceptions of "gains" or "losses" [Kahneman et al., 1982] by wording a criterion in terms of losses to one reference point, in terms of gains to a different one or by biases according to the number of sub-criteria or the hierarchical level of the criteria to be valued (cf. [Belton and Stewart, 2002]).

Apart from the classical weighting techniques, such as direct ratio, SWING [v. Winterfeld and Edwards, 1986], SMART [Edwards, 1977; v. Winterfeld and Edwards, 1986], SMARTER [Barron and Barret, 1996; Edwards and Barron, 1994], eigenvector method [Saaty, 1980], specialised methods are discussed in the case of environmental impacts.

However, for the valuation of different ecological criteria the discussion of weighting issues leads to the fundamental questions:

- Should there be a weighting at all?
- If so, which weighting method should be used?
- Which weights should be put on different criteria?

Scientific research can provide support for the decision maker in his/her quest for better understanding of the interdependencies in the weighting of environmental criteria. However, this discussion is highly controversial and it is important to note that some authors favour a more technical approach, whilst others stress the importance of detailed stakeholder involvement because of context sensitivity and the significant influence on the overall results.

Well known approaches (cf. [Geldermann, 1999; v. Berkel and Lafleur, 1997; Soest et al., 1998]) addressing the issue of valuation of potential environmental impacts are

- Cumulative Energy Demand,
- Eco Indicator method,
- Environmental Pressure Indicators,
- MIPS ((cradle to grave) Material Input per Unit Service),
- Calculation of shadow prices based on abatement costs,
- Determination of weights based on eco-taxes,
- Panel methods,
- Total relevance using verbal predicates based on ecological relevance and specific contribution.

Additionally, the aspects of shifting potential impacts from one environmental medium (air, water, soil) to another is analysed through cross-media evaluations [EIPPCB Cross-Media]. However, often high quality environmental impact data is missing and the impact assessment can only capture a simplified representation of the complex ecological inter-dependencies and toxicological issues.

3.1.4.2 Preferential Information within Criteria

Preferential information within criteria, i.e. intra-criteria preferences, create normalised data of the decision table to achieve comparability between the different criteria. The different attributes are measured in their respective scales, but the attribute values must be harmonised in order to reflect the perception of the different parameter values. "The purpose of all multi-criteria methods is to enrich the dominance graph" [Brans and Mareschal, 2005], i.e. to reduce the number of incomparibilities R (cf. Equation 3.4). This is done completely via *distance measures*, i.e. norms, *value functions (Multi Attribute Value Theory (MAVT))* or *utility functions (Multi Attribute Utility Theory (MAUT))* or partially via pairwise comparisons *(Outranking Relations).*

In contrast to methods based on value or utility functions, which associate to each individual attribute value a score between 0 and 1, the *pairwise comparisons* are based on deviations between attribute values to model the preference structure of the decision maker. An essential part of the modelling is the extension of the pairwise dominance relations by comparisons based on preference functions. The preference functions describe the subjective view and attitude of the decision maker, i.e. his/her preferences using preference function $P_j(.,.) : A \times A \rightarrow [0,1]$ for each criterion. These functions are "models describing the relative importance or desirability of achieving different levels of performance for each identified criterion" [Belton and Stewart, 2002] by incorporating value judgements about the decision makers' preferences.

3.2 Definition of a Metric

Based on the efficiency definition given in the last section a metric is defined as a multi-criteria approach to evaluate and discuss resource efficiency. Different technology combinations, characterised by the consumption of several resources, are compared. Two major aspects are to be pointed out:

1. The metric considers a target value for each resource. This target value compromises a minimal consumption of the resource. To a certain extent, these theoretical minimal target values can be determined using the pinch analysis approaches described in Chapter 2.

2. The metric is part of a multi-criteria decision support process. Consequently, it considers explicitly preferential information such as the relative importance of the different resources (cf. Section 3.1.4).

The following nomenclature will be used within this section:

Table 3.2: Nomenclature for the Metric

Variable	**Name**
R	set of all resources $R = \{r_1, r_2, \ldots, r_n\}$
τ_κ, τ_ν	points within $\mathbb{R}^n$
$\|\tau_\kappa\|$	norm of τ_κ
$r_{i\kappa}$	resource consumption of resource i at the point τ_κ, $i = 1, \ldots, n$ ($n \in \mathbb{N}$) and $r_i \in \mathbb{R}$
r_{i0}	resource consumption of resource i at current level
$r_{i\,pinch}$	resource consumption of resource i at theoretical minimal level
$r_{i\,limit}$	resource consumption of resource i at maximal acceptable level

Table 3.2: Nomenclature for the Metric (cont.)

Variable	**Name**
$r^{\mu}_{i\lambda}$	resource consumption of resource i of technology combination T^{μ}_{λ}
S_0	Pareto surface S at the level of the current technology combination T^0_0
S_λ	Pareto surface S at the level λ; $S \in \{S_0; S_1; \ldots; S_\lambda; \ldots; S_{pinch}\}$
S_{pinch}	Pareto surface S at the minimal level of resource consumption of all resources r_i (i.e. point within $\mathbb{R}^n$)
T^{μ}_{λ}	technique combination μ at Pareto surface level λ
T^0_0	current technique combination
D	domain of the acceptable technique combinations, $D \subset \mathbb{R}^n$
Θ	set of all available technique combinations T^{μ}_{λ}
Θ_D	set of all technique combinations T^{μ}_{λ} within D
d_λ	distance of the Pareto surface S_λ to the pinch point (S_{pinch})
$d^{\mu}_{i\lambda}$	distance of the resource consumption of resource i from its pinch point $r_{i\,pinch}$ according to technology combination T^{μ}_{λ}
w_i	preference to resource r_i
δ_{MOPA}	efficiency improvement over the current status according to MOPA
$\delta_{i\,MOPA}$	efficiency improvement by component over the current status according to MOPA for resource i

3.2.1 Definition of a Distance Measure

Relevant topology, terminology and definitions for the distance metric are given in the following. Based on the general conditions of any metric an overall improvement potential is described. A distance measure will be defined providing the basis for the determination of a measure for the degree of efficiency. This efficiency metric illustrates the savings potential for the different resources considered and provides a base to compare different technical options. The relative assessment is based on the target values identified within the framework of Multi Objective Pinch Analysis (MOPA) (cf. Chapter 2.4). For the subsequent multi-criteria analysis and process design the efficiency measure can be used to derive either a combined attribute of all resources (i.d. δ_{MOPA}) or a set of attributes for each resource by component (i.d. $\delta_{i\,MOPA}$).

A metric $d(\cdot\,,\cdot) : \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}$ defines a distance between two points in $\mathbb{R}^n$ and a norm $\|\cdot\| : \mathbb{R}^n \rightarrow \mathbb{R}$, describing the length of a vector, induces a metric by $d(x, y) =$

$\|x - y\|, x, y \in \mathbb{R}^n$ in the vector space $\mathbb{R}^n$. The general conditions of a metric $d(\cdot, \cdot)$ and a norm $\|\cdot\|$ are fulfilled [Kelley, 1975].

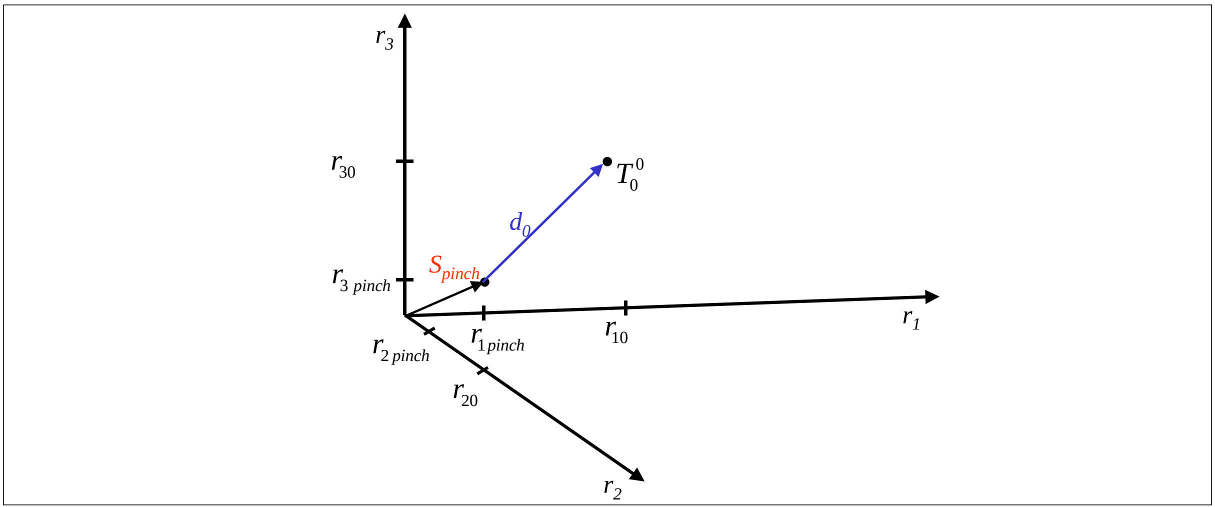

Figure 3.2: Pinch Point S_{Pinch} and Current Technology Combination T_0^0 in the $\mathbb{R}^3$

The parameter $n \in \mathbb{N}$ represents the number of different resources considered, i.e. mass and energy flows, and therefore the dimension of the given problem. In terms of multi-criteria analysis the different resources correspond to the different evaluation criteria. As described in the previous chapter the pinch points, i.e. the theoretical minimal consumption targets $r_{i\ pinch}$ of each resource r_i, can be calculated. These pinch points are the coordinates of S_{pinch} (cf. Equation 3.6, Figure 3.2). S_{pinch} is a point in the $\mathbb{R}^n$ and the target of all further investigations.

$$S_{pinch} = \begin{pmatrix} r_{1\ pinch} \\ r_{2\ pinch} \\ \dots \\ r_{n\ pinch} \end{pmatrix} \tag{3.6}$$

Just as for S_{pinch}, the point of current resource consumption of the considered resources can be described by a vector. The current consumption is realised by a combination of different technologies referred to as T_0^0. The current consumptions r_{i0} are the coordinates of the technology vector:

$$T_0^0 = \begin{pmatrix} r_{10} \\ r_{20} \\ \dots \\ r_{n0} \end{pmatrix} \tag{3.7}$$

Taking any two points τ_κ,τ_ν $(\kappa, \nu \in \mathbb{N})$ within $\mathbb{R}^n$, such as

$$\tau_\kappa = \begin{pmatrix} r_{1\kappa} \\ r_{2\kappa} \\ \dots \\ r_{n\kappa} \end{pmatrix} \tag{3.8}$$

where τ_κ is defined by a certain resource consumption of each resource $r_{1\kappa}$ as its coordinates. The norm $\|\tau_\kappa\|$ of the vector τ_κ is defined as

$$\|\tau_\kappa\| = \sqrt{\sum_{i=1}^{n} (w_i \cdot r_{i\kappa})^2} \tag{3.9}$$

taking into account the weighting of the different resources, i.e. criteria. Incorporating the weights w_i a modified Euclidean norm can be defined for the length of a vector. The preference of a certain resource r_i is expressed via a weighting factor w_i, whereby the sum of all weighting factors equals one ($\sum_i^n w_i = 1 \wedge w_i \geq 0 \ \forall i$). In this context the Euclidean, i.e. *2-norm*, is incorporated because the direction of the deviation is considered to be less important. Other norms, such as *1-norm*, *max-norm*, can be used and are discussed in the context of DEA and MCA [Kleine, 2001].

Using this norm the distance $d(\tau_\kappa, \tau_\nu)$ of two points τ_κ, τ_ν is:

$$d(\tau_\kappa, \tau_\nu) = \|\tau_\kappa - \tau_\nu\| \tag{3.10}$$

In particular, the distance d_λ from τ_κ $(\tau_\kappa \in S_\lambda)$ to the pinch point S_{pinch} is:

$$d_\lambda = d(\tau_\kappa, S_{pinch}) = \|\tau_\kappa - S_{pinch}\| \tag{3.11}$$

3.2.2 Determination of an Aggregating Measure

Incorporating the general metric the distance d_0 from the current technology combination T_0^0 (and therefore from the Pareto surface S_0) to the pinch point S_{pinch} is:

$$d_0 = d\left(S_0, S_{pinch}\right) = \|S_0 - S_{pinch}\| \tag{3.12}$$

An aggregated normed distance d_λ^{norm} is consequently derived:

$$d_\lambda^{norm} = \sqrt{\sum_{i=1}^{n} \left(w_i \cdot \left| \frac{r_{i\,\lambda}^{\mu} - r_{i\,pinch}}{r_{i\,0}^{0} - r_{i\,pinch}} \right| \right)^2} \tag{3.13}$$

The normed distance d_0^{norm} from the current consumption to the pinch point S_{pinch}, $d_0^{norm} = \|S_{pinch} - T_0^0\|$, characterises the compact domain $D \in \mathbb{R}^n$. This region in $\mathbb{R}^n$ is a bounded and closed subset of $\mathbb{R}^n$.

In fact $\mathbb{R}^n$ and the subspace domain D are continuous, but only discrete points T_λ^μ within $\mathbb{R}^n$ that can be realised by a technology combination are relevant. All these points build the set Θ of available technology combinations from which the points of the subset Θ_D, $\Theta_D \subset \Theta$, become points for further investigation.

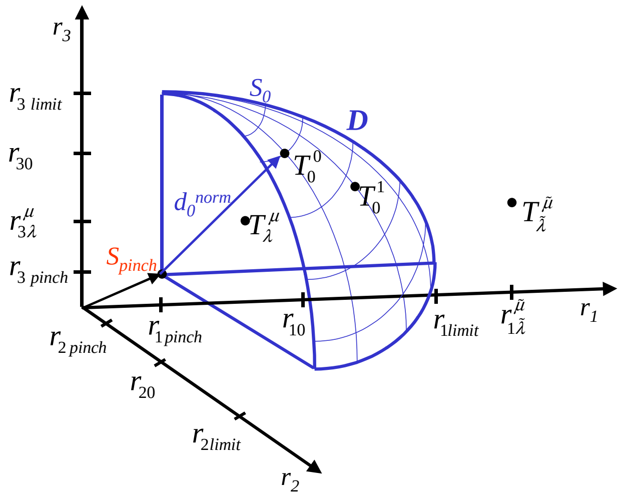

Figure 3.3: Domain D of Acceptable Technique Combinations T_λ^μ in the $\mathbb{R}^3$

The distance d_0^{norm} illustrates the overall savings potential of all resources. The actual realised savings potential compared to the current status is expressed by δ_{MOPA}. It is a percentage between 0% and 100% and can be interpreted as the potential realised, where the current status or any change to T_0^μ would be 0%, and a theoretical change to the pinch point S_{pinch} would be 100% respectively. If an improvement from T_0^0 to the point T_λ^μ exists (cf. Figure 3.4) then δ_{MOPA} is:

$$\delta_{MOPA} = \frac{d_0^{norm} - d_\lambda^{norm}}{d_0^{norm}} \tag{3.14}$$

Consequently, δ_{MOPA} is a measure of the distance to the pinch point taking into account the weights of the various resources i and eliminating the different scales of measurement. A change within the same Pareto surface would yield no improvement ($\delta_{MOPA} = 0$) .

Since process improvements are considered, only technology combinations T_λ^μ that have a shorter distance than the current distance are analysed, $d(S_{pinch}, T_\lambda^\mu) \leq d_0$. Technology combinations exist (e.g. T_0^1 in Figure 3.3) that use less of one resource but more of another, however, they share the same distance to S_{pinch}. All points with the distance d_0 span the Pareto surface S_0 around the pinch point. Points below the theoretical minimal consumption level are impossible. The closed domain D is defined by $\{T_\lambda^\mu : d(S_{pinch}, T_\lambda^\mu) \leq d_0 \wedge r_i \geq r_{i\,pinch} \forall i\}$. Consequently, the domain D is shaped like an eighth of an ellipsoid.

The surface S_0 describes the characteristics of the decision maker's preferences and not the technical feasibility. An illustrative example can be seen in the recovery of VOC: If the current status is T_0^0 and resource 1 is energy and resource 2 is VOC, the line between the $r_{1\,limit}$ and the $r_{2\,limit}$ is the Pareto curve between r_1 and r_2 and visualises the trade-off between those resources according to a decision maker who is willing to increase r_1 by x units in order to reduce r_2 by y units. However, the technical alternatives can be entirely different. In addition to the described case (in general increased consumption of energy in order to reduce VOC consumption), points inside the domain D, such as T_λ^μ, or outside, such as $T_{\tilde{\lambda}}^{\tilde{\mu}}$, can represent the technical alternatives.

A distance d_λ^{norm} and a corresponding Pareto surface S_λ can be assigned for each technology combination T_λ^μ within the domain D. Depending on the preferences between the resources, the resource consumption of one resource can be higher than the current consumption, but only to a certain extent. The point where the Pareto surface S_0 intersects the edge of the domain D parallel to the axis r_i defines the maximal acceptable level of resource consumption for the considered resource r_i (i.e. $r_{i\,limit} = r_{i\,pinch} + d_0$).

3.2.3 Impact of Different Weightings on the Domain D

It is important to note that the shape of the domain D depends on the considered set of processes and decision maker's preferences. Consequently, the profile of D is different even for similar applications and depends highly on the considered case study.

The determination of the weighting factor is complex since it involves much technical expertise in addition to knowledge about the special requirements of the local context considered. For example, different perceptions about water might lead to different weightings depending on the water supply in the specific region.

A first approach would be to employ similar methods to those used in life cycle analysis [Guinée et al., 2002] to derive the weighting factors and modify these to reflect the decision maker's preferences. If one resource (e.g. r_1) is less weighted than another (e.g. r_2), comparatively more units of r_1 are required to counterbalance one unit of resource r_2. In

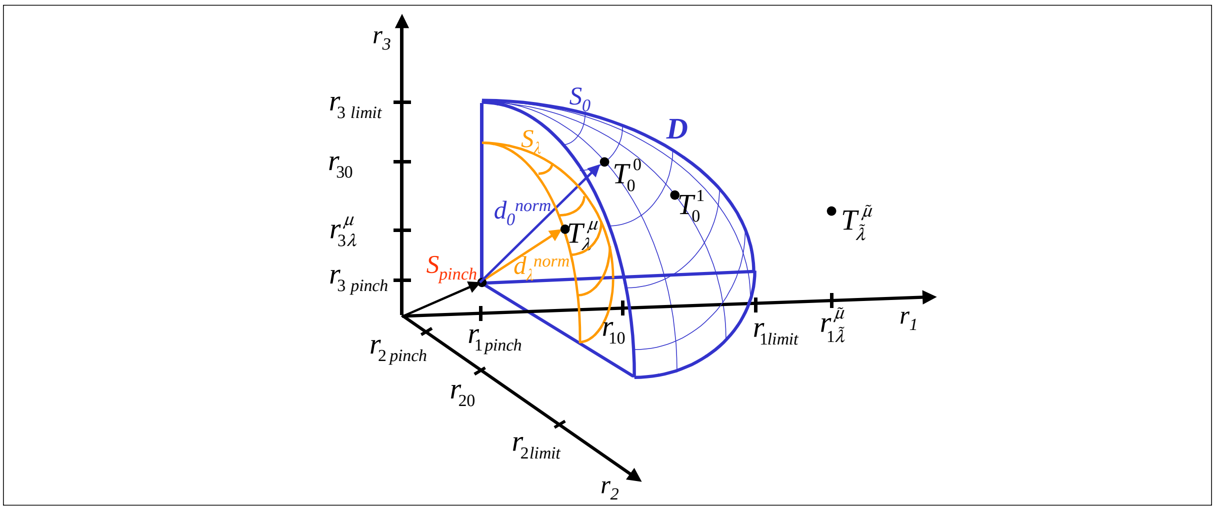

Figure 3.4: Domain D with Pareto Surfaces S_λ in the $\mathbb{R}^3$

this case the domain D is prolongated in the direction of the less weighted criteria and assumes the shape of an eighth of an oblate spheroid.

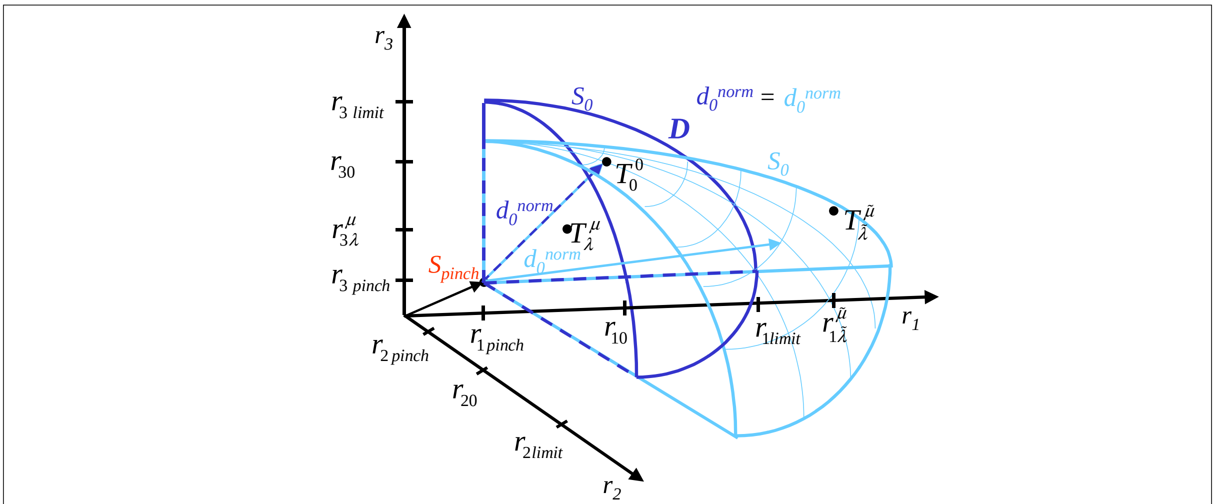

Figure 3.5: Domain D with Pareto Surfaces S_λ in the $\mathbb{R}^3$

Furthermore, the weighting of the different considered resources plays an important role in the consideration of the problem and the definition of the savings potential. On the one hand, there exist points (e.g. T_λ^μ in Figure 3.4) which use less of each resource than the technology combination of the current process layout. Obviously, these points represent a process improvement according to the current status. On the other hand, however, there exist points (e.g. $T_{\lambda}^{\tilde{\mu}}$ in Figure 3.4) which use less of one resource (e.g. resource r_3), but more of another (e.g. resource r_1). Whether or not these technology combinations should be considered in the process layout planning depends on the weighting between the different resources. The weighting illustrates for example the trade-off between a higher energy consumption and a lower water consumption with respect to the current process layout.

Hence, by changing the weightings the formerly excluded technology combination $T_{\lambda}^{\tilde{\mu}}$ would now be within the domain D of technology combinations to be considered for the process layout planning (cf. Figure 3.5).

The distance d_0 is a modified Euclidean norm incorporating the weights for the different resources considered and therefore the distances d_0^{norm} and d_0^{norm*} have the same length (cf. Figure 3.5). Consequently, the combined distance measure including the weighting or each resource and its weighting separately are the input criteria for the following techno-economic assessment of the technology options.

3.2.4 Discussion of the Application of a Metric

It must be pointed out that the considerations are based on a relative efficiency measure depending on the selected criteria and the selected alternatives. Consequently, both the definition of S_{pinch} and T_0^0 in combination with the weighting and the selected Euclidean norm highly influence the shape of the domain D. Hence, even if no statement is made concerning the technology combinations and only existing technology combinations are considered the assessment is limited by the simplified parameter and system boundary selection.

Several examples show that the definition of the system boundaries and the technically correct modelling are essential for a technology assessment. One example is the implementation of end-of-pipe emission reduction measures, which can be implemented downstream in the process in contrast to process integrated measures involving the re-engineering of the complete process across the supply chain, making the assessment very complex since all required parameters (e.g. solvent content) for process changes must be considered. For example the selection of coating material for the coating of metal or plastic parts using solvent-based vs. waterborne coatings significantly influences the energy consumption in the corresponding drying step and hence the layout of the heating and waste gas system [Geldermann et al., 2005].

Consequently, further aspects must be included and the impact assessment of LCA must be combined with multi-attribute optimisation and decision support [Azapagic and Clift, 1999; Geldermann and Rentz, 2004; Seppälä et al., 2002]. Thus, economic criteria such as investments and operating costs must be included, which also depend highly on the region considered. Consequently, a multi-criteria approach incorporating country specific data and enabling sensitivity analysis is required (cf. Section 3.3). In general, the number of dimensions n of the metric is flexible and can be extended with further quantitative data. However, there are also qualitative data (such as operation experience, quality, etc.) to be considered. Hence, more explicit MADM methods can be used to compare the different alternatives of technology combinations and to provide sensitivity analyses [Bertsch et al., 2006b].

The attributes for the MADM method would be the different resource potentials considered by component. Also, the preferences of the decision maker (i.e. w_i) would be considered separately. As a result, the distance by component $d_{i\lambda}^{\mu\, norm}$ is not characterised by the weighted Euclidean norm (cf. Equation 3.9), but by an unweighted value. The realised savings potential by component $\delta_{i\ MOPA}$ is expressed in terms of the distance $d_{i\lambda}^{\mu\, norm}$:

$$\delta_{i\ MOPA} = d_{i\lambda}^{\mu\, norm} = \| \frac{r_{i\lambda}^{\mu} - r_{i\, pinch}}{r_{i\,0}^{0} - r_{i\, pinch}} \| \tag{3.15}$$

Besides the absolute values the realised savings potential δ_{MOPA} and the realised savings potential $\delta_{i\ MOPA}$ can now be used for the subsequent multi-criteria analysis and the process design. Using this measure a techno-economic assessment of the process modification can be performed. The economically valued $\delta_{i\ MOPA}$ is the available funding for investment in unit operations, such as heat exchangers, in order to realise the new technology combination [VDI 3800].

However, the identification of the techno-economic-environmental process improvement potential using a simple metric offers adequate possibilities in order to assess the different technologies.

3.3 The Approach of PROMETHEE

The problem of defining resource efficiency is discussed in this section based on the multi-criteria method PROMETHEE[9] [Brans et al., 1984; Brans and Vincke, 1985; Brans et al.,

[9] **P**reference **R**anking **O**rganization **METH**od for **E**nrichment **E**valuations

1986; Brans and Mareschal, 2005]. Beginning from the efficiency definition given in Section 3.1.1 the fundamental idea of PROMETHEE and its proposed approach for resolving the incomparabilities are discussed. For this purpose, PROMETHEE requires preferential information about relationships between the criteria and about each criterion. The accrued complexity requires sophisticated sensitivity analysis to guide the decision maker and to illustrate the impacts of his modelling. Especially the determination of preferential parameters is quite often underestimated. In this chapter various new sensitivity analyses for the outranking approach PROMETHEE are presented and discussed with respect to their advantages as well as their limitations.

It is well known that different decision makers prefer different decision support methods. For example, in many practical applications multi-attribute value theory (MAVT) [see e.g. Keeney and Raiffa, 1976] is also suitable. However, in principle, a MAVT analysis is subject to the same questions as an analysis in PROMETHEE addressed in this thesis. It is important both to investigate the modelling preferential information to resolve incomparabilities and to address sources of preferential and data uncertainty.

3.3.1 Preference Modelling

The fundamental idea of PROMETHEE is a dominance relation based on *preference*, *indifference* and *incomparability* (cf. Equations 3.2 - 3.4) aimed at reducing the number of incomparabilities by employing preferential information to identify efficient solutions.

The PROMETHEE algorithm is based on the deviations of the attribute values. The decision table is called D and D_j is the vector of all differences of attribute values for criterion j. The goal of PROMETHEE is the identification of a ranking by resolving incomparabilities of efficient alternatives. This problem is addressed via weighting factors as inter-criteria preferential information (cf. Section 3.3.1.1) and *preference functions* as intra-criteria preferential information (cf. Section 3.3.1.2).

3.3.1.1 Weighting of the Criteria

The relative importance of a criterion j is reflected in its weighting factors w_j. In the following normed weights are considered:

$$\sum_{j=1}^{k} w_j = 1 \tag{3.16}$$

Even so there exist specialised weighting approaches for outranking methods (e.g. cf. [Vansnick, 1986; Bana e Costa et al., 1997]) similar methods are applied as in classical approaches (cf. Section 3.1.4.1).

3.3.1.2 Preference Functions

The preference function $P_j(.,.) : A \times A \rightarrow [0,1]$ is based on the difference in the attribute values of two alternatives a_1 and a_2 ($d_j(a_1,a_2) = g_j(a_1) - g_j(a_2)$). In the case of a criterion that must be maximised, the alternative a_1 outranks the alternative a_2 if the difference $d_j(a_1,a_2)$ is positive. Consequently, if a decision maker prefers a_1 over a_2 he has no preference for a_2 over a_1 ($P_j(a_1,a_2) > 0 \Rightarrow P_j(a_2,a_1) = 0$).

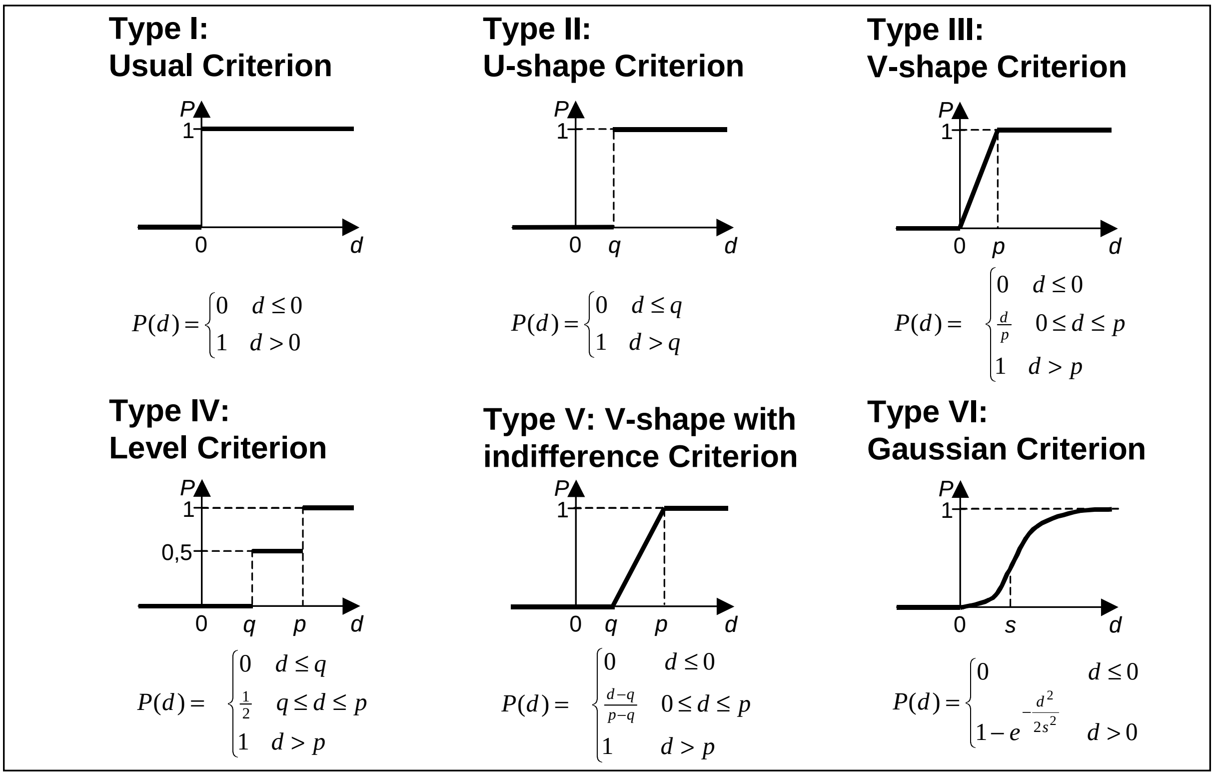

Figure 3.6: Types of Preference Functions $P(d)$ [Brans and Mareschal, 2005]

Decision support methods such as PROMETHEE, however, are usually used in situations in which the decision makers cannot specify their preferences exactly, thus it is also the task of the applied method to formally structure and model the preferences which exist in a diffuse way. Usually six generalised preference functions are proposed and defined by threshold values of indifference (q) and strict preference (p), or an inflection point s as in the case of a Gaussian distribution [Brans and Mareschal, 1994]. Figure 3.6 shows the six generalised preference functions of PROMETHEE. The decision maker can choose a preference function for each criterion and depending on the selection must define certain preference parameters.

Using the generalised preference functions the indifference value q is regarded as the largest negligible difference by the decision maker. The smallest deviation, which the decision maker considers to be sufficient for a full preference, is called strict preference threshold p. Thus, q is relatively small in comparison to the attribute values of the considered criterion, whereas p is in general at the upper end of the value range. However, the inflection point s of the Gaussian preference function is located between the indifference value q and the preference value p. Preferences are strengthened for minor differences by a small value for s near q while preferences are reduced by a value close to p.

However, both parameters q and p can also be defined and interpreted depending on the uncertainty and the quality of the attribute data [Rogers and Bruen, 1998]. The indifference value q can be interpreted for example as the minimum and correspondingly p as the maximum uncertainty value. Inaccuracies from incorrect attribute data are not clear without ambiguity up until the indifference value q, while starting from p certainly full preference exists [Maystre et al., 1994].

Specially defined or generally accepted values for the parameters q, p and s, or methods to define them, are found extremely rarely in literature concerning multi-criteria decision theory. The reason for this is based on the understanding that there are neither "correct" values for the parameters nor is there a "correct" way to define these [Kangas et al., 2001]. The parameter values always depend on the specific decision problem as well as the preferences and assessment of the decision maker. If it is difficult for the decision maker to define such parameter values a moderator and/or an experienced analyst is of help, i.e. *homme d'etude*.

Since no objective preferences exist and value judgements are, at least partially, formed only during the modelling process, the multi-criteria method should enable the decision maker to better comprehend his underlying assumptions and model his own preferences [Belton and Stewart, 2002; Basson, 2004]. Nevertheless, it is complex to make decisions about the preference parameters and understand their effects by defining a certain value. Therefore, default values based on the attribute values are proposed in this thesis if the decision maker cannot identify a starting point. However, in this case the proposed default values have a high uncertainty and sensitivity analyses are necessary in order to understand the effect of changing the proposed values [Treitz et al., 2006b,a].

If no value is given by the decision maker the following default values are proposed based on the mean and the standard deviation of the attribute values concerning criterion j:

$$q = |mean\{|D_j|\} - std\{|D_j|\}| \tag{3.17}$$

$$p = mean\{|D_j|\} + std\{|D_j|\} \tag{3.18}$$

Depending on the attribute values, these methods result in relatively high limits for indifference and relatively low limits for the strict preference value p. Therefore, the default values tolerate relatively high differences as indifferent, and on the other hand ascertain already relatively small differences a full preference.

For the parameter s the entire range of possible attribute values is considered:

$$s = \frac{1}{2}(max\{D_j\} - min\{D_j\}) \tag{3.19}$$

Various other parameter definitions seem reasonable (for example 5 % of the minimal attribute value for q ($q = \frac{1}{20}(min\{|D_j|\})$) or the maximal difference ($p = max\{|D_j|\}$) for p) and it is highly controversial whether proposals of parameter values should be made at all. By ascertaining default values to the preference parameters the decision maker can identify values in a meaningful range and analyse the robustness of his choice.

3.3.2 The Aggregation Model of PROMETHEE

The positive outranking flow $\Phi^+(a)$ (cf. Equation 3.20) expresses how much alternative a is preferred to, i.e. outranks, all other $(n-1)$ alternatives $x \in A$. Whereas the negative outranking flow $\Phi^-(a)$ (cf. Equation 3.20) expresses how much all the other alternatives are favoured compared to alternative a. Consequently, $\Phi^+(a)$ and $\Phi^-(a)$ both are positive (i.e. $0 \leq \Phi^+(a), \Phi^-(a) \leq 1$)

$$\Phi^+(a) = \frac{1}{n-1} \sum_{j=1}^{k} \sum_{x \in A} [P_j(a,x)]w_j \tag{3.20}$$

$$\Phi^-(a) = \frac{1}{n-1} \sum_{j=1}^{k} \sum_{x \in A} [P_j(x,a)]w_j \tag{3.21}$$

Considering $\Phi^+(a)$ and $\Phi^-(a)$ the net outranking flow $\Phi(a)$ is the overall comparison (i.e. $-1 \leq \Phi(a) \leq 1$):

$$\Phi(a) = \Phi^+(a) - \Phi^-(a) \tag{3.22}$$

Consequently, the PROMETHEE algorithm provides two approaches for ranking the alternatives [Brans and Mareschal, 2005]:

- The *PROMETHEE I ranking* preserves all incomparabilities and illustrates the results as a partial ranking combining the rankings induced by $\Phi^+(a)$ or $\Phi^-(a)$.
- The *PROMETHEE II ranking* balances the positive and negative flows to a complete order.

The positive and negative outranking flows already consider the weighting of the different criteria. By focussing on one alternative a the single criterion net flows $\Phi_j(a)$ express the quality of a with respect to all criteria individually:

$$\Phi_j(a) = \frac{1}{n-1} \sum_{x \in A} [P_j(a,x) - P_j(x,a)] \tag{3.23}$$

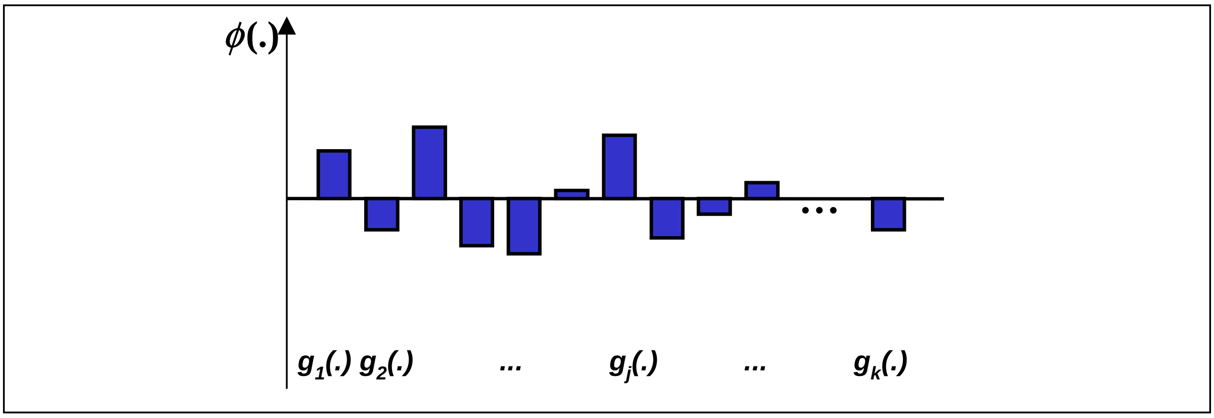

Figure 3.7: Profile of an Alternative [Brans and Mareschal, 2005]

Figure 3.7 shows the single criterion net flows $\Phi_j(a)$ of an alternative a. It expresses the strengths and weaknesses of an alternative. All individual $\Phi_j(a)$ are pooled in the matrix M $(n \times k)$. Thus, each line in M represents an alternative and each column a criterion. Different criterion scales do not affect M, since M is dimensionless, and because it is based on the values of the respective preference functions. Likewise, M is independent of the criterion weights.

3.3.3 Sensitivity Analyses in PROMETHEE

Sensitivity analyses play an important and relevant role in decision making and "the learning and understanding which results from engaging in the whole process of analysis is far more important than numerical results." [Belton and Stewart, 2002]. Especially in group decision making acceptance is increased by starting with preliminary results and iteratively refining the decision support model. In multi-criteria decision support sensitivity analyses are used to investigate both the data uncertainty and the preferential uncertainty of the decision maker(s). This is done to assess how robust the results react to changes of data and parameters. When modelling value judgements especially, it is important to carry out sensitivity analyses in order to iteratively re-model the decision problem and to facilitate learning about the given problem as proposed in [ISO 14040]. Sensitivity analyses investigate how the results of a model change with respect to variations in the input parameters [Saltelli et al., 2000] and are therefore essential in any multi-criteria decision analysis problem. The motivation behind sensitivity analyses are amongst others [French, 2003]:

- to support the elicitation of judgemental inputs to an analysis;
- to guide the making of decisions;
- to explore and build consensus;
- to build understanding about a given problem.

While decision support by PROMETHEE is also available in several existing standard MCA software packages, such as Promcalc [10] or Decision Lab [11], the major drawback of these packages is the possibility to handle the different types of uncertainties arising in a decision process in an adequate way. Therefore, the analyses are based on an implementation of PROMETHEE in *MATLAB*™ [12].

By applying the PROMETHEE technique several standard but also new sensitivity analyses can be carried out (cf. Table 3.3). On the one hand the robustness of a decision can be investigated by analysing the inter-criteria preferential information: By varying the weighting of one criterion j from zero to 100 %, by calculating sensitivity indicators $\delta_{j,a,b}$ for the switch in the ranking position of two selected alternatives a and b, by changing all weighting factors simultaneously within certain weighting intervalls, or by determining

[10] see [Brans and Mareschal, 1994]
[11] see http://www.visualdecision.com/dlab.htm
[12] for further information see: http://www.mathworks.com

stability intervalls based on δ_j^- and δ_j^+ for a fixed ranking of a certain number of best alternatives the definition of the inter-criteria preferential parameters is supported. On the other hand the robustness of intra-criteria preferences, i.e. the preference function, can be investigated by evaluating all possible preference type combinations or by carrying out a *Monte Carlo Simulation (MCS)* using specific uncertainty levels, such as $\pm 10\,\%$, for the parameters q, p, and s. Furthermore, not only consideration of uncertainty in the value judgements of the decision maker but also in the process data must be addressed by evaluating the distinguishability between the different alternatives considered (cf. Table 3.3).

The introduced sensitivity analyses for the outranking approach PROMETHEE and their applicability will be discussed in detail throughout this Chapter. The consideration of preferential uncertainty and data uncertainty has been addressed for multi attribute value theory, too. Possibilities to handle and visualise data uncertainties in MAVT have for instance been proposed by [Basson and Petrie, 2007; Geldermann et al., 2006a]. Approaches that allow the use of weight intervals in MAVT instead of crisp weight values are for example described in [Mustajoki et al., 2005; Bertsch et al., 2006a]. Furthermore, the variation of value function parameters (in analogy to the variation of the type of the PROMETHEE preference function) has for instance been suggested by [Mavrotas and Trifillis, 2006; Bertsch et al., 2006a]. However, the literature so far is mostly limited to analyses within one MCDA approach. Having decision processes in groups in mind where different members prefer different MCDA approaches, a comparison of the results of the different "schools of thought" can be helpful to investigate the robustness of a decision with respect to the different approaches [see e.g. Stewart and Losa, 2003; Geldermann and Rentz, 2000; van Huylenbroeck, 1995; Zhang, 2004].

3.3.4 Sensitivity Analyses for Preferential Data

The evaluation of the inter-criteria preferences, i.e. the weighting factors, is essential for the evaluation of the uncertainty in preferential information, since the weighting highly influences the results of the multi-criteria analysis. Consequently, analytical methods for the evaluation of the weighting factors and stability intervals of the results are discussed (cf. Section 3.3.4.1). Furthermore, enumerative and simulation based approaches are applied to evaluate the uncertainty in the model parameters of the intra-criterion preferential information (cf. Section 3.3.4.2).

Table 3.3: Sensitivity Analyses for PROMETHEE

Variable	**Fixed**	**Method**	**Output**	**Source**
weight (one criterion)	preference parameter and type	change of weight within $[0, 1]$	$\Phi_{net}(a)$ (line plot)	[Geldermann, 1999]
weight (one criterion)	ranking of two selected alternatives a and b	analytical determination of maximal change	sensitivity indicator $\delta_{j,a,b}$	[Zhang, 2004]
weights (all criteria)	preference parameter and type, weighting limits	convex hull off all valid weighting vectors	area in GAIA plane	[Brans and Mareschal, 1995]
weights (all criteria)	ranking of a selected number of best alternatives	maximal change of all weighting factors	stability intervals $[w_j - \delta_j^-, w_j + \delta_j^+]$	[Zhang, 2004]
preference type (one criterion)	preference parameter	variation of preference type	$\Phi_j(a)$ (line plot)	new
preference type (all criteria)	preference parameter and weighting	variation of all preference types for all criteria	$\Phi_{net}(a)$ (line plot)	new
preference parameter (one criterion)	preference type	MCS (uniform distribution)	$\Phi_j(a)$ (line plot)	new
preference parameter (all criteria)	preference type and weighting	MCS (normal distribution)	$\Phi_{net}(a)$ (box plot)	new
attribute values	preference parameter and type, weighting	MCS (normal distribution)	scatter plot	new

3.3.4.1 Sensitivity Analysis for the Inter-Criteria Preferences

The most frequently applied analysis technique for decision problems plots the output value, i.e. $\Phi_{net}(a)$ in PROMETHEE, versus the weighting of a selected criterion in a two-dimensional graph [Geldermann et al., 1999]. The graph in Figure 3.8 shows the alternatives as straight lines. Thus, the effect on Φ is illustrated for the different alternatives by a variation of the weighting from 0 to 100 % of the selected criterion. Although only one parameter is explicitly changed (the weight of the selected criterion), implicitly the other criterion weights change as well.

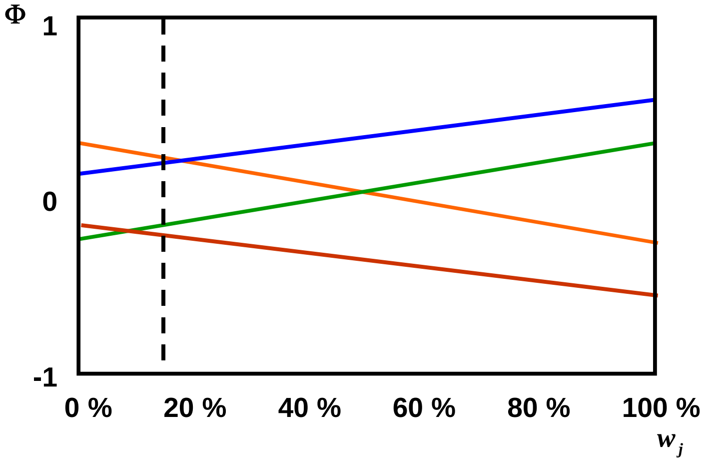

Figure 3.8: Sensitivity Analysis of the Weighting of a Selected Criterion

The gradient of the lines represents the influence of the selected criterion on the performance of the alternatives. A negative / positive gradient corresponds to negative / positive correlation on the output value $\Phi_{net}(a)$ by the selected criterion. At the intersections of the lines a change in the ranking of the alternatives takes place. Therefore, the whole range can be divided into sections with different rankings. Within these insensitivity or stability intervals the weighting of the selected criterion can be changed and it will have no impact on the ranking [Mareschal, 1998]. The stability interval around the current weighting of the selected criterion and all possible rankings, for example up to 10 rankings, first three positions) can be calculated and used to inform the decision maker about the robustness of his weighting factor definition. Therefore, further examination of the weighting factors for an insensitive criterion can be avoided [Geldermann et al., 2003].

Furthermore, interactive software tools enable the decision maker to change the weighting of a selected criterion (i.e. *walking weights*) via a scroll bar. On the one hand the required (spare) weight can be obtained (reallocated) from (to) all other criteria, but on the other hand only from (to) selected criteria. Not only the weights of each criterion are shown in a bar chart, but simultaneously the $\Phi_{net}(a)$ flows of the considered alternatives are shown in a bar chart with the height of each bar (i.e. Φ) changing with the weighting.

Additionally, sensitivity indicators $\delta_{j,a,b}$ can analytically be calculated for each criterion j. The sensitivity indicator $\delta_{j,a,b}$ ($1 \leq a \leq b \leq n$ and $1 \leq j \leq k$) denotes in absolute terms or as a percentage the smallest change of the current weighting w_j of criterion j, such that the ranking order of the alternative pair a and b is reversed [Zhang, 2004]. Consequently, for a $n \times k$ decision table D a total number of $\frac{k \cdot n(n-1)}{2}$ sensitivity indicators can be calculated and the indicator with the smallest absolute value $|\delta_{j,a,b}|$ marks the most sensitive criterion [Geldermann et al., 2003, 2006e]. The ranking is stable concerning criterion j if no indicator $\delta_{j,a,b}$ can be determined.

To evaluate the robustness of the ranking with respect to all weighting factors simultaneously, the sensitivity indicators $\delta_{j,a,b}$ can be used in an optimisation model to determine stability intervals based on δ_j^- and δ_j^+ in which the positions in the ranking order of a predetermined number of best alternatives, for example the group of the best three alternatives, remains unchanged [Zhang, 2004]. In this case the weighting w_j of criterion j can be changed within the interval $[w_j - \delta_j^-, w_j + \delta_j^+]$ for all criteria $j = 1, \ldots, k$. The calculation of the stability intervals is based on a linear optimisation approach maximising the stability intervals [Zhang, 2004]:

$$max \sum_{j=1}^{k} (\delta_j^- + \delta_j^+) \tag{3.24}$$

The optimisation is subject to no change in the ranking position of a predetermined number of best alternatives [see Zhang, 2004, for a detailed description].

In addition to the described analytical evaluation spider diagrams are used for the visual comparison of several alternatives considering all criteria simultaneously [Vetschera, 1994]. In case of PROMETHEE the single criterion net flows $\Phi_j(a)$ of individual attributes are shown on criterion axes, which proceed symmetrically from a common centre from -1 to 1 [Rosenau-Tornow, 2005]. Figure 3.9 shows a fictitious example. The number of axes corresponds to the number of criteria. A line for each alternative forms a polygonal traverse connecting the attribute values whose relative position shows the quality of an alternative.

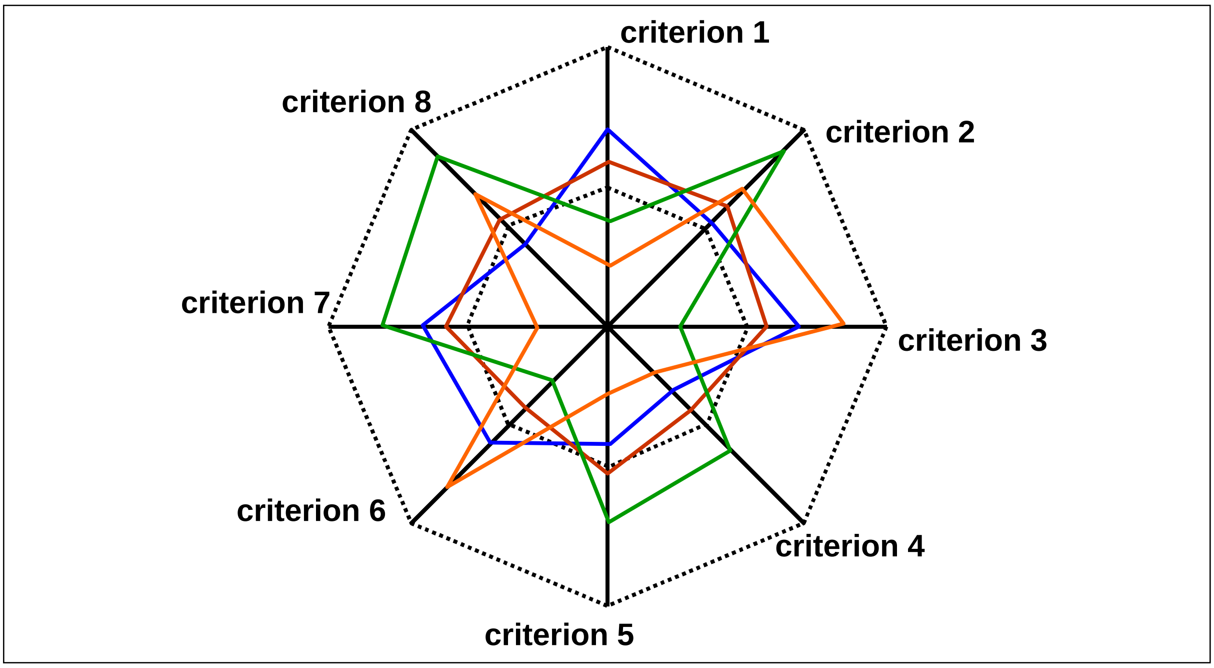

Figure 3.9: Spider Diagram of Φ of All Criteria and All Alternatives of the Decision Problem

The purpose of a spider diagram is less to present precise data values but more to impart a holistic, overall impression of the decision problem [Vetschera, 1994]. Depending on the decision context it can be reasonable to prefer a well-balanced alternative with average performance in all criteria than the identified best, but possibly very differentiated, alternative. Since the general overview becomes increasingly confusing with a growing number of criteria or alternatives, an aggregation of the attribute values is inevitable in such cases. Here factor-analytic techniques can be employed (cf. Section 3.3.5).

3.3.4.2 Sensitivity Analyses for Intra-Criterion Preferences

Extensive sensitivity analyses are necessary to capture not only the uncertainty in the inter-criteria preference values, but also in the modelling of the decision makers' preferences concerning the intra-criterion preferences. Therefore, special sensitivity analysis for preferential uncertainties within the outranking approach PROMETHEE are essential. The decision maker can define a preference function by type and depending on the type by a preference parameter. For example, the selection of preference type 1 requires no further parameter definition whereas the selection of preference type 5 requires the definition of parameters q and p (cf. Section 3.3.1.2). The differences in the attribute values can be added to the graph of the selected preference function, which clearly facilitates the determination of the preference function parameters, since the decision maker can directly see the effect of his preference type selection and parameter value definition.

The preferential uncertainties concerning the intra-criterion preferences are here addressed by a complete enumeration of all possible preference type combinations for the kind of preference type and by *Monte Carlo Simulation (MCS)* for the evaluation of the preference parameters of the preference function in the following. Under the term Monte Carlo Simulation statistic procedures of random sampling are summarised, which approximate the effects of uncertainties of the input values onto the output values which could analytically not be regarded. First, a sufficiently large number n of random numbers is drawn according to a certain distribution for one or more selected variable(s) of the decision model. Thus, it is accepted that the values distribute themselves statistically around an expected value (within an interval) which is assumed to be likely for the input data. Possible distribution types are in general for example the Normal, Uniform, Poisson, Binomial or Exponential distribution or others. Besides the simulation of the uncertainty of the regarded values, the aim is to identify potential risks and errors afflicted with the decision analysis results.

A different approach to address the uncertainty in preferential information in multi-criteria methods is carried out by fuzzy approaches [Carlsson and Fullér, 1996; Ribeiro, 1996]. Employing trapezoidal fuzzy intervals for the preference parameters, fuzzy preference flows can be used to represent the decision problem within the outranking approach PROMETHEE [Geldermann et al., 2000b]. The ranking of the alternatives is ultimately based on the defuzzified fuzzy preference flows.

However, the use of fuzzy approaches as opposed to probabilistic and Monte Carlo approaches is discussed controversially in literature. It should be emphasised that the methods described in this thesis are aimed at communicating and visualising the uncertainties associated with the results of the decision analysis in contrast to the illusory preciseness of deterministic results remaining after a procedure such as the defuzzification (or after calculating expectation values in the case of probabilistic approaches). Thus, using the methods described in this thesis, it is possible to explicitly illustrate the spread of the results - i.e. the ranges in which the results can vary for the spread due to preferential uncertainties or for the spread resulting from data uncertainties.

Thus, in order to address the difficulty of selecting a preference type and defining preference parameters for each criterion $g_j(\cdot)$, four new sensitivity analyses are proposed in this thesis. The first two sensitivity analyses focus on the type of preference function and are based on preference type combinations. The second two sensitivity analyses evaluate the robustness of the decision based on the preference parameters using MCS. For each sensitivity analysis the ratio is calculated for which an alternative is ranked first.

- *Sensitivity Analysis of the Type of Preference Function of the Selected Criterion:*

  A line diagram visualises the single criterion net flow Φ_j for all alternatives by variation of all six possible preference types. In case no individual preference parameters are set the default values (cf. Section 3.3.1.2) are used. Since it is possible that in a line diagram one alternative is completely covered by another alternative warning messages are useful in a graphical representation.

- *Sensitivity Analysis of all Combinations of the Types of Preference Function for all Criteria:*

  The total net flow Φ considering all criteria is plotted as a line diagram by varying all six possible types of preference function for each alternative for all criteria. $\Phi(a)$ is calculated for all alternatives and all 6^k different combinations of preference functions. Again, in case no individual preference parameters are set the default values are used.

- *Sensitivity Analysis of the Preference Parameter(s) of the Selected Criterion:*

  For this analysis the single criterion net flow $\Phi_j(a)$ of all alternatives is calculated by variation of the preference parameter q and/or p as well as s. The uncertainty is given as a percentage, such as 10 % or 90 % uncertainty. Values for the parameters are generated using a Monte Carlo Simulation with a uniform distribution within the interval $\pm$ the value of the uncertainty level around the original parameter value. In the case of preference type 1 no analysis is carried out since the preference function does not depend on a preference parameter. In the case of a preference function requiring two parameters two line plots are shown. When changing the uncertainty level the effects on $\Phi_j(a)$ can be observed.

- *Sensitivity Analysis of the Preference Parameters of all Criteria:*

  A box plot of the total net flow Φ for all alternatives is shown for a variation of all preference parameter values using the uncertainty interval. This analysis can explore how Φ is dependent on the preference parameters. In this case all preference parameter values are generated using a MCS approach with a normal distribution. The standard deviation is assumed to be half of the uncertainty indicated. Thus, the interval including twice the standard deviation corresponds to the uncertainty interval around the original value and covers 95.4 % of all values. This interval is also called the 2σ range.

The edges of the boxes are the lower and upper quartiles and within the box, i.e. the interquartile range, the deterministic value is visualised. The middle line of the deterministic value is equal to the height of the bar of each alternative in the analysis using the deterministic values. The whiskers show the minimal and maximal $\Phi(\cdot)$ of all samples. This analysis considers the selected preference type and does not vary this selection. Consequently, if preference type 1 is selected for all criteria there is no variation in the height since no parameter is used in preference type 1.

3.3.5 Principal Component Analysis for Sensitivity Analyses

Decision problems usually represent complex circumstances, often characterised by a multiplicity of variables. The resulting high-dimensional data sets can only be analysed and illustrated graphically using suitable statistical procedures such as the *Principal Component Analysis (PCA)* [Timm, 2002; Härdle and Simar, 2003]. In general, the principal component analysis is an attempt to obtain a reduction of the number of correlated variables. The resulting uncorrelated variables, the principal components, successively describe a maximum of variance.

3.3.5.1 Basics of the Principal Component Analysis in PROMETHEE

In the case of PROMETHEE the PCA is based on the matrix M of the *single criterion net flows* $\Phi_j(a)$ in which the strengths and weaknesses of an alternative can be analysed for each criterion individually. By calculating the eigenvectors of the covariance matrix of $M'M$ and building a matrix of all eigenvectors, sorted by the magnitude of the eigenvalues, the axes can be transformed. The transformation represents a rigid rotation of the old axes into the new principal axes based on the matrix of the sorted eigenvectors. Consequently, the new principal components span a rotated coordinate system in comparison to the original system. Both coordinate systems are k-dimensional. The desired reduction of dimension is reached by using only a subset of the principal components.

The question of how these components should be combined arises, whereby even considering the reduction of the number of dimensions, as much information as possible is preserved. It must be pointed out that the spread (i.e. the variance) of the new linear combinations is a measure for the represented information by the linear combinations [Härdle and Simar, 2003]. Therefore, it can be concluded that the eigenvector ν_i of the largest eigenvalue (i.e. λ_1) of $cov(M'M)$ is the result of the optimisation problem for finding a representative of the maximal variance. Thus, the linear combination with the largest variance is called the 1^{st} principal component. Perpendicular to ν_1 is the eigenvector ν_2 of the second largest eigenvalue λ_2 (2^{nd} principal component), representing the largest part of the remaining total variance. By projecting the alternatives from the $\mathbb{R}^n$ onto the plane of the 1^{st} and 2^{nd} principal component, the dimension is reduced while preserving the maximum information in the $\mathbb{R}^2$ (cf. Figure 3.10).

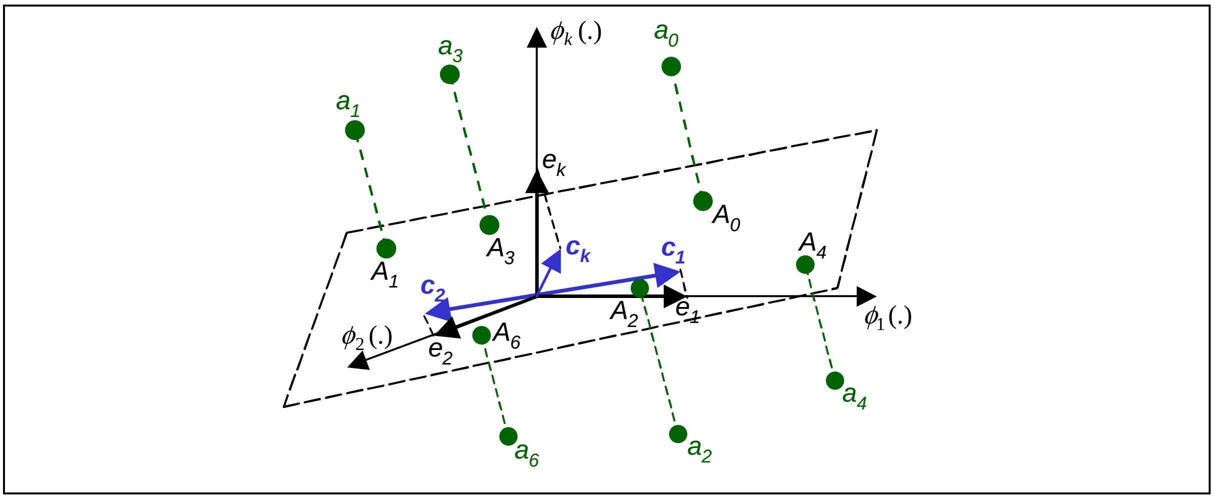

Figure 3.10: Projections on the GAIA Plane [Brans and Mareschal, 2005]

The sorted eigenvalues are therefore a measure for the ratio of the total variance, represented by the principal components. Thus, it can be calculated how much variance (and/or information) is represented by the 1^{st} and 2^{nd} principal component. Often, more than 60 % or even 80 % of the total variance is represented by the first two principal components [Brans and Mareschal, 2005] and consequently a meaningful visualisation is possible. Nevertheless, the ratio depends on the number of alternatives and number of criteria. Hence, there still exist many cases where less information is represented by the first two components and thus it is questionable whether the visual representation is meaningful for the decision problem [Basson, 2004].

Besides the total variance ratio the correlation of the new principal axes with the original axes is of interest. The coefficient of correlation describes how well the j^{st} variable (criterion axis) is represented by the PCA. The decision maker can use this information to ascertain how well the criterion (j^{st} variable) is represented by the 1^{st} and 2^{nd} principal component.

In PROMETHEE the PCA approach is incorporated and the plane of the 1^{st} and 2^{nd} principal component is called the *GAIA*[13] *plane* [Brans and Mareschal, 1990]. It must

[13] **G**eometric **A**nalysis for **I**nteractive **A**id

be pointed out that the application of the PROMETHEE algorithm to the original data from matrix D compared to the single criterion net flows $\Phi_j(a)$ of M has little influence on the representation of the decision problem on the GAIA plane [Brans and Mareschal, 1990]. The projection of D onto the GAIA plane leads only to negligibly different results than the projection of M, if one refrains from considering some unimportant reflections and the rotation of the graph.

3.3.5.2 Interpretation of the GAIA Plane

The alternatives are plotted as points in the GAIA plane with the unit vectors of the original coordinate axes as straight lines emanating from the origin (henceforth called *criterion axes*) (cf. Figure 3.11). Since the alternative vectors are usually longer than one, the points of alternatives are projected relatively far away from the origin for a growing number of criteria, the criterion axes appear comparatively small and the interpretation is more difficult. Therefore, the alternative vectors are optionally normalised. In this case only the end points of the unit vectors of each alternative are projected and the alternatives move toward the origin. Since the relative positions remain unchanged the meaning is unaffected. The centre of the alternatives lies in the origin of the projection, meaning that an imaginary alternative with exactly average quality aspects regarding each criterion would be projected to the new origin [Belton and Stewart, 2002].

Alternatives projected close together in the $\mathbb{R}^2$ show likely similar characteristics, and correspondingly, strongly different alternatives are likely to be projected far from each other. Alternatives which are plotted in the direction of one criterion axis show good performance regarding this criterion. Applied to the criterion axes this implies that their length is a measure of the influence of the respective criterion on the decision problem, i.e. the longer the unit vector of the projected criterion is on the plane, the more this criterion affects the differentiation between the alternatives. Furthermore, it can be stated that criteria whose criterion axes approximately point in the same direction are positively correlated, whereas negatively correlated criteria have opposite orientations in the plane. Orthogonal criterion axes, however, mean independence of the criteria with respect to their impact [Brans and Mareschal, 1994]).

Furthermore, the GAIA plane can be used to illustrate how representative the criteria selection is and to evaluate the independence of the criteria with respect to the considered alternatives. For example in Figure 3.11 criterion axes in all directions exist, whereas in Figure 3.12 no criterion axes in favour of the alternatives A_2, A_7, A_8 exist. Since no aspects are considered supporting A_2, A_7, A_8, these alternatives will come off badly, even

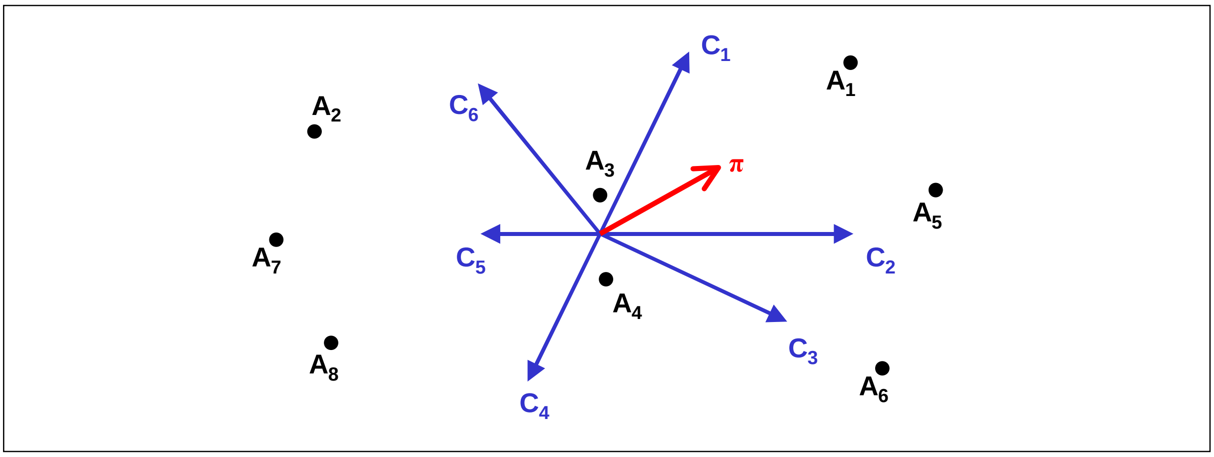

Figure 3.11: Alternatives and Criteria in the GAIA Plane [Brans and Mareschal, 2005]

though they might be applied technologies in practice (for a more detailed discussion see [Treitz et al., 2005]).

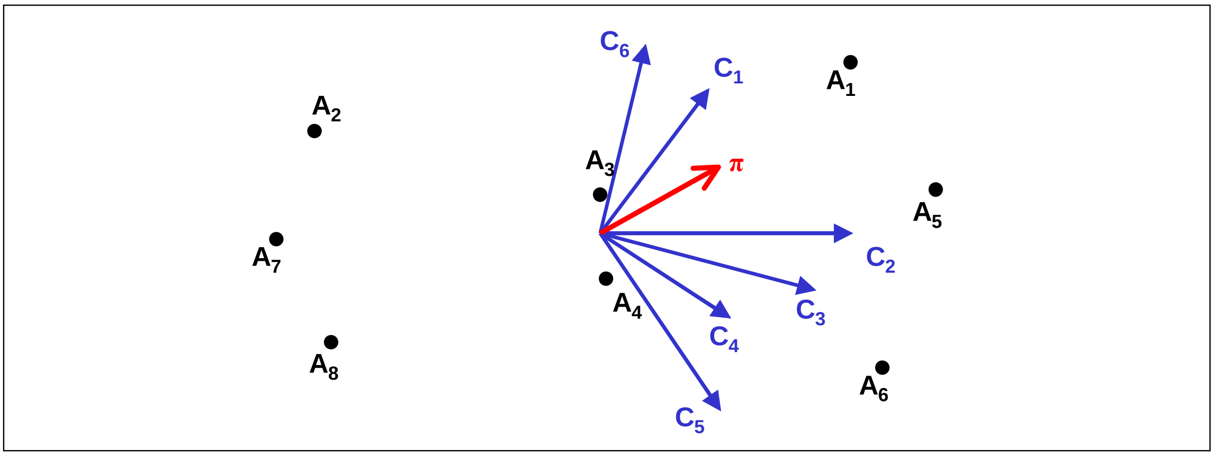

Figure 3.12: Alternatives and Criteria Selection in the GAIA Plane

Within this context it can be helpful to further consider two fictitious alternatives on the plane which facilitate the interpretation:

- *IDEAL* alternative, which achieves optimal performance regarding all criteria, as opposed to the
- *NADIR* alternative, which shows worst performance concerning each single criterion.

The worth of these two practically unattainable points lies in the fact that the decision maker can assess the quality of an alternative based on its relative position compared to the IDEAL and/or NADIR. Alternatives which are close to the IDEAL, have high Φ flows and are preferred, while alternatives in the proximity of the NADIR do not correspond to the preferences of the decision maker.

3.3.5.3 Decision Axis π in the GAIA Plane

Besides the projections of the alternatives and criterion axes the unit vector of the weighting vector $\vec{w}$ can be projected as the *decision axis* π on the GAIA plane. As the name already suggests π is the substantial graphic decision instrument in the GAIA plane. The incorporation of the PROMETHEE preference functions into GAIA does not appear to add substantially to the geometrical representation of the alternatives, criteria and their interrelationships. The real value of GAIA lies in the idea of projecting a weighted sum of the normed flows as a direction vector in the plane in which the criteria and alternatives are plotted [Belton and Stewart, 2002].

Φ of an alternative can be determined by dropping a perpendicular on $\vec{w}$. Therefore, the ranking of the alternatives is determined by the order of the intersection points on the decision axis $[-\pi, +\pi]$ (cf. Figure 3.13). The value of Φ of an alternative is equal to the distance of the intersection point on π to the origin. Optimal performance of an alternative is equivalent to a maximal Φ of one (worst performance of an alternative conversely is equivalent to a Φ of -1), so that the intersection point of the projections of the IDEAL and/or NADIR on π lies at the two ends of $[-\pi, +\pi]$.

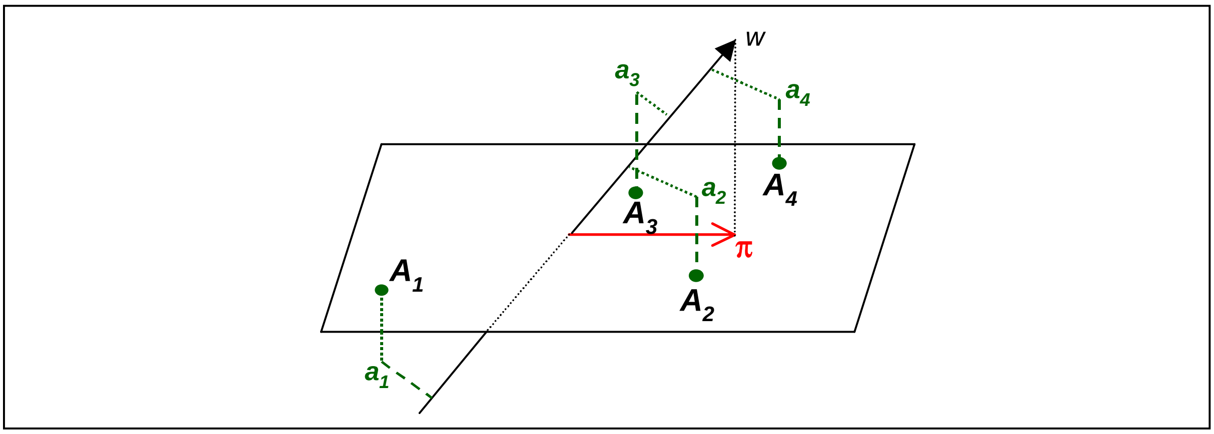

Figure 3.13: PROMETHEE II Ranking and PROMETHEE Decision Axis with Decision Stick π [Brans and Mareschal, 2005]

By changing the current weighting $\vec{w}$ (for example using walking weights) the decision maker navigates π over the plane. Thereby the Φ flows of the alternatives and the projections of the alternatives on π and possibly the ranking change. It must be stressed that the unit vector of $\vec{w}$ by definition always has the same length, the length of its projection however changes. The position of π thereby determines the *decision power*: In case the unit vector of $\vec{w}$ is relatively flat in relation to the plane and therefore π is relatively long, those alternatives which are on the plane far in the direction of π can be considered as optimal. However, if the unit vector of $\vec{w}$ is almost orthogonal to the plane, π will be short. In this case the criteria probably have a strong contradictory interaction so that the determination of the preferential alternative represents a problem solvable only with difficulty.

However, projection on only two dimensions partly leads to interpretation problems: Although in general the alternatives that lie in the direction of π show high Φ flows and thus are preferred by the decision maker, the relative positions of the alternatives to π do not necessarily match with their rank. With regard to the distance in particular, this means that far-off alternatives lying in the direction of π are not necessarily better than those that lie closer. The reason for this is that the perpendicular vectors of alternatives on $\vec{w}$, are not orthogonal on π. Thus, the perpendicular vectors of alternatives to $\vec{w}$ can intersect on the projected plane. The loss of information here becomes obvious and especially for large k the plane does not represent the decision problem adequately. In order to be able to determine an unambiguous ranking of the alternatives, the projected perpendicular vectors of the alternatives are plotted into the plane.

3.3.5.4 PROMETHEE VI Area Δ in the GAIA Plane

In practice multi-criteria problems are often characterised by the fact that an accurate weighting $\vec{w}$ is difficult for the decision maker(s) [see Geldermann et al., 1998; Geldermann, 2006a]. Due to the inherent degree of subjectivity contained within the weights it is often difficult for the decision maker to be precise about their values [Belton and Stewart, 1999]. Even though the PROMETHEE algorithm does not offer guidelines for the determination of the criterion weights w_j, the framework nevertheless allows the decision maker to define weighting intervals $[w_j^-, w_j^+]$ instead of exact weighting factors w_j. The exact weighting is extended by intervals in the following way [Brans and Mareschal, 2005]:

$$0 \leq w_j^- \leq w_j \leq w_j^+ \leq 1, j = 1, \ldots, k \tag{3.25}$$

Geometrically, this results in a body in the $\mathbb{R}^n$ instead of one point (i.e. the head of the weighting vector $\vec{w}$). This body is axis-parallel and its edges are limited by the weighting interval limits. By definition all components of each weighting vector $\vec{w}$ must always add up to one (cf. Equation 3.16), which defines a hyperplane in the $\mathbb{R}^n$. Again, expressed geometrically, this means that the axis-parallel body intersects with the defined hyperplane. This results in a convex polygon of the dimension $\mathbb{R}^{n-1}$, which contains all valid weight combinations within the given intervals representing the convex hull of all valid weighting vectors.

The calculation of this convex hull is a time-consuming problem for larger k because all intersection points of the axis-parallel body with the hyperplane must be determined. An edge of the axis-parallel body is given by $k-1$ interval limits and one variable component. In the calculation all possible combinations are formed whereby $k-1$ arbitrary elements of lower and upper interval limits are taken and one variable element, which is the remainder to one and thus not necessarily an interval limit. Each combination represents an edge of the axis-parallel body. From a geometric viewpoint, only those edges that run from a corner under the hyperplane to a corner above the hyperplane intersect with the hyperplane. All other edges run completely over (sum of the components is larger than one) or under (sum of the components is smaller than one) the hyperplane. Consequently, these edges must not be considered further. The number of all combinations that must be calculated in order to identify the number of valid combinations can become exceedingly high. Nevertheless, this appears to be the most appropriate method since other methods, such as ordering the weighting factors in advance, etc., seem to be more time-consuming in the end. Therefore, a simplified approximation of Δ is implemented (considering all combinations of upper and lower weighting interval limits without the condition of a valid weighting vector but with normalisation of the weighting vector before projection) reducing the calculation time for large k significantly. Moreover, an evaluation of an reduced area Δ considering only selected criteria (cf. Section 3.3.3) is possible.

The convex hull of all valid unit weighting vectors can be projected on the GAIA plane, too (cf. Figure 3.14). The generated convex polygon Δ on the GAIA plane is called the *PROMETHEE VI Area* or even sometimes *Human Brain (HB)*, since it visualises the perceptions of the decision maker [Brans and Mareschal, 1995]. It surrounds π and marks the range in which π can move as long as it stays within the defined interval limits[14].

[14] One known inadequacy concerns the representation of the PROMETHEE VI area Δ on the GAIA plane. In a first step all valid corner points of a convex polygon in the $\mathbb{R}^{n-1}$ are calculated for the representation of the area. This polygon corresponds to the range within which the head of the decision stick moves in the k-dimensional space, if the criterion weights are changed only within the weight interval limits. Thus, π leaves the polygon only if at least one of its components lies outside of its limits. On the GAIA plane, however, it is not the decision stick but the projection of the unit vector of w that is displayed. By definition the unit vector has the length one. Accordingly, the polygon must be normalised for the projection so that the unit vector does not leave the new normalised polygon as long as all weights are within the preassigned weight intervals. Such a normalisation, however, is problematic since the

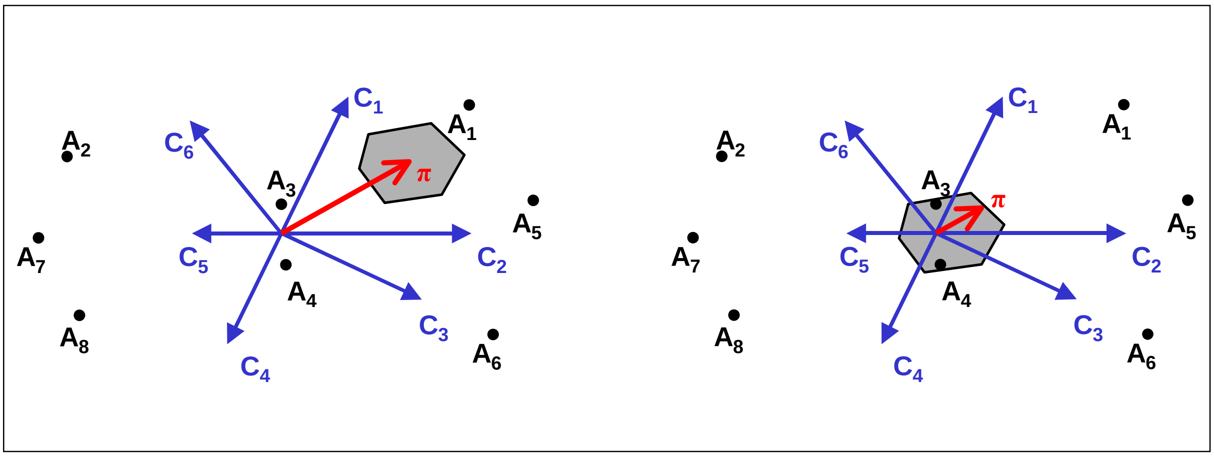

Figure 3.14: PROMETHEE VI Area Δ for a Hard (left) and Soft (right) Decision Problem [Brans and Mareschal, 2005]

First conclusions can be drawn from the position of Δ concerning the "difficulty" of the problem [Brans and Mareschal, 1995]:

- Δ does not include the origin of the GAIA coordinate system. Therefore, the area lies in the direction of the decision axis and in this case all valid weight combinations point approximately in the same direction. Thus, all alternatives lying in that direction are preferred and the problem can be solved relatively easy and represents a *soft problem* [Brans and Mareschal, 1995].
- Δ includes the origin of the GAIA plane. Thus the decision axis can point into each direction and preferential alternatives can lie in each direction. In this case a more precise weighting is necessary to identify a compromise solution. Consequently, it is more difficult to make a decision and therefore is called a *hard problem* [Brans and Mareschal, 1995].

unit vector moves concentrically around the origin. Consequently, the edges of the new normalised polygon must likewise be concentric. Due to the high complexity of such a calculation and the minor differences in comparison to the realised calculation, the modification was omitted. Consequently, only the corner points of the original polygon are normalised and projected on the GAIA plane. The edges of the normalised polygon thereby remain as straight lines and are not changed to concentric functions. Therefore, it can occur that π leaves Δ even though all weights lie within the interval limits. In this case Δ is calculated correctly, but only corner points are normalised and not the entire polygon. Possibly, the decision maker can additionally display the simplified and estimated PROMETHEE VI area, which shows better results in part than the accurately computed but insufficiently normalised area.

Nevertheless, it is questionable whether or not the PROMETHEE VI Area and the decision axis π provide an adequate method for decision makers to determine exactly if the variation of certain weights has an impact on the ranking of the alternatives. Consequently, it would be helpful if the stability intervals, i.e. the intervals corresponding to the simultaneous change of all criteria $[w_j - \delta_j^-, w_j + \delta_j^+]$ $\forall j = 1, \ldots, k$, would be projected onto the GAIA plane, too. By a comparison of the projected area of the defined weighting intervals with the projected area of the stability intervals the decision maker can assess the robustness of the ranking order. Furthermore, by allowing the assignment of general weight distributions and not "only" weight intervals to the attributes the concept of the PROMETHEE VI area could be extended and possibly allow a more accurate representation of the decision makers' preferences. However, difficulties exist concerning the practical realisation of this idea. While the convolution of the (potentially different) marginal distributions does not appear to be problematic from a theoretical point of view, an operationally applicable implementation, taking into account a constraint (i.e. the sum of the weights of all attributes is equal to one), has not been mentioned in literature up until this point [Bertsch et al., 2006a].

3.3.5.5 Consideration of Data Uncertainties

The goal of the analysis techniques presented thus far was to evaluate the sensitivity of the output values with respect to the preferential input parameters. However, the uncertainty of the data has not yet been addressed sufficiently. All attribute values are deterministic values in the decision table D but can be characterised by an individual uncertainty. The uncertainty can be characterised by an uncertainty level as a percentage, such as 10 % or 90 % of the deterministic value. Instead of using deterministic attribute values for each alternative with respect to each attribute, a set of different attribute values is drawn for each alternative with respect to each attribute by MCS. Hence, when calculating the relative differences of the attribute values (also called relative *preference differences*), a set of different values is generated for each pairwise comparison instead of only one individual value.

Therefore, each alternative is not only represented by one point on the GAIA plane, but as a scatter plot. In this case attribute values are generated using a *MCS* approach with a normal distribution[15]. The standard deviation is assumed to be half of the uncertainty indicated like in the MCS approach for preferential uncertainties.

[15] Since no further information about the distribution of the attribute values is given a normal distribution is selected.

With this approach a *distinguishability analysis* [Basson and Petrie, 2004, 2007] can be carried out. It explores whether or not a meaningful evaluation of different alternatives is possible based on the considered criteria and considering all uncertainties in the data. The distinguishability of alternatives can be explored graphically using PCA plotted in the GAIA plane. Therefore, each alternative is not only represented by one point on the GAIA plane, but as a scatter plot (cf. Figure 3.15). Through the simulation of various parameter values for each attribute value not only one deterministic point is illustrated in the GAIA plane, but a point set reflecting the range of variation due to the underlying data uncertainty. Even though the PCA provides an adequate tool for the assessment of the distinguishability of alternatives it can only capture linear dependencies.

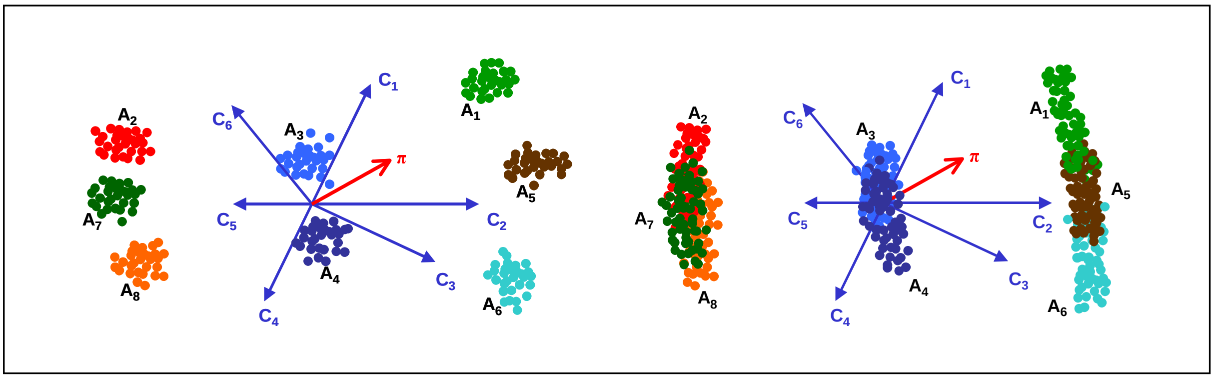

Figure 3.15: Distinguishability Analysis (schematically)

The distinguishability of the alternatives can be assessed depending on the extent to which the alternatives overlap on the plane. Furthermore, it is possible to identify the criteria responsible for the overlap, the range of overlap and to calculate a *distinguishability index (DI)* for decision support [Basson, 2004].

3.3.6 Summary of the Sensitivity Analyses in PROMETHEE

The presented approaches allow an exploration of the impact of uncertainty in the process data as well as in the value judgements of the decision maker(s). The results of the different analyses lead to a deeper understanding of the decision problem itself. Consequently, the decision maker is able to evaluate the influence of the chosen preference parameters and to investigate the sensitivity in an uncertain data set. In particular, the extensive possibilities of analysing the effects of the preferential uncertainties are very important. By allowing the assignment of weighting intervals the concept of *walking weights* and the

PROMETHEE VI Area seem to provide a more adequate model of human preferences than sharply defined values.

Even so it is quite discussed in decision theory to ascertain default values for preferential parameters, for example the "starting values" for the preference parameters p, q and s, this step enables the use of extensive sensitivity analyses. In the same way, the possibility of exploring the impact of variable preference function types contributes to a facilitation of decision processes. Unfounded doubt that does not directly affect the results can be eliminated and attention can be focussed on the differences that do matter in terms of the results [French, 2003; Bertsch et al., 2006a].

To summarise, it should be noted that complex decision situations usually require input from different disciplines and fields of expertise, which must be brought together in some form. The described approaches seek to enhance decision processes and consensus building. They can be applied in a straightforward way in any context where multi-criteria methods are used to support decision makers or their advisers in resolving complex decisions.

3.4 Summary

The definition of resource efficiency from an applicability point of view is complex since various parameters must be considered and representative ones selected. By considering a multitude of different input and output parameters the relative definition of efficiency as stated in Section 3.1 does not help to compare a few individual technical options because most of the alternatives are called efficient based on incomparability. Hence, methodologies are required to extend the efficiency definition to reduce the incomparabilities.

One approach is Data Envelopment Analysis (DEA), which generates an efficiency frontier from the considered alternatives and defines a distance measure as a measure for the degree of inefficiency. Another approach is multi-criteria analysis resolving incomparabilities by incorporating preferential information in the relative measurement of efficiency.

A crucial point of the DEA is the determination of the efficiency frontier, thus the *virtual* efficient method of production to which the real existing organisations are compared to. The parameter λ determines, how organisations can be scaled up and down or combined. This leads to serious problems, especially in the evaluation of a small number of techniques.

Even if the application of DEA is useful for the ex-post evaluation of many similar organisations, it is not appropriate for the comparison of technologies in a technique assessment.

Three major drawbacks can be identified: The classification of the efficiency of a certain technology can be forced by the

1. alternatives considered
2. the evaluation criteria used and
3. the assumption concerning the set of possible technology combinations.

Consequently, it is necessary to acknowledge in a multi-criteria analysis the subjectivity and uncertainty in the selection process of criteria, alternatives and distance measure in order to transparently model the assessment process. Hence, when considering the assessment and evaluation of different technological options it can be concluded that the exact definition of efficiency, considering for example recycling etc., is of minor importance. However, the selection of appropriate criteria and alternatives and the modelling of the decision makers' values is of major importance.

The techno-economic assessment of a process design by determination of the various targets by pinch analyses simultaneously including country specific economic parameters and perceptions is achieved in the multi-criteria evaluation. The combination of the different pinch analysis approaches for intra- and inter-company production networks in one integrated comprehensive model, the *Multi Objective Pinch Analysis (MOPA)* provides the framework to address the trade-off between a full and adequate level of integration.

A metric is described to roughly assess techniques using a distance measure and weighting factors between the criteria considered. The application of the multi-criteria approach PROMETHEE is presented to resolve the incomparabilities between alternatives by preferential information between the criteria (weighting factors) and within criteria (preference functions).

The developed sensitivity analyses allow an exploration of the impact of uncertainty in the process data as well as in the value judgements of the decision maker(s). The optimisation and assessment methodology is demonstrated in the next chapter with a case study (cf. Chapter 4). The case study shows the application of the various pinch analysis modules and a subsequent multi-criteria assessment with both the metric and the PROMETHEE approach.

Chapter 4

Application of Multi Objective Pinch Analysis to Bicycle Production

The pinch analysis approach in connection with multi-criteria analysis provides a consistent assessment method for different mass and energy flows within a company, an industry park or even throughout a supply chain network. It consequently strives for a more comprehensive approach to optimise the system's performance than focussing on single operational units. By determining savings potentials, an assessment of possible process layout modifications is possible. A case study from industrial bicycle coating in China is used to demonstrate the application of the methodology proposed[16].

By applying the methodology developed, decision support can be provided for the production process design of single companies and inter-company networks to improve resource efficiency. First, the realisation of savings potentials based on target values is discussed. Individual target values for energy, water and solvents consumption are calculated based on the pinch analysis and different unit operations are discussed concerning the realisation of the individual savings potentials. Second, an overall assessment is provided by using a multi-criteria approach combining the individual target values. Comprehensive sensitivity analyses are carried out to examine the robustness of the decision and to gain a deeper understanding of the decision problem. In a third step, the scope of application

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[16] As two major emerging economies, China and Chile are the research focus of the project *"PepOn: Integrated Process Design for the Inter-Enterprise Plant Layout Planning of Dynamic Mass Flow Networks"*. The project is funded by the VolkswagenStiftung within its promotion initiative for interdisciplinary environmental research. The case study provides a consistent data set for a reference company to apply the methodology. However, the data is consolidated using a series of different case studies in Chile and China within the PepOn project [Geldermann et al., 2006c, 2007b] and profits from a selection of on-site field investigations in China and Chile.

is extended to an inter-company cooperation within the context of a model of an industry park. The individual companies of the industry park are briefly introduced and the savings potentials are assessed based on target values considering the mass and energy flows of the whole park. The chapter concludes with a discussion about the findings and implications for the bicycle company.

4.1 Background and General Setting

In the case study the serial coating of bicycles in China is investigated. The main question to be answered is if it is worthwhile to modify the paint application process in order to increase the resource efficiency. Furthermore, the context of the company within an industry park is evaluated. Here, a model of an industry park is used with exemplary companies from China and Chile.

4.1.1 Introduction of the Case Study

The developed methodology considers country specific data, but even though the country specific aspects of industrialising countries are considered here, the methodology can be applied to production networks in general. By focussing on mass and energy flow data the identified savings potentials are based on the currently used techniques of a specific country. By not considering the special circumstances of particular countries, "one-size-fits-all policies" [Steenblik and Andrew, 2002] are less likely to succeed and a transfer of clean technologies[17] is limited. This aspect is also emphasised in the *Agenda 21*, which states that "environmentally sound technologies are not just individual technologies, but total systems which include know-how, procedures, goods and services, and equipment as well as organisational and managerial procedures" (UNEP [1992], chapter 34, art. 34.3)[18]. Therefore, country-specific data, i.e. socio-economic, cultural and environmental priorities and key financial parameters, must be considered.

[17] The transfer of clean technologies refers to the application of existing technologies for a new use, or by a new user for economic gain and lower environmental impact [Schollenberger et al., 2005; Agmon and Glinow, 1991].

[18] The *Agenda 21* is the result of several UN-Conferences which took place between 1972 and 1992. It has been signed by 179 countries on the United Nations Conference on Environment and Development in Rio de Janeiro in 1992.

4.1.1.1 Situation in China

China and Chile[19] are used as representatives for other industrialising and developing countries since they face similar financial and environmental challenges[20] as others, such as for example Guatemala, Nicaragua, Tanzania, Vietnam or Zimbabwe as an UNEP study shows [Ciccozzi et al., 2003]. However, newly introduced environmental legislation in China[21] of the *State Environmental Protection Agency (SEPA)* by the *Cleaner Production Promotion Law* in 2003 and in Chile of the *"Comisión nacional del medio ambiente" (CONAMA)* by the *Environmental Framework Act* in 1994 show the ambition of these two important industrialising countries to improve their environmental performance.

Nevertheless, a significant structural difference exists between China and Chile. In China state-owned enterprises are the major constitutive type of enterprise and in addition the *Township and Village Enterprises (TVE)* play a significant role in the Chinese economy besides privately-owned companies. A detailed analysis about the institutional framework in China covering cultural, political-legal, and environmental aspects and include an analysis of the economic policy and its implication to an environmental incentive system, in particular energy efficiency, is provided in [Banks, 1994; Badelt, 2005; Steger et al., 2003; Geng and Yi, 2005; Zeng et al., 2005; Geldermann, 2006b]. Furthermore,

[19] During the military dictatorship of Pinochet between 1973 and 1999 the increased dynamic growth of Chile started accompanied with environmental deterioration. Starting with the democratic development of the country in 1990 and the increasing entanglement of the Chileanian economy with the world markets new cleaner production strategies, in Spanish "Producción Limpia", were adopted and companies can be certified according to sector specific emission limits. Especially the rapidly increasing per capita energy consumption challenges the environmental policy in Chile. Even though Chile achieved a considerable trade volume of salmon and wine production, the extraction of copper is still the backbone of the Chilean economy. Major environmental impact with respect to global metal cycles are site dependent and consequently it is necessary to consider local impacts from the mining stage in an overall assessment [Giurco, 2005].

[20] With respect to other points, there exist of course major differences between industrialising and developing countries and as the European Parliament notes in an resolution on prospects for trade relations between the EU and China ((2005/2015(INI)), 13.10.2005, http://www.europarl.eu.int), there is a growing unease of developing countries about the effects on their markets, which are most vulnerable to Chinese exports as the discussion about dumping prices and anti-dumping regulations in the sector of various consumer and preliminary products (for example textiles, shoes, colour television receivers, bicycles) shows.

[21] Legislation especially focussing on different media were enacted before 2003 in China for example by the *Environment Protection Act* in 1989, the *Water Pollution Protection Act* in 1984 and revised in 1996, the *Air Pollution Protection Act* in 2000, the *Solid Waste Pollution Protection Act* in 1995 and the *Noise Pollution Protection Act* in 1996 [Zeng et al., 2005]. Most regulations do not contain specific emission limits [Zeng et al., 2005], but if they contain standards, most of them are unrevised limits from the Soviet Union.

the relevance of the different stakeholder groups, for example the State Environmental Protection Agency (SEPA), local environmental protection agencies (EPA), energy suppliers, and customers is analysed in [Badelt, 2005]. Up to now major changes of the economic system and only minor changes in the political system prevail in China since the reform and opening policy in 1978 [Zeng et al., 2005]. Consequently, there exists a tight entanglement between political, economic, and administrative sectors leading to inefficient operating control, corruption and absence of the economic principle [Badelt, 2005]. Size and ownership significantly determine for example the energy efficiency in a company because due to the higher economic pressure the demand for energy efficiency improvements in privately owned companies is stronger than in state owned. But even though the production increases annually in China leading to higher energy demand, the specific energy consumption per production unit improves since the size of the companies and the number of privately-owned companies increases [Badelt, 2005]. Major driver for the implementation of cleaner production techniques in China is the motivation to enter international markets requiring certain environmental standards [Zeng et al., 2005].

4.1.1.2 Sector of Bicycle Production in China

The production capacity for bicycles in China is over 80 million bicycles per year by actually producing around 66 million in 2004. The bicycle producers in China face a considerable decline in domestic sales from around 40 million per year in the past to only 22 million bicycles in 2004.[22] Nevertheless, the production of bicycle and parts and components for bicycles considerably increased in the last years with worldwide 55 % – 60 % of all bicycles being produced in China. However, there are considerable regional differences: In the USA 96 % of the bicycles sold today are coming from China, whereas in the EU the market share of Chinese bicycles is only around 4 % in 2003/2004 (cf. Table 4.1). In new markets, e.g. electric powered bicycles, bicycle producers in China created a significant market share globally.

[22] China Business Information, Ein Informationsportal des Deutsch-Chinesischen Zentrums in Leipzig (DCZL),http://www.china-business-information.de

Table 4.1: Data of Bicycle Production and Consumption in the EU in [units] [EC 2005/1095]

Indicator	**2000**	**2001**	**2002**	**2003**	**04/2003 03/2004**
consumption in EU	17 348 000	15 236 000	15 695 000	17 336 000	18 037 000
production in EU	12 700 000	11 028 000	10 083 000	10 165 000	10 160 000
sales EU products	11 718 000	10 035 000	9 175 000	9 100 000	9 300 000
market share EU	67 %	66 %	58 %	52 %	51 %
imports from PRC	128 091	257 728	561 706	707 351	733 901
market share PRC	0.73 %	1.68 %	3.58 %	4.08 %	4.07 %

Some of the bicycle producing companies in China are situated in *Export Processing Zones (EPZ)* and face a binding export obligation included in their investment licenses and furthermore, all exporting producers face significant state interference concerning export prices and quantities [EC 2005/1095]. This resulted in price-dumping accusations and an investigation of the European Council, which finally imposed anti-dumping duties of 30.6 % on bicycle imports originating in China into the EU in the year 1993. Following an anti-circumvention investigation in 1997 this regulation was extended to certain bicycle parts. In 2000 the anti-dumping duty was confirmed according to a new review. The last review for bicycles originating from China was in 2005 considering an investigation period (IP) in 2003/2004. In that review the export prices of China were compared to *normal values* of Mexico and a dumping marging of 48.5 % was identified[23] and became effective as an anti-dumping duty[24] [EC 2005/1095]. However, the import of bicycles and bicycle parts from China into the European Union plays only an underpart. Major importing country for the EU is Taiwan with a total market share of 14.5 % of the total sales in the EU.

[23] The weighted average duty rate of the sample was 36.8 %, but because of a low level of cooperation no exeptions for sample companies were made and all companies were assigned the maximal value of 48.5 %.

[24] The same regulation imposes anti-dumping duties of 34.5 % on companies in Vietnam with the exeption of one cooperating company with an anti-dumping duty of 15.8 %. Furthermore, the regulation (EC) No 397/1999 of the European Council imposes anti-dumping duty on imports of bicycles originating in Taiwan with rates ranging from 2.4 % to 18.2 % (weighted average duty rate of 5.4 %). There were also anti-dumping duties effective in the sector of bicycle production for Indonesia, Malaysia and Thailand in the years 1996 - 2002.

One reason for imposing anti-dumping duties was the low profitability of 3.6 % of the European bicyles producing sector with respect to a minimum assumed profitability of 8 % during the investigation period (IP) in 2003/2004 [25] [EC 2005/1095]. The anti-dumping duty was increased in 2005, even though the average profitability of existing European bicycle producers increased in comparision to the investigation in 2000. This increase was mainly caused by both restructuring and closing of businesses and a higher share of imported bicycle parts, such as coated frames, which are frequently cheaper than in-house production (cf. Table 4.2).

Table 4.2: Cost Data of Bicycle Production in the EU [EC 2005/1095]

Indicator	**2000**	**2001**	**2002**	**2003**	**04/2003 03/2004**
sales price [€/per unit]	124	127	120	115	122
cost of production [€/per unit]	119	122	115	110	117
wage costs per employee [€/a]	23 575	25 846	27 130	27 593	28 153

Consequently, with a production of over 100 million bicycles per year worldwide and the share of about 66 million bicycles produced in China, this sector represents an important part in the economic development of China as the second leading trading partner of the European Union.

4.1.2 Process Characteristics of the Bicycle Coating Process

The case study analyses a reference installation of a typical bicycle production facility of a middle sized firm in China (approximately 850 000 bicycles in 2004, 1 million in 2005 and estimated 1.2 million in 2006) and is one of four bicycle companies at the "bicycle road"[26] in Ludu, a suburb of Taicang[27]. In the reference company up to 130 000 bicycles

[25] **I**nvestigation **P**eriod (IP) for the anti-dumping regulation was 1 April 2003 to 31 March 2004

[26] Around 3.6 million bicycles and bicycle parts and components were produced in 2004 along a nine kilometre long road by four bicycle companies and approximately 60 bicycle components producers in Ludu [Lu, 2005].

[27] The development of an eco-design concept for the *Ludu Bicycle Park* is one of the exemplary projects of the *Taicang Eco-City Development Plan* of the College of Environmental Science and Engineering of the Tongji University in Shanghai [Bao et al., 2005; Lu, 2005]

are produced per month in peak times and approx. 50 000 in low times by 800 to 1 000 employees [Guo, 2005].

4.1.2.1 The Coating of Bicycles

The focus of the analysis are the paint application steps of the production process. Even though the company produces completely assembled bikes, the construction of the frames as well as the assembling and the packaging steps are not taken into account. The coating of bicycle frames is important for protecting the frame, for example against corrosion and chemical deterioration, and for maintaining the best possible optical quality.

In order to fulfil these requirements the following sequence of process steps is widely established:

- pre-treatment (degreasing, passivation, several water cleaning steps and phosphating);
- filler application;
- topcoat application:
  - single layer application (rare),
  - double (basecoat and clearcoat) layer application (primarily),
  - special coatings (metallic) (rare).

Several coating layers are applied through a spraying process building up a sequence of layers on the frame. Only if two or more different colours are used the basecoat application is split in different chromophoric steps, which are applied primarily in wet-wet application. Consequently, this requires the application of at least three co-ordinated coating layers. After the pre-treatment and each coating application step, forced drying is necessary. Thus, energy input is required and solvent emissions are generated if liquid paints are used. Basically, a trade-off between reduced VOC-input and energy consumption can be observed. Therefore, the drying process following the coating of the bicycle frame and fork is central to the application of the pinch analysis and the setting of minimal costs and energy targets [Geldermann et al., 2006b].

In the reference company the bicycle frames and forks go through several batch-wise pre-treatment steps and a discontinuous drying process in an oven. Next, the frames pass on a conveyer band through three coating steps (filler application, basecoat application and

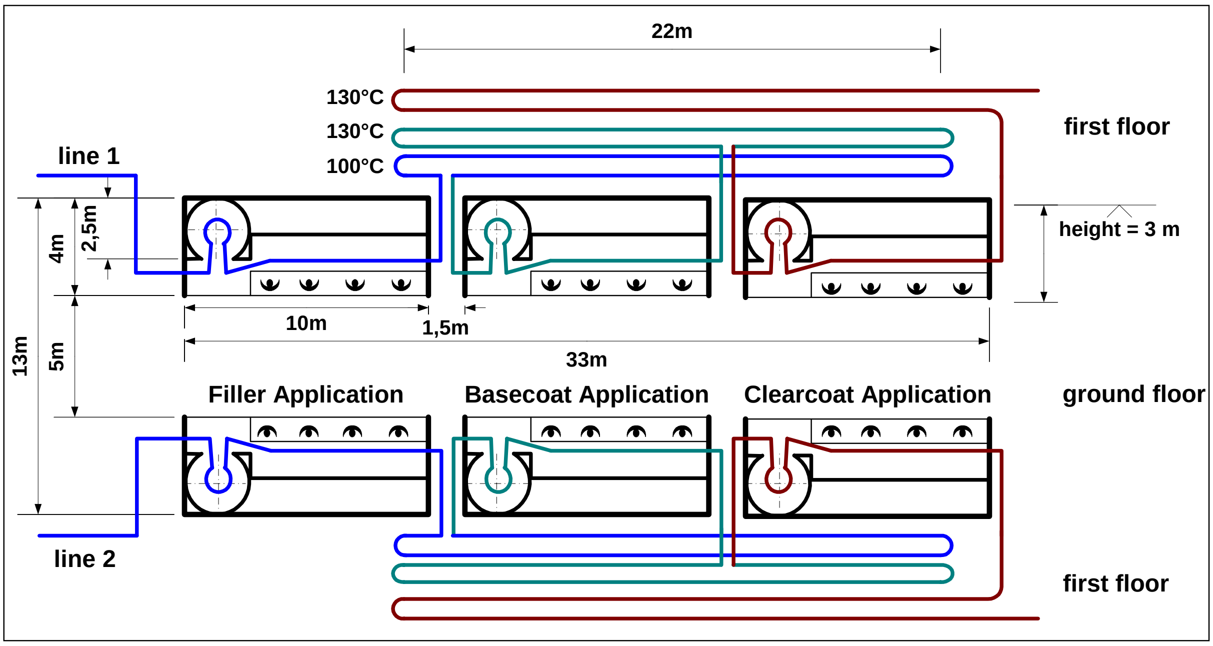

Figure 4.1: Process Layout of the Coating Section of the Bicycle Production

clearcoat application) each followed by a drying step (cf. Figure 4.1). As shown in Figure 4.1 each coating step consists of an automatic application step with a high-speed rotating disc in an Ω-loop and a manual application step. A maximum of four workers can stand simultaneously in the touch-up zone of the coating cabin to spray individual parts of the frame which might not have coated properly by the disc. In the reference company two equal coating lines are located along a corridor. The spray booths with their flash-off zones and the drying ovens have a separate waste gas system (cf. Figure 4.2). After each coating step the conveyer band transports the bicycle frames up to the first floor, where the drying ovens are located. The general measurements can be found in Figure 4.1.

4.1.2.2 Process Parameters for the Coating Step

In industrial coating fillers and paints are in general supplied not ready for application but with a lower solvent content than required (e.g. solvent content of filler delivered: 47 %). Thus, additional solvents are used to adjust the viscosity of the paint right before the application (e.g. solvent content of filler ready for application: 76.5 %). Furthermore, additional solvents are required for cleaning equipments such as spray guns. Here, a multi-component solvent is used for all three application steps (cf. Table 4.3). The material properties of the pure components, such as the parameters to model the curve of the heat capacity of the component depending on the temperature, come from the CHERIC[28] database according to their CAS No[29].

Table 4.3: Multi-component Solvent Composition

Solvent	**CAS No**	**mole fraction**	**formula**	C_{org}	**molar weight [kg/kmol]**
m-Xylene	95-47-6	55 %	C_8H_{10}	0.91	106.16
Ethyl Acetate	141-78-6	20 %	$C_4H_8O_2$	0.55	88.10
Toluene	108-88-3	20 %	C_7H_8	0.91	92.14
Benzene	71-43-2	5 %	C_6H_6	0.92	78.11
Solvent Mix	-	-	-	0.84	98.35

The solvents used are Xylene, Ethyl Acetate, Toluene, and Benzene [Guo, 2005]. The temperature dependent properties (heat capacity, saturation pressure etc.) are assumed to be similar to an ideal gas and are approximated by pure component specific parameters. The mass flow stream in kmol/h is considered to be constant throughout the whole drying process. Relevant for emission limits is the total organic carbon, C_{org}, which is easier to measure technically than individual solvent concentrations[30]. Therefore, C_{org} in mgC/m^3 is primarily used as a threshold reference, as for example in German legislation [BMU-31.BImSchV].

The quantities of released solvents are calculated based on annual consumption averages (cf. Table 4.4) and are verified using measurement data of the lasting dried paint on the frame[31] and the respective solvent content based on a total surface of one bicycle set of 39.7 dm^2 (surface frame: 33.8 dm^2; surface fork: 5.9 dm^2) of a comparable case study

[28] **CH**emical **E**ngineering **R**esearch **I**nformation **C**enter, Korea Thermophysical Properties Data Bank, http://www.cheric.org/

[29] All chemical elements can be identified by a CAS No. The **C**hemical **A**bstracts **S**ervice registry numbers are copyright by the American Chemical Society and uniquely identify each chemical component.

[30] Itemisation of individual solvent concentrations would require enormous effort and high costs. Thus, flame ionisation detector (FID) instruments or silica gel is used for analysing the waste gas composition by determining the total carbon content.

[31] Another important aspect in spray coating is the application efficiency. Depending on the geometry of the object in regular spray coating the application efficiency is 30 % – 50 %, by support of HVLP spray guns the efficiency can be improved to 50 % – 70 %. With electro-static support the application efficiency can even be as high as 60 % – 85 % [Ondratschek, 2002]. However, these values seem to be too high for the coating of bicycle frames.

	1 Filler	2 Drying 1	3 Paint	4 Drying 2	5 Clear Coat	6 Drying 3
T [°C]	16	100	16	130	16	130
Air [Nm^3/h]	64 000	600	64 000	600	64 000	600
VOC [kg/h]	14.86	7.65	24.06	12.39	6.54	3.37
VOC [mgC/Nm^3]	197	9 438	318	15 282	86	4 157

Figure 4.2: Parameters of the Bicycle Coating Application

[Schollenberger and Treitz, 2005]. As specified by the coating company $\frac{2}{3}$ of the solvent emissions emerge in the coating cabin and flash off zones and $\frac{1}{3}$ of the solvent emissions emerge in the drying oven. However, the proportion of solvent emissions in the drying oven seems to be quite high compared to other studies [32] where $92\,\% - 96\,\%$ of the solvent emissions emerge in the coating cabins and flash-off zones and only $8\,\% - 4\,\%$ in the drying ovens.

The major environmental impacts during the drying process are caused by energy consumption and volatile organic compound emissions from solvents in the coating material. In the current process layout each stream is heated up separately and is released after the drying tunnel using independent fresh air sources[33] for each oven.

This current production process layout is compared to a new process layout using the waste heat of the drying process being released. In the new process layout the air flows of the drying ovens are preheated using the released heat and consequently the overall energy consumption is reduced. Further measures for improving the general energy efficiency such as for example improved insulation may be possible, but are not included in this case study. For example delays resulting from malfunctions and downtimes in the production facilities cause an automated shut-down of the heating in the drying ovens and an ensuing cooling these down, which might be slowed down with appropriate insulation. Increased energy consumption due to these downtimes, which might be substantial, is not considered in

[32] Within the PepOn project several case studies were investigated on-site in close cooperation with companies in Chile, China and Germany. A special focus was put on the estimation of solvents emission within the diploma thesis by Robert Kolotilo ("Untersuchung der Sensitivität der Lösemittelemissionen bei Änderung der Massenbilanz am Beispiel einer Lackierstraße für Plastikanbauteile", Institut für Industriebetriebslehre und Industrielle Produktion, Universität Karlsruhe, 2005) and Alexander Hercher ("Technische und wirtschaftliche Möglichkeiten der Minderung von Lösemittelemissionen am Beispiel eines industriellen Lackierbetriebes in Chile", Institut für Industriebetriebslehre und Industrielle Produktion, Universität Karlsruhe, 2005)

[33] Annual average daytime temperature for Shanghai is 15.8 °C, German Weather Service, www.dwd.de

Table 4.4: Settings for the Case Study

Indicator	Amount	Unit
Effective working time	400	min/d
Working days	260	d/a
Filler consumption	50 220	1/a
Basecoat consumption	84 240	1/a
Clearcoat consumption	27 540	1/a
Additional solvent consumption	54 000	1/a
Solid content undiluted filler	47 %	%
Solid content undiluted paint	50 %	%
Solid content undiluted clear coat	64 %	%
Mixing ratio additional solvent/filler	1: 3	-
Mixing ratio additional solvent/paint	1: 3	-
Mixing ratio additional solvent/clear coat	1: 3	-
Density undiluted filler	1.20	kg/dm^3
Density undiluted paint	0.98	kg/dm^3
Density undiluted clear coat	0.94	kg/dm^3
Density additional solvent	0.9	kg/dm^3

the following model. Furthermore, auxiliary processes such as the preheating of drying ovens, the cleaning of tools, or the mixing of the filler or paint do exist in addition to the main painting process, but are not regarded in the following. Nevertheless, they may also provide significant potential for the conservation of resources [Neugebauer et al., 2005].

4.1.3 Process Design Options and Evaluation Criteria

Modifications in the processes of various SME and TVE in China are necessary within the next years in order to increase efficiency, to improve environmental performance, and to comply with existing and new legislation[34]. Considering various design modifications

[34] In its resolution on *Prospects for EU-China Trade Relations* the European Parliament "recognises that many of China's environmental problems stem not from lack of laws but from lack of law enforcement", and addresses "the many outstanding areas of concern ... in the field of Intellectual Property Rights (IPR) enforcement, ..., transparency and environmental, social and health standards" and additionally calls on the European Commission "to make use of the EU countries' political and economic influence in

and variants (Thermal Oxidiser vs. Regenerative Thermal Oxidiser (RTO)) four different generic process design options aiming at emission reduction can be identified to be compared to the *Status Quo*: a complete shift to waterborne coatings concerning the basecoat as a process integrated measure and the two additive measures of thermal incineration, i.e. thermal oxidation, and the recovery of the solvents by condensation. Additionally, the complete technique shift to powder coatings is discussed as a separate measure:

- Status Quo (T_0)
- Waterborne Basecoats (T_1)
- Thermal Incineration (T_2)
- Condensation (T_3)
- Powder Coating (T_4)

The status quo represents the current process layout and has no solvent emission reduction measure installed. The development of new coatings, for example waterborne, high solid or powder coatings, and new coating application tools, for example HVLP[35] spray guns or high-speed rotating discs, were caused by more stringent environmental legislation concerning solvent emissions in the serial coating of metal parts [Rentz et al., 2003; Geldermann et al., 2004] and in the sector of vehicle refinishing [Schollenberger, 2006]. Waterborne coating systems for bicycles are state-of-the-art for filler and basecoat systems, but are not available for clearcoat systems. The waterborne coatings still contain solvents, but have a considerably lower solvent content (10 % - 15 % compared to 50 % - 80 % of regular coatings). However, waterborne coating systems often contain biocides for long-term stability and therefore may represent a potential health risk during application and handling[36]. The second option as a proven technology is thermal incineration, which offers a safe, reliable, and efficient method for the removal of a wide range of VOC (except halogenated hydrocarbons) [Rentz et al., 2003]. They undergo oxidation in a combustion

order to bring about a change in China's attitude towards compliance with international trade rules." ... Addressing inter alia the worker's rights, social dumping and the high levels of pollution the European Parliament "urges the Chinese government, under pain of seeing trade with the EU being severely restricted, to play a full and positive role in promoting sustainable development, both inside China and globally". (European Parliament Resolution on Prospects for Trade Relations between the EU and China (2005/2015(INI)), 13.10.2005, European Parliament Public Register of Documents, Document P6_TA(2005)0381, http://www.europarl.eu.int)

[35] **H**igh **V**olume **L**ow **P**ressure

[36] The use of biocidal products as preservatives is regulated by the European Parliament Directive 98/8/EC concerning the placing of biocidal products on the market.

chamber at temperatures between 700 °C and 1 000 °C, to a certain extent with the addition of fuel. Removal efficiencies up to 99 % and even above can be achieved [Rentz et al., 2003]. The third option considered is a condensation system. The advantage of a condensation system is the recovery of the solvents used in the application and reuse resulting in a potential economic benefit [Geldermann et al., 2006d]. The last option is a switch of techniques to powder coatings, which are solvent-free systems that require electrostatic application procedures and are therefore primarily suitable for metal bodies, such as bicycle frames. Powder coating systems provide some inherent positive properties: Since they are free of solvent emissions, no water is necessary in order to absorb coating particles in the coating cabins and less waste is generated compared to liquid spray coatings since a recycling of the coating material is possible[37] (up to 95 %) [Rentz et al., 2003]. Even though there exists a high application efficiency and the high proportion of circulating air in the coating booth results in a reduction of energy consumption, the investment for a change to powder coatings is must be considered.

Further process design alternatives, such as for example catalytical incineration, a biofilter, a bioactive scrubber, or a zeolite wheel[38] are not considered in the following [see e.g. Rentz et al., 2003; Geldermann et al., 2004, for further information and a techno-economic assessment].

Following the procedures of a techno-economic assessment [Geldermann, 1999] various criteria are taken into account in the evaluation of the process design options to be assessed. For an evaluation in reference to a sustainable development a whole range of different criteria from various perspectives can be considered with respect to functionality, economy, environmental quality, safety and societal quality [VDI 3780]. With respect to a selection of an appropriate process design in the context of emission abatement techniques, major criteria are amongst others the required efficiency of the VOC emission reduction, the characteristics of the waste gas (composition, volume flow, VOC concentration), the technical-economic service life and the quality requirements of recovered solvents [Rentz et al., 2003].

For the following case study the criteria for the evaluation consider the mass and energy flows of the company and the evaluation is based on a relative assessment of the

[37] A recycling of liquid paints within the automatic application step in the Ω-loop is also possible, but requires higher effort.

[38] A zeolite wheel can be used as a concentrating system to purify low loaded waste streams. The cleaning of the gaseous waste stream is accomplished by a adsorption of the VOC in the hydrophobic zeolites and the continuous or discontinuous release by a smaller air stream at high release temperature. However, due to the moisture in the gaseous waste stream caused by the water curtains in the coating cabins and the coating particles caused by the overspray, filters have to be installed.

alternatives compared to target values for each criterion which are calculated using the pinch analysis approaches. The criteria represent only a selection of relevant criteria for the evaluation of the resource efficiency of the different production process design options and are specifically:

- Energy [kWh/h] (Energy)
- Water [m^3/h] (Water)
- Solvents [mgC/m^3] (VOC)
- Investment [€] (Invest)
- Operating Costs [€/a] (Costs)

Since the criteria cover only the decision relevant aspects of the design options, only differences between the options are taken into account. Unchanged process steps for all options, for example the welding before the coating and the assembling and packaging after the coating, and all the involved parameters, such as the energy use of these process steps, are neglected. The change in operating costs considers for example the amount and value of the recovered solvents and include the operating cooling costs for the condensation installation. In case of a switch to powder coatings the decision relevant operating costs and the investment in comparison to the status quo are taken into account.

4.2 Determination of Target Values

In this section the target values for heat integration, water reuse and solvents recovery are calculated using the pinch analysis approaches as described in Chapter 2. The target values are discussed in comparison to current resource consumption in terms of the savings potential they provide and the possibilities how they could be realised by installation of specific unit operations. The individual savings potential constitute the base for the multi-criteria assessment integrating the various targets in one overall assessment in Section 4.3. All calculations and analyses are performed using *MATLAB*™ and its *Optimization Toolbox*. For the numerical integration 0.1 K steps are used to approximate the heat capacities.

4.2.1 Determination of the Energy Target Values

For the determination of the energy target values the thermal pinch analysis approach based on an implementation in $MATLAB^{TM}$ using the transport algorithm of Operations Research as described in Section 2.1 is applied. The energy savings potentials identified for the different process design options are discussed with respect to available unit operations for realising the theoretical savings potential.

4.2.1.1 Application of the Thermal Pinch Analysis

The thermal pinch analysis of the reference bicycle company is based on three cold streams C_1, C_2, C_3 requiring heating and two hot process streams H_1, H_2 requiring cooling. In the following only the process streams of the three continuous drying ovens are used, since the process streams in the coating cabins and flash-off zones do not require heating at all and the drying step of the pre-treatment requires a special batch-wise analysis. Table 4.5 shows the specific temperatures and the components of the different gaseous streams. The drying air of the processes requiring heating is taken from the outside air supply. 33 % of the solvents are emitted in the drying ovens and are therefore relevant for the heat integration scenario. The minimal temperature difference between the hot and the cold composite curve is assumed to be $\Delta T_{min} = 10$ K.

The current process layout requires a heating by hot utilities of 275 MJ/h (= 76 kWh/h). All waste heat is released without being re-used. As Figure 4.3 illustrates the pinch points are situated at the bottom of the hot and cold composite curve. There exists a wide range of overlapping composite curves illustrating the theoretic possible heat integration of 249 MJ/h (= 69 kWh/h) leaving a minimal requirement of hot utility at the upper end of the composite curve of around 25 MJ/h (= 7 kWh/h). Hence, the theoretical savings potential is about 90 % and the major heating requirement for the ovens could be met by heat integration of the hot waste gas[39].

[39] The individual solvent components and the air flow are considered with their temperature specific parameters. However, the humidity in the air is not considered.

Table 4.5: Data for the Thermal Pinch Analysis

Stream	T_{in} **[K]**	T_{out} **[K]**	r [m^3]	**Component**	**CAS No**	**mole fraction**
C_1	289	373	667	Oxygen	7782-44-7	0.21
				Nitrogen	7727-37-9	0.79
C_2	289	403	667	Oxygen	7782-44-7	0.21
				Nitrogen	7727-37-9	0.79
C_3	289	403	667	Oxygen	7782-44-7	0.21
				Nitrogen	7727-37-9	0.79
H_1	403	373	1 333	m-Xylene	95-47-6	$3.24E^{-03}$
				Ethyl Acetate	141-78-6	$1.18E^{-03}$
				Toluene	108-88-3	$1.18E^{-03}$
				Benzene	71-43-2	$2.94E^{-04}$
				Oxygen	7782-44-7	0.21
				Nitrogen	7727-37-9	0.79
H_2	393	300	2 000	m-Xylene	95-47-6	$1.60E^{-03}$
				Ethyl Acetate	141-78-6	$5.83E^{-04}$
				Toluene	108-88-3	$5.83E^{-04}$
				Benzene	71-43-2	$1.46E^{-04}$
				Oxygen	7782-44-7	0.21
				Nitrogen	7727-37-9	0.79

However, as discussed in Section 2.1.2 a distinction must be made between a thermodynamic and an economic approach. As introduced in Section 2.1.1.3 the grand composite curve shows the aggregated heating and cooling requirements of the analysed system and can be used to optimise the use of additional utilities.

The thermodynamic analysis shows that there do not exist any external cooling requirements in this analysis (cf. Figure 4.4). The aggregated external heating requirements are shown with respect to the required temperatures. These energy demands cannot be covered by heat integration, but must be supplied by additional utilities.

However, the economic analysis shows less heat integration of 194 MJ/h (= 54 kWh/h) and a higher demand of external heating utilities of 80 MJ/h (= 22 kWh/h). In this case external cooling requirements exist, balancing the heat demand and supply of the system.

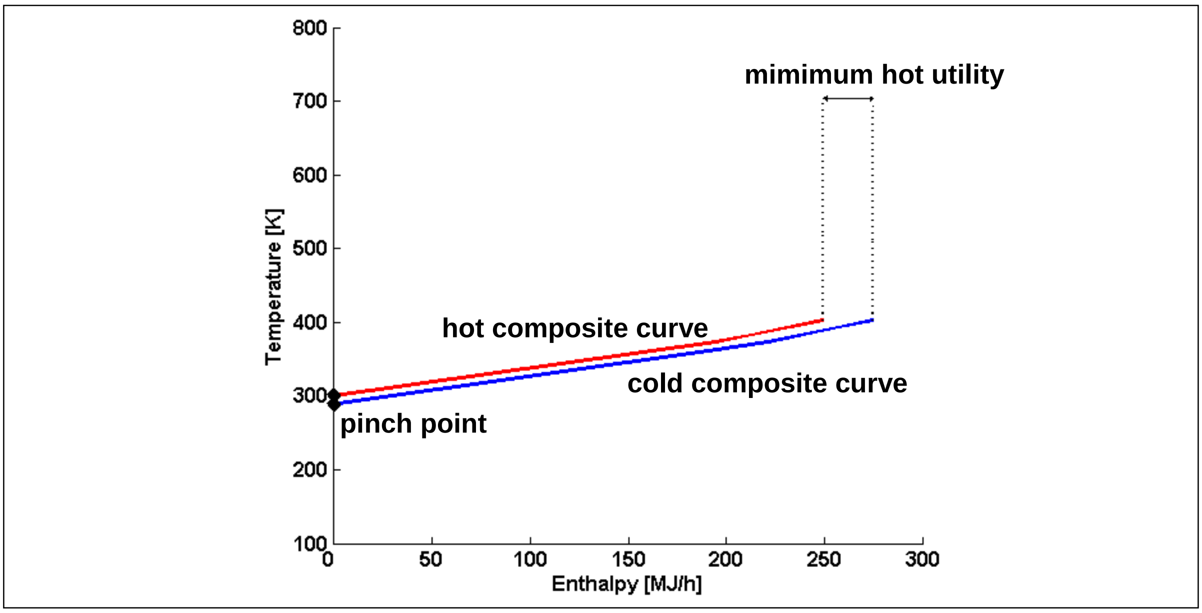

Figure 4.3: Composite Curves of the Thermal Pinch Analysis

In the economic approach less heat integration is used (70 % vs. 90 %) and therewith taking advantage of a higher temperature gradient in the heat exchanger resulting in a smaller heat exchanger surface area and utimatly in lower costs for the heat exchanger.

In this case an optimisation concerning the selection of different heating utilities is not reasonable, since a gas-powered heating system is available at the bicycle company and other additional alternatives do not provide potential for economic improvement. A split between different hot utilities may provide the possibility to use cheaper utilities in lower temperature ranges, but would require more heat exchanger and more equipment resulting in unreasonable effort.

4.2.1.2 Discussion of Unit Operations

After the determination of the thermodynamic and economic targets by using the thermal pinch analysis approach an adequate unit operation must be identified to realise the existing savings potentials. Given the economic optimal solution requiring only around 22 kWh/h heating utility, a significant energy savings potential can be identified. The heat transfer table (cf. Table 4.6) shows which flows can be connected. For example the heating duty of the cold stream C_1, which is the drying air of the filler oven at 100 °C, is completely satisfied by heat integration. The cold process streams C_2 and C_3 are only

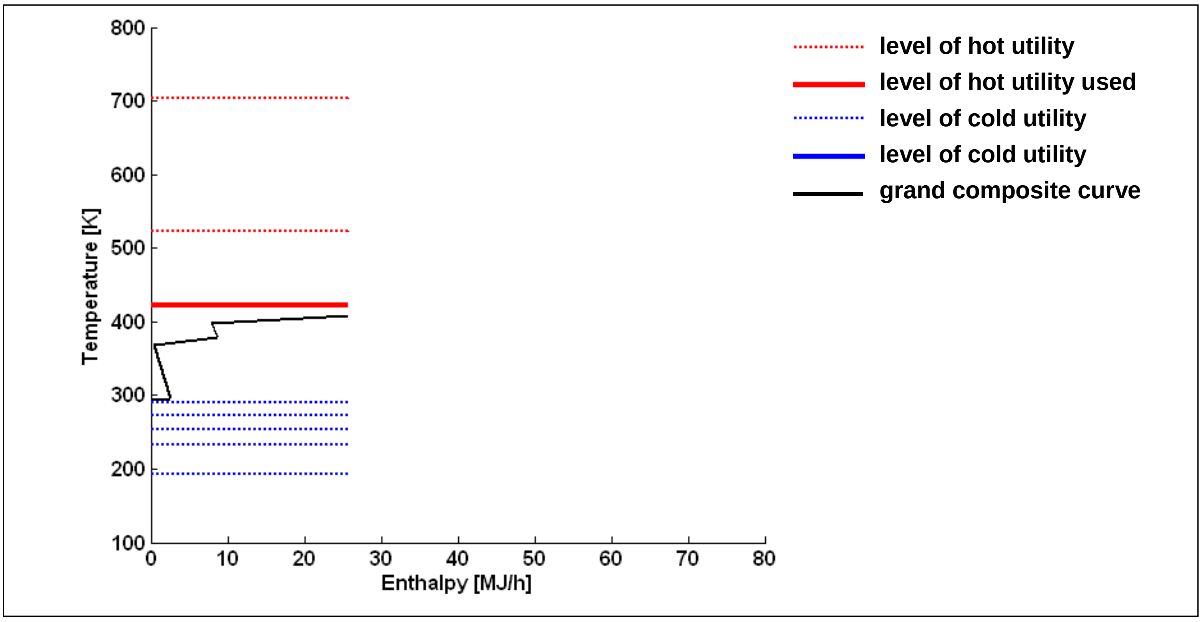

Figure 4.4: Grand Composite Curve of the Thermodynamic Approach *of the Thermal Pinch Analysis*

partially covered by heat integration and the remaining requirements are fulfilled by the hot utility.

Table 4.6: Heat Transfer Tableau of the Economic Analysis of the Thermal Pinch [MJ/h]

	H_1	H_2	hot utility
C_1	54 758	10 247	8 858
C_2	0	65 004	35 552
C_3	0	65 004	35 552
cold utility	0	54 613	-

As the heat transfer tableau suggests several heat exchanger would be necessary for combining the cold and hot process streams. However, in this special case the gaseous waste streams can be combined to one single stream and all the cold process streams can be combined to one single stream for pre-heating the air of the drying ovens. By considering the different temperature levels and mass flow streams the parameters for modelling the gaseous waste streams can be adjusted. Consequently, only one heat exchanger is required reducing considerable the investment of the heat exchanger and the necessary

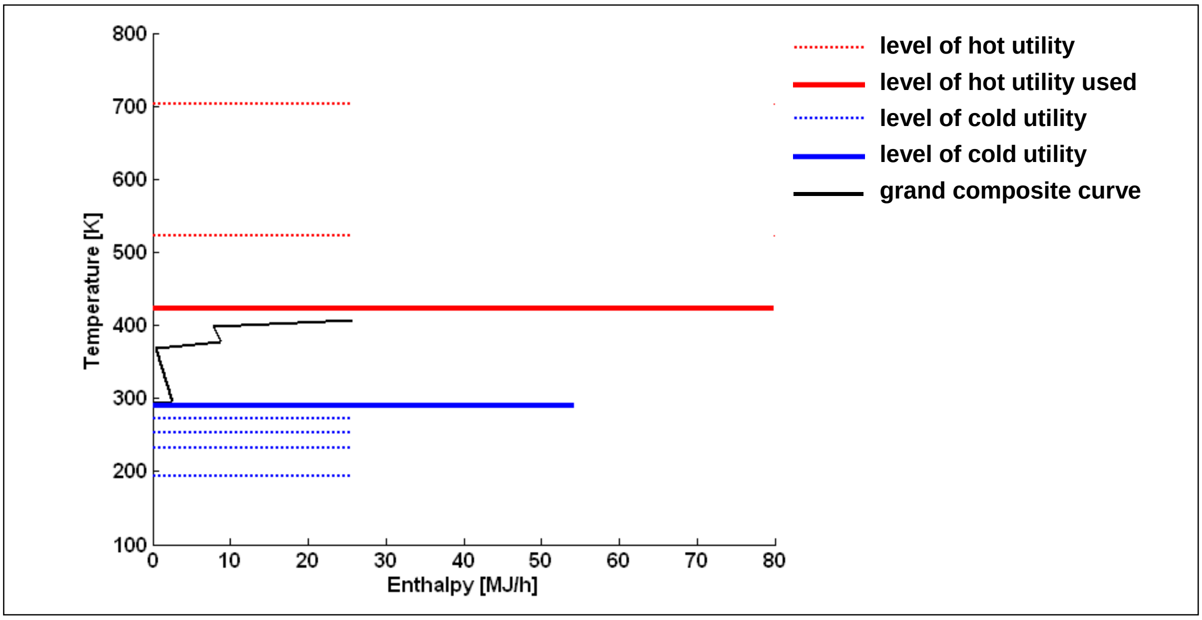

Figure 4.5: Grand Composite Curve of the Economic Approach *of the Thermal Pinch Analysis*

piping. Furthermore, the temperatures of the hot process streams can be adjusted for the exclusive consideration of the best heat integration resulting in no cooling requirements by specifically cooling the hot process streams down to only 48 °C. If the aim of the analysis is the calculation of the energy requirements for a condensation system for the solvents in the gaseous waste stream, different cooling utilities must be discussed (cf. Section 4.2.3).

A gas-gas heat exchange is characterised by low heat transfer coefficients and thus requires large heat exchange surfaces. Because of this the surface area of gas-gas heat exchanger is extended by fins within the heat exchanger [VDI]. In this case a welded, stainless steel plate heat exchanger[40] would be suitable with an exchange surface area of 124 m^2 by 167 plates realising 54 kW for the 2 000 m^3 of all process streams. The heat transfer coefficient for this gas-gas heat exchanger is 0.014 kW/m^2K and therewith in the range of typical values of 0.01 kW/m^2K - 0.035 kW/m^2K [VDI].

In a countercurrent flow arrangement of a recuperative heat exchanger the gaseous waste is cooled down from 120 °C to 48 °C and herewith it is possible to pre-heat the fresh air supply from 16 °C to 89 °C.

[40] Within the PepOn project several diploma thesis were carried out in China in cooperation with the Tongji University in Shanghai and local companies. The diploma thesis of Stefan Weiler focused on heat integration ("Optimierung der Stoff- und Energieströme am Beispiel eines Industrieparks in China", Institut für Industriebetriebslehre und Industrielle Produktion, Universität Karlsruhe, 2005)

Total investment for the installation can be estimated by the investment for the heat exchanger plus the piping installation. The costs for the heat exchanger is assumed to be 10 000 €. This leads to a complete surface dependent costs of 115 €/m^2. The costs for the piping installation depends on the distances of the chimneys at the roof of the bicycle company. Currently, eight chimneys are at the roof of the company (two for the pre-treatment drying ovens, and two for each of the three continuous drying ovens). The fresh air supply is also taken from an channel located at the roof of the company. Consequently, it is necessary to connect the gaseous waste streams with a heat exchanger at the roof of the company and the fresh air channel. By assuming a stainless steel pipe with a diameter of 200 mm a total length of 60 m is required to connect the streams. Considering additional insulation and connecting parts, such as for example 90° bends, T-pieces and mountings, the installation of the heat exchanger would require further 9 000 € of material and 11 000 € of labour costs[41]. Consequently, the total investment would sum up to 30 000 €. Assuming a price for natural gas of 416 €/t savings of approx. 3 800 €/a can be achieved resulting in a positive net present value.

4.2.1.3 Characterisation with respect to Energy

As determined in the last section in case of *Condensation* or *Waterborne Basecoats* an investment of 30 000 € is considered and energy savings of 54 kW are realised (cf. Table 4.7). In case of *Thermal Incineration* a special heat exchanger is not reasonable since temperatures of 982 °C must be reached to burn the solvents and a cooling down of the waste gas of the drying ovens is not useful. In this case a heat exchanger system within the thermal incinerator is considered realising 50 % heat recovery (cf. Section 4.2.3). Thus, the ratio of the heating of the drying ovens is considered here with 38 kW.

Table 4.7: Characterisation of the Energy Target Values

	Status Quo	**Waterborne Basecoats**	**Thermal Incineration**	**Conden-sation**	**Powder Coating**
Energy [kWh/h]	76	22	38	22	25
Investment [€]	0	30 000	-	30 000	35 000

[41] For the installation an European wage level is assumed. However, the wage level in China is considerably lower, but specific data for the individual installation steps were not available for China.

The option *Powder Coating* requires higher temperatures because of an higher film thickness to burn in the coatings. Thus, the investment highly depends on the existing drying ovens. If the existing drying ovens are able to reach temperatures of 150 °C, as assumed in the following, only minor changes in the investment have to be considered with respect to the heat integration compared to the proposed heat exchanger and 35 000 € are taken into account in the following for a heat exchanger installation of 75 kW of the total required 100 kW. If the drying ovens have to be renewed an investment of approx. 250 000 € would be required.

4.2.2 Determination of the Water Target Values

By the application of the water pinch analysis a reduction of water consumption and of wastewater generation is aimed at with reusing water in the pre-treatment step through cascading, the application of regeneration processes, such as for example ultra-filtration or ion exchanger, or the recycling of water streams by using regeneration processes, e.g. filter press, with a closed recycling loop.

In the bicycle production the water consumption can be almost solely traced back to the batch-wise pre-treatment and the coating application. In the pre-treatment of the bicycle frame and fork the adherence is improved between the bicycle parts and the subsequent coating layers by dipping the bicycle parts in different baths and rinsing them with water and deionised water (cf. Table 4.8).

The analysis revealed that it is difficult to find a common key contaminant for the different operations, since various metals, salts from the cleaning agents and solvents are used in the different operations[42]. Nevertheless, the conductance and the pH-value seemed to be the most appropriate values for describing the pre-treatment steps, in which the phosphating is one exception since this process step can be characterised by total acid value, and the COD value is the best value to describe the water used in the coating application.

[42] Within the PepOn project several diploma thesis were carried out in China in cooperation with the Tongji University in Shanghai and local companies. The diploma thesis of Andreas Leicht focused on water integration (”Anwendung von Methoden des Operations Research zur Optimierung des Wassereinsatzes in der Industrie”, Institut für Industriebetriebslehre und Industrielle Produktion, Universität Karlsruhe, 2005)

Table 4.8: Characterisation of the Pre-Treatment

Operation	**Minimal** pH**-Value**	**Maximal** pH**-Value**	**Minimal Conductance [μS/cm]**	**Maximal Conductance [μS/cm]**
degreasing	11.2	11.8	-	-
water rinsing 1	2.5	8	0	10 000
water rinsing 2	6.5	10	0	5 000
passivation	7.8	8.4	1 100	3 300
water rinsing 3	5	8	0	5 000
water rinsing 4	6	8	0	500
surface activation	8.7	9.8	-	-
phosphating	-	-	-	-
deionised water rinsing 1	5.2	7.8	0	50
deionised water rinsing 2	5.2	7.8	0	50

The pre-treatment of the bicycle parts consists of several steps: In the degreasing process contaminations are removed from the surface. The application of organic solvents is limited in that step to manual degreasing of small and/or working pieces with a complex geometry [Rentz et al., 2003]. In general the degreasing is done with water-based cleaning agents. Several rinsing operations are applied throughout the pre-treatment. The substrates proceed through an phosphatation bath to both increase the adhesion of the coating layers and prevent interferences in the coating process to failures on the surface [Rentz et al., 2003]. Here, iron and zinc phosphating processes are the most applied ones. In the last step before the actual coating a passivation is carried out in order to extend the effect of protection against corrosion and to improve adherence [Rentz et al., 2003]. After the pre-treatment the frames are dried batch-wise in an oven at 140 °C.

In the coating application large amounts of water are used as water curtains to capture the overspray in the coating application and to wash out the particles from the air in the coating cabin. High volumes of air are drawn twice through the water curtain, i.e. venturi washer, to collect the coating particles and solvents. Around 15 m^3/h are required for this operation in each of the six coating cabins. However, the water is regenerated by a filter press and only 1.8 m^3/h of fresh water is required.

4.2.2.1 Application of the Water Pinch Analysis

Table 4.9 shows the mass load and the limiting parameters of the different process steps of the pre-treatment, which are relevant for the water pinch analysis providing the base for the determination of target values[43]. The limiting fresh water flow rate is based on averaged values considering the bath volume and frequency of alteration of the different baths, such as for example the bath volume of the *water rinsing 1* is assumed to be 25 m^3 and must be changed four times a year, resulting in 0.058 m^3/h. The $C_{lim,out}$ corresponds to the maximal conductance in Table 4.8 and the $C_{lim,in}$ is determined by the durability of a bath and the contamination from zero to maximal conductance[44] during that period[45]. Considering $C_{lim,out}$ and the minimum fresh water flow rate $fresh_{lim}$, the contamination $\Delta m_{i,total}$ can be calculated (cf. Table 4.9). In addition the minimal flow rate r_{lim} is determined based on the minimal amount of water at the level $C_{lim,in}$ to remove $\Delta m_{i,total}$, which corresponds to the bath volume[46].

If all processes of the pre-treatment would be fed by fresh water the total water demand would be 0.762 m^3/h adding up the last column in Table 4.9. By considering all limiting process parameters for each pre-treatment step the composite curve for the system's total water demand can be shown based on the mass load to be transferred within the maximal inlet and maximal outlet concentration (cf. Figure 4.6). The minimal fresh water supply, illustrated as the line with the flattest slope, defines the base to determine the possible savings potentials based on the assumption that all processes are fed by minimal fresh water and no recycling is used.

[43] The diploma thesis of Maximilian Wurdack focused on the modelling of regeneration and recycling processes by the water pinch analysis ("Techno-ökonomische Bewertung von Einsparpotentialen am Beispiel von Wasserströmen in einem Industriepark", Institut für Industriebetriebslehre und Industrielle Produktion, Universität Karlsruhe, 2006)

[44] In general the water pinch analysis is based on the contaminant load, which must be removed through a washing process. Taking into account the contaminant load to be removed, the minimal water flow rate can be determined. However, since the contaminant load varies from piece to piece and this information is in general not available, the contaminant load is calculated based on the determined minimal water flow rate. For this case study it is assumed that the minimal fresh water flow rate corresponds to the maximal duration and volume of a bath

[45] The conductance in $\mu S/cm$ can be transformed into ppm as a measure for the total dissolved solids, whereby the rate depends on the actual components in the water, the temperature and the concentration and no fixed conversion factor can be applied [Wiegran, 2000]. In the following an average conversion factor of 2 $\mu S/cm$ = 1 ppm is used.

[46] The minimal water flow rate r_{lim} for a dipping bath means that the bath at $C_{lim,in}$ can only be used one more hour and the contamination is raised from $C_{lim,in}$ to $C_{lim,out}$. Thus, if only water at the level of $C_{lim,in}$ is available for reuse, the complete bath must be changed to remove $\Delta m_{i,total}$.

Table 4.9: Data for the Water Pinch Analysis

No.	**Operation**	$\Delta m_{i,total}$ $[kg/h]$	$C_{lim,in}$ $[ppm]$	$C_{lim,out}$ $[ppm]$	r_{lim} $[m^3/h]$	$fresh_{lim}$ $[m^3/h]$
1	water rinsing 1	0.289	4 988.46	5.000	25.0	0.058
2	water rinsing 2	0.144	2 494.23	2.500	25.0	0.058
3	passivation	0.457	1 627.15	1.650	20.0	0.277
4	water rinsing 3	0.289	2 497.11	2.500	100.0	0.115
5	water rinsing 4	0.029	249.71	250	100.0	0.115
6	deionised water rinsing 1	0.002	24.94	25	30.0	0.069
7	deionised water rinsing 2	0.002	24.94	25	30.0	0.069

By allowing theoretical maximal reuse within the limits, the total water demand of the system would be only 0.4 m^3/h defined by the reciprocal of the slope of the water supply line, which touches the limiting composite curve at the pinch point at 2 500 ppm. The water supply line defines the maximal slope without an intersection of the limiting composite curve. The limiting composite curve consists of almost horizontal lines defining the concentrations of the different pre-treatment baths.

In the case of reuse of water, which means that water in baths with a lower contaminant concentration at the end of the cleaning process are moved to the first cleaning steps, with higher contaminant concentration, the overall wastewater has a concentration of $C_{out} =$ 3 280 ppm leaving the processes if reuse is used to a maximal extend. The slope of the minimal fresh water supply line is lower than the water supply line reusing the water illustrating the higher flow rate and the savings potential through reuse.

By considering available regeneration operations, such as for example an ion exchanger or ultra-filtration reducing the concentration from $C_{pinch} = 2\,500$ ppm to 250 ppm, the fresh water demand can be lowered to 0.19 m^3/h (cf. Figure 4.7). In the case of regeneration reuse the outlet concentration increases to 3 986 ppm. In addition to the original water supply line and the minimal fresh water supply line Figure 4.7 shows the limiting composite curve of the water supply using a regeneration process. Below C_0 and above C_{pinch} the composite curve illustrates the fresh water supply of 0.19 m^3/h in the middle range the composite curve has a lower slope illustrating the contaminant reduction by the regeneration process. Consequently, in the case of regeneration and reuse it is possible to reduce the fresh water flow rate compared to the case of pure reuse without cutting the limiting water profile.

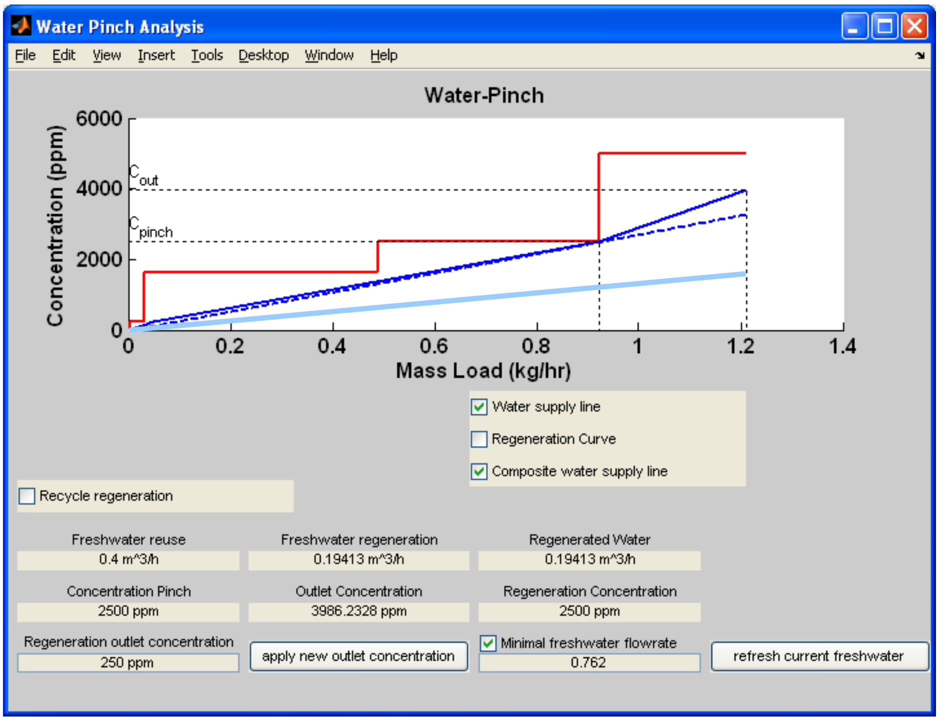

Figure 4.6: Composite Curves of the Water Pinch Analysis with Reuse

By introducing a recycling of the water it is possible to reduce the fresh water demand to 0.14 m^3/h, which is just the sum of the water demand of the two deionised water rinsing steps. These two steps cannot be fed by recycled water since they require lower contaminant concentration than can possibly be achieved by the recycling process. However, the outlet concentration of the water increases to 4 600 ppm. The slope of the fresh water for the recycling ("recycling water" in Figure 4.8) is higher than the slope of the regenerated water within the recycling loop ("regenerated water" in Figure 4.8). Through the recycling process the inner loop has an internal water flow rate of 0.26 m^3/h, whereas the fresh water supply is only 0.14 m^3/h. The composite water supply line illustrates the sum of the profiles and stays under the limiting composite curve.

4.2.2.2 Characterisation with Respect to Water

The target values concerning the water consumption are based on the water pinch analysis for the pre-treatment steps, the minimal water supply for the water curtains due to evaporation and the process characteristics of the different techniques. The current consumption is based on the different water consuming process steps of the pre-treatment

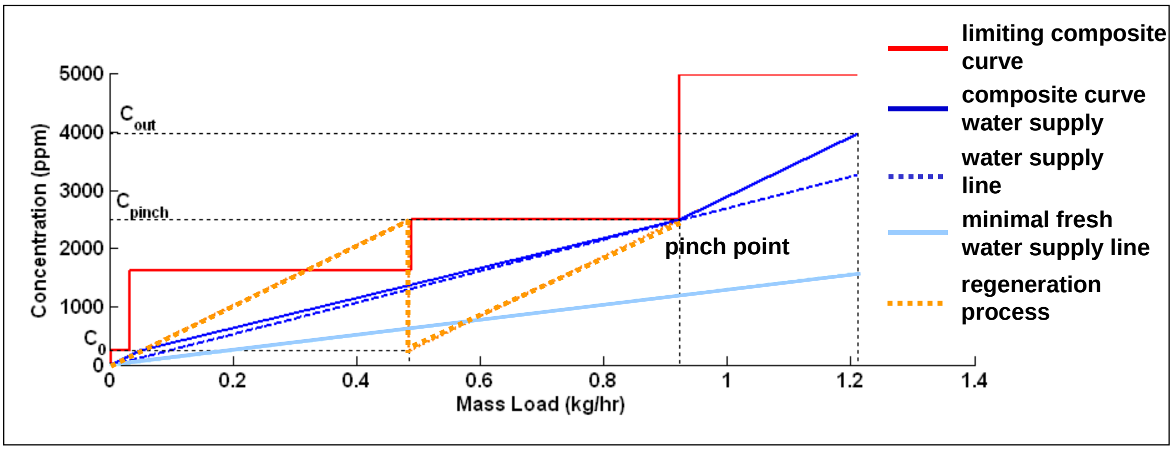

Figure 4.7: Water Pinch Analysis with Regeneration - Reuse

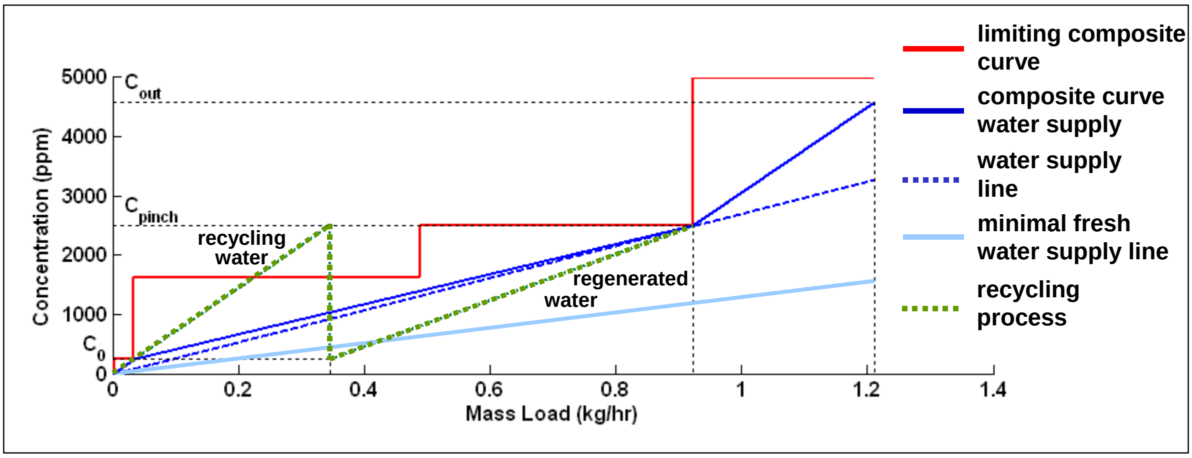

Figure 4.8: Water Pinch Analysis with Regeneration - Recycling

using the minimal fresh water flow rate[47] of 0.762 m^3/h and the current consumption of the water curtains in the coating section of 1.8 m^3/h. Thus, the in the *Status Quo* a fresh water demand of 2.562 m^3/h exists. However, in general the fresh water demand of the water curtains can be reduced to 200 L/d for each of the six coating cabins to balance the loss of evaporated water resulting in a minimal water consumption of 0.18 m^3/h. In general it is possible to neutralise the wastewater of the pre-treatment steps and reuse the wastewater in the coating section. Thereby, no wastewater is generated in the overall process since the solids are filtered out and dried resulting in solid waste. The grease separated from the water can be burned in a power station, and the sludge of the pas-

[47] Since no specific consumption values are available for the pre-treatment steps, the minimal fresh water flow rate is taken as a base for comparison.

sivation and degreasing must be brought to landfill. However, further investigation is required if this is possible in the plant of the reference company and thus, this option is not considered in the following.

Through various process improvement measures (like the introduction of regeneration and recycling techniques or the extension of life-time of pre-treatment baths) the use of water can be lowered to 0.14 m^3/h for the pre-treatment section and 0.18 m^3/h for the water curtains as the target for the analysis requiring an investment of 15 000 € (cf. Table 4.10). In case of the options *Thermal Incineration* and *Condensation* this results in an overall performance of 0.32 m^3/h.

Table 4.10: Characterisation of the Water Target Values

	Status Quo	**Waterborne Basecoats**	**Thermal Incineration**	**Conden-sation**	**Powder Coating**
Water [m^3/h]	2.56	0.46	0.32	0.32	0.28
Investment [€]	0	30 000	15 000	15 000	30 000

In the case of a change to *Waterborne Basecoats* two additional deionised water rinsing steps are required, since the waterborne paints have worse adhesion than solvent-based coatings. Thus, the water use for this option is 0.18 m^3/h for the water curtains and 0.28 m^3/h for the pre-treatment steps (0.46 m^3/h overall). The installation of the two additional deionised water baths is considered with an additional investment of 15 000 €. In case of a switch to *Powder Coatings* the water curtains are not used any more. However, as in the case of waterborne basecoats an improved pre-treatment is required. Using an improved pre-treatment it is possible to apply a two layer coating without a filler application. Since powder coatings in general result in higher film thickness it is possible to use an integrated filler system in the basecoat powder application. Consequently the fresh water demand of the pre-treatment is 0.28 m^3/h.

4.2.3 Determination of the Solvent Target Values

In this section the focus of the analysis is on the identification of target values of the condensation system by the solvents pinch analysis approach for the solvent emissions in the gaseous waste streams. In a first step the target values are identified followed in a second step by an economic analysis of the target values for the condensation system and in a last step unit operations are suggested to realise the proposed savings potentials.

4.2.3.1 Application of the Solvents Pinch Analysis

The calculations of the thermal condensation of solvents can be described as a heat exchange problem and thus can be evaluated by the pinch analysis approach for the recovery of solvents as shown in Section 2.3. The analysis is based on temperature-concentration relationships depending on the temperature-sensitive saturation pressure curves of the considered multi-component VOC.

In the following it is assumed that the coating system would be changed to a Benzene-free coating system[48] by an installation of a condensation installation. Furthermore, the minor content of Ethyl Acetate would be replaced to have less different but higher concentrated solvents in the waste gas. Consequently, the Xylene content is kept constant and the mole fraction of the Toluene is increased by the former Benzene and Ethyl Acetate ratio keeping the total amount of solvents used constant (cf. Figure 4.2 on page 106).

Even though most of the solvent emissions are generated in the coating cabins and flash-off zones, the solvent concentrations in the gaseous waste streams of the coating cabins are considerably lower due to the high air flows compared to the solvent concentration in the waste gas of the drying ovens. The high air flows are necessary to speed up the sinking of the coating particles in the air resulting from the overspray. The average solvent concentration in the gaseous waste stream of the coating cabins and flash of zones is $5.4 \cdot 10^{-5}$ kmol/kmol air and in the gaseous waste stream of the drying ovens $2.6 \cdot 10^{-3}$ kmol/kmol air. Thus, only $\frac{1}{3}$ of the solvents, i.e. the gaseous waste stream of the drying ovens, are considered for the condensation and the coating cabins and the flash-off zones are not relevant for the condensation because of the low solvent concentration in the waste gas.

The calculation considers the temperature dependent heat capacities of the waste gas and the partly cleaned waste gas after condensation. Furthermore, the heat of condensation is taken into account as well as the heat capacity of the condensed liquid solvents. In addition

[48] Benzene is an important industrial solvent and is commonly used as an additive in gasoline. Since it is a human genotoxic carcinogen and "there is no identifiable threshold below which there is no risk to human health", all industrial fields are encouraged to substitute Benzene (European Parliament Directive 2000/69/EC). In industrial metal coating Benzene can be substituted by Toluene, which is basically a Benzene ring with a functional CH_3-group instead of one hydrogen or Xylene substituting two hydrogen with functional CH_3-groups.

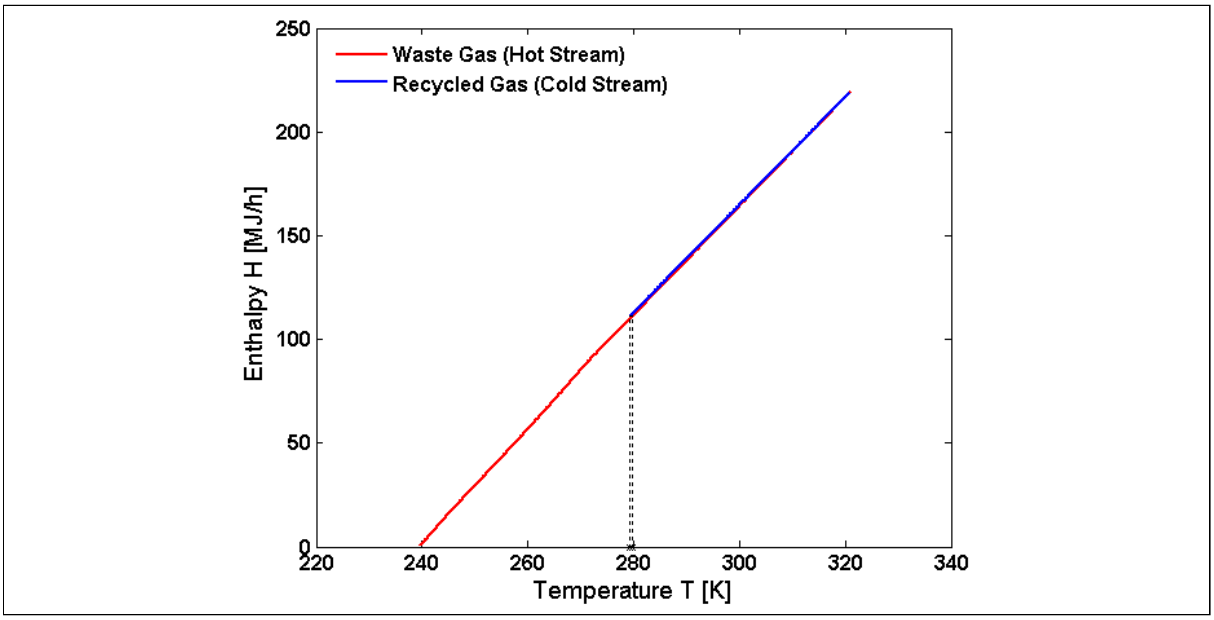

Figure 4.9: Hot and Cold Composite Curves of the Solvents Pinch Analysis

to the heat integration described in Section 4.2.1 the condensation requires further cooling of the waste gas of the drying ovens. Thus, the temperature range to be considered for the calculation of the condensation is given by the supply temperature of the waste gas T^S (in this case 48 °C (= 321 K)) as the upper bound and the maximum of the system dependent temperatures (freezing point of the coolant, minimal system temperature, freezing point of solvent etc.) as the lower bound. Here the installation of a mechanical cooling unit is considered[49]. Thus, the minimal operating temperature of the mechanical cooling plus the minimal temperature difference ΔT_{min} at -38 °C (= 235 K) defines the lower bound of the temperature range $T_{LowerEnd}$. Consequently, the condensation system covers the dehumidification component from supply temperature of the waste gas of 321 K to 278 K, the condensation component from $T_{UpperEnd} = 278$ K to the optimal endpoint temperature T_{End} (minimal 235 K) and the internal heat integration component from $T_{End} + \Delta T_{min}$ to 321 K (cf. Figure 2.14 on page 44). Consequently, the hot and cold composite curves of the thermal condensation system summarise the cooling and heating requirements of the complete condensation system (cf. Figure 4.9).

If the waste gas is cooled down the concentration is constant until condensation starts and the solvent concentration in the waste gas sinks. The actual starting point of condensation depends on the solvent concentration of the individual solvents in the waste gas and the

[49] For a different company using the single solvent Xylene in a further case study the condensation to cryogen temperatures with liquid nitrogen (N_{2_l}) is examined [Schollenberger and Treitz, 2005].

resulting partial pressures of the individual components. The concentration of Xylene is $1.44 \cdot 10^{-3}$ kmol/kmol air and of Toluene is $1.18 \cdot 10^{-3}$ kmol/kmol air which results in an overall concentration[50] of 9 625 mgC/m^3 (= $2.6 \cdot 10^{-3}$ kmol/kmol air). This concentration accrues from the solvents contained in the paint and the solvents used for dilution. The flow rate of the waste gas is 2 000 m^3/h. The calculation shows that the condensation of Xylene in the waste gas starts at 270.9 K ($T_{UpperEnd}$ in Figure 4.10) and of Toluene at 245.3 K. The integrals of the heat balance are solved in $MATLAB^{TM}$ numerically with a linear approximation in 0.1 K steps.

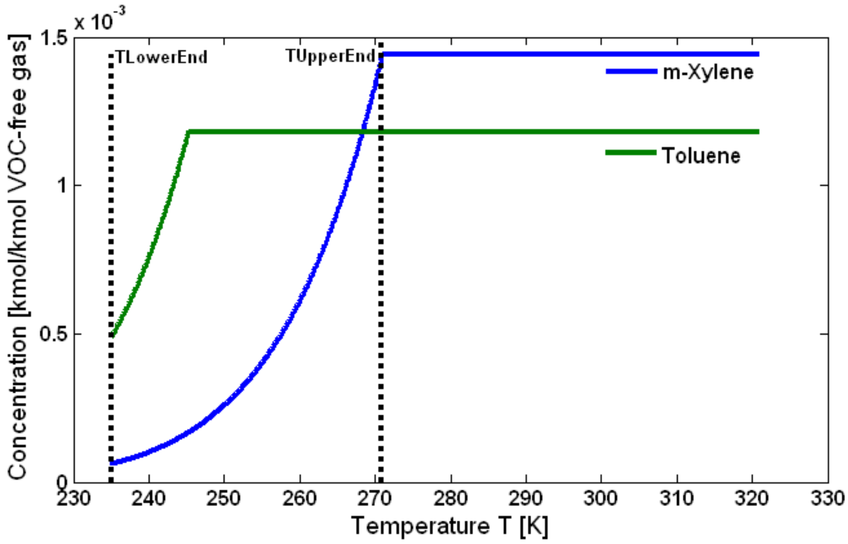

Figure 4.10: Concentrations of m-Xylene and Toluene in the Waste Gas

The endpoint temperature of condensation $T_{End} = 239.4$ K can be translated in a remaining solvent concentration in the waste gas after condensation. At T_{End} the concentration of Xylene is $9.5 \cdot 10^{-5}$ kmol/kmol air and of Toluene is $7.2 \cdot 10^{-4}$ kmol/kmol air as Figure 4.10 shows. This corresponds to a C_{org} in the waste gas of the drying ovens of 3 300 mgC/m^3 after condensation from originally 9 625 mgC/m^3. The remaining solvents in the partly cleaned cold gas lead combined with the air flows of the coating cabins to overall solvent emissions of 233 mgC/m^3 at an air flow of approx. 194 000 m^3/h waste air. By using N_{2_l} as a coolant the minimal temperature of the condensation system would be the freezing point of Xylene at 225 K and C_{org} could be even reduced down to 844 mgC/m^3 for the waste gas of the drying ovens (207 mgC/m^3 overall).

The advantage of a condensation of VOC from a waste gas stream is that air pollution control and solvent recovery in liquid state are achieved simultaneously within one apparatus.

[50] Xylene and Toluene have the same C_{org} ratio of 0.91.

However, complex systems and cooling temperatures[51] well below −100 °C are required to fulfil for example German legislation, since condensation only takes places "when the temperature of a cooling surface is below the dew point of the vapour of the respective concentration" [Rinner et al., 2002]. With a decreasing concentration lower temperatures are necessary to condense the remaining solvents from the waste gas. Nevertheless, it is possible to use only a condensation system to fulfil legal requirements and emission reduction rates up to 99.8 % can be achieved [Rinner et al., 2002]. However, as the analysis showed in this case the overall limit would be 844 mgC/m^3. The emission reduction rate is limited by the freezing point of Xylene. By installing a more complex system with de-icing units a cooling to even lower temperatures and higher emission reduction rates is possible.

4.2.3.2 Economic Evaluation of the Solvents Pinch Analysis

The objective of the analysis is to determine the economic reasonable amount of solvents to be recovered. This can be translated into an endpoint temperature of the condensation T_{End} at which this recovery target is reached. The costs for running the condensation are calculated as total annual costs comprising fixed costs for the installation of heat exchangers and operating costs for the additional cooling.

The amount of heat to be integrated and the heat to be dissipated depend on the endpoint temperature of the condensation. The costs for the heat exchanger is determined by specific surface dependent costs. There are no operating costs, for example for maintenance, for the heat exchanger of the integration unit and no heat transfer losses are included in the analysis. In case of the cooling unit of the condensation system the use of electric power based on the specific heat transfer coefficient of the mechanical cooling unit is regarded. The condensed solvents are also cooled to T_{End} since an advance extraction is not considered. Parameters such as for example the geometry of the heat exchanger are not explicitly considered.

The minimal temperature gradient ΔT_{min} for the use of mechanical cooling between the raw gas and the partly cleaned waste gas depends in this special case only to a limited extend on the end point of condensation. The solution is driven by the trade-off between the amount of recovered solvents and therefore the revenues for the solvents and necessary investment in heat exchanger and operating costs for the cooling. For each endpoint temperature of the condensation within the condensation range from 270.9 K down to 235 K and for each ΔT_{min} within an assumed range (2 K - 60 K) the total annual costs

[51] These cryogenic temperatures can for example be achieved with liquid nitrogen.

are determined. The analysis reveals that the optimal temperature gradient for the heat integration is 40 K between the partly cleaned cold gas and the condensation waste gas stream.

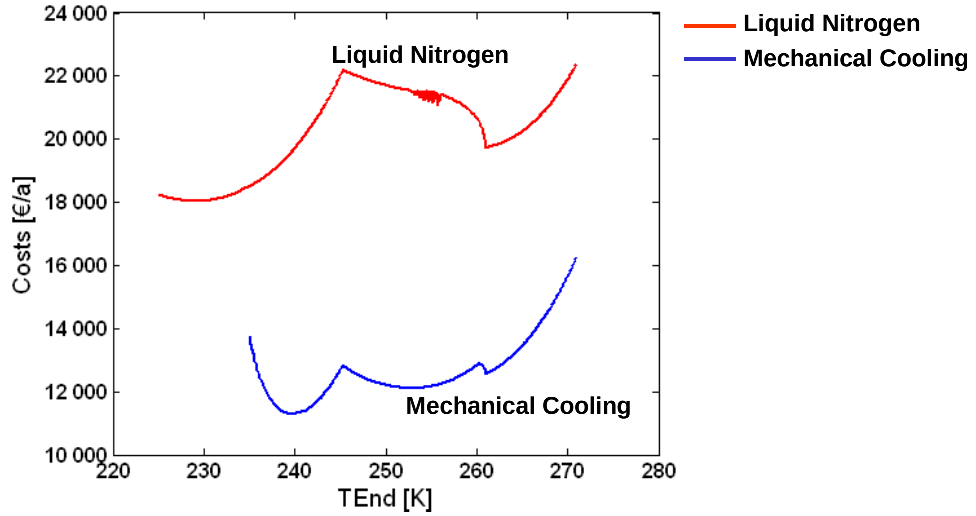

Figure 4.11: Total Annualised Costs Depending on the Endpoint Temperature of Condensation

To identify the best operating point of the condensation system the operating costs for the cooling, the annualised direct costs for the heat exchangers and the value of the recovered solvents must be determined for each condensation temperature. Thus, taking into account the operating costs of the mechanical cooling unit (12 230 €/a) and the annualised direct costs for the three heat exchangers, the total annualised costs are 27 500 €/a (assuming a 10 % interest rate and an economic life time of 5 years). By assuming a value of 0.56 €/kg for the recovered solvents, i.e. this corresponds to 60 % of the original price, savings of 16 000 €/a can be realised, leading to a minimum of 11 300 €/a at the best operating point of 239.4 K (cf. Figure 4.11). Thus, instead of spending 45 000 €/a only 29 000 €/a must be spend for solvents. The condensation with N_{2_l} is more expensive than the mechanical cooling, as Figure 4.11 illustrates, but it is possible to reach lower temperatures[52].

The investment for a condensation unit consists of the direct costs for the three heat exchangers (dehumidification unit 11 000 €, cooling unit 27 000 € and integration unit 16 000 €), freight (3 %), taxes (5 %) and the direct (foundations, piping) and indirect

[52] Assuming a de-icing unit the analysis would not be limited by the freezing point of Xylene and even lower temperatures would be possible using N_{2_l}.

(engineering, start-up) installation costs. Thus, the total investment for the condensation system would be 95 000 €.

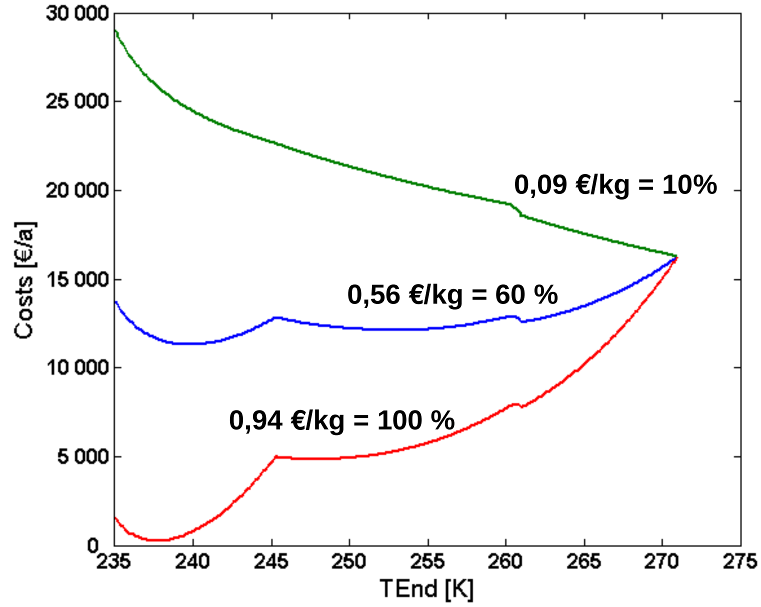

Figure 4.12: Sensitivity Analysis for the Value for Recovered Solvents

Depending on the quality requirements of the process the recovered solvents can be used either in the same process or for a different application or in a combined solution. Since the solvents from the paint can also be recovered it is possible that more solvents are recovered as are necessary for the process.

Figure 4.12 shows the sensitivity of the overall annualised costs to the value of the recovered solvents. Since the recovered solvents can be used only to a limited extend directly in the process the value of the recovered solvents is assumed to be 0.56 €/kg only 60 % of the original price. But as Figure 4.12 indicates the total annualised costs are sensitive to the value of the recovered solvents. However, as the sensitivity analysis for a price of 0.94 €/kg (= 100 % of the original price) shows there exists no significant change in the endpoint temperature of condensation. Whereas the costs rise disproportionately high by cooling down assuming a price of only 10 % of the original price.

The sensitivity of the overall costs to the annualised costs for running the heat exchanger depends on the surface dependent price for the heat exchanger and the energy for the mechanical cooling. Figure 4.13 shows different combinations of investment and operating costs for the heat exchanger. Only by significantly reducing the costs for the heat exchanger by a given value for the recovered solvents it is possible to reach a balance

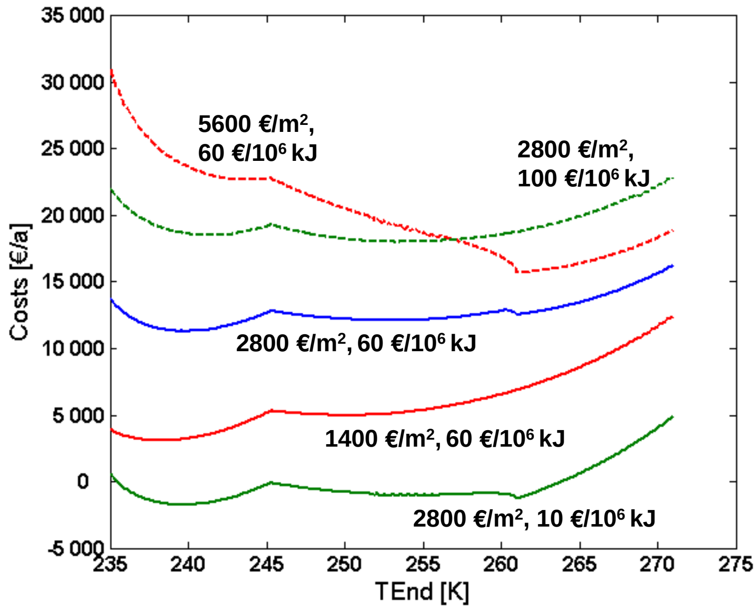

Figure 4.13: Sensitivity Analysis of Surface Specific Costs and Operating Costs for the Coolant

of the costs and the realised savings. Figure 4.13 does not include the total investment considering all investment components, hence it is possible to reach a balanced running of the heat exchanger even though the total investment is still not cost effective.

The sensitivity of the total annualised costs with respect to the concentration of solvents in the waste gas is shown in Figure 4.14. There is a significant effect on the overall total annualised costs concerning the concentration of the solvents. Figure 4.14 shows the original solvent concentration and a 5 times higher concentration. Since the total annualised costs is very sensitive to the concentration of the solvents a combination of a condensation system of mechanical cooling, which is cheaper than a condensation system with liquid nitrogen cooling (cf. Figure 4.11), with a concentration component, for example a zeolite wheel, or a secondary measure after the condensation, for example an active carbon filter, to fulfil ultimately the legal requirements may provide economic advantages compared to a sole cryogenic system. The condensation process is only economic if the solvent concentration in the exhaust gas is in the range of the saturation concentration at high temperatures and if the volume of exhaust gas is as small as possible for energy reasons [Rentz et al., 2003]. A basic problem is that the solvent proportion may exceed the emission limits for the explosion prevention. In this case the installations must be operated with inert gas (typically nitrogen) as carrier gas instead of air. For the case study the explosion limits are not relevant. If the exhaust gas contains several components with

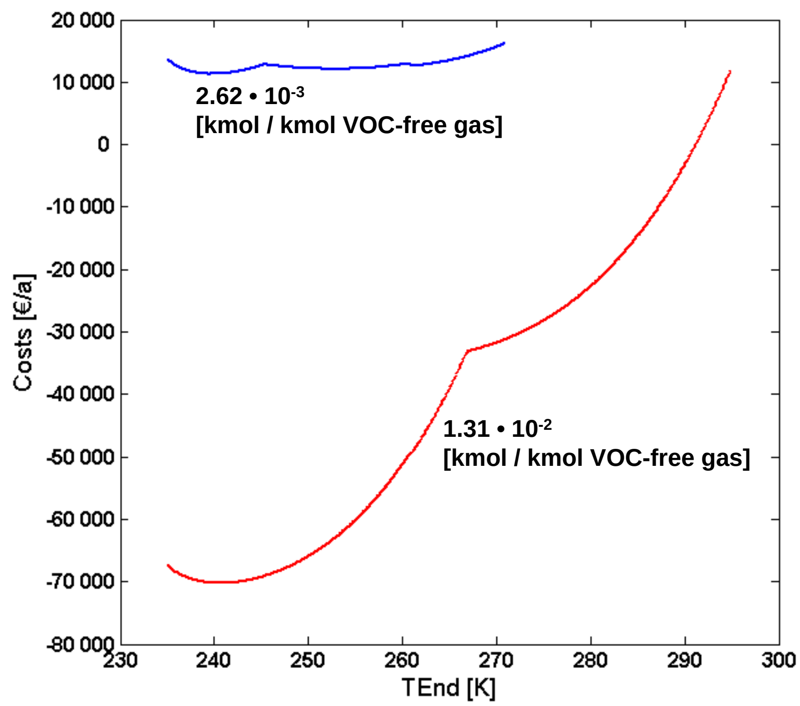

Figure 4.14: Sensitivity Analysis of the Concentration of Solvents in the Waste Gas

similar vapour pressure curves, a selective separation of components is often not possible [Schultes, 1996]. A limiting factor for the applicability of condensers is the energy demand that is necessary for reaching the dew point of the substances to be condensed.

4.2.3.3 Characterisation with Respect to Solvents

As identified in the last section, at the best operating point an reduction in the overall solvent emissions to 233 mgC/m^3 can be achieved with a condensation system. The overall investment results in 140 000 € considering the *heat integration* option (30 000 €) and the *water regeneration-recycling* option (15 000 €) and the *solvents recovery* option (95 000 €) (cf. Table 4.11).

The thermal incineration is quite effective compared to the condensation leading to emission reduction rates of 99 % of the initial concentration of the waste gas, but faces a high investment[53]. If an incinerator is installed only for the 2 000 m^3/h waste gas of the

[53] The initial investment is calculated considering the incinerator, auxiliary equipment, direct installation costs, such as for example foundations and piping, indirect installation costs, such as for example engineering and start-up costs and an internal heat recovery of 50 % in the incinerator installation. The price is determined according to the formula provided in [Rentz et al., 1999b]

drying tunnels an investment of 186 000 € would be required. However, if an thermal incineration system is installed for the total waste gas of 194 000 m^3/h the investment of an thermal oxidiser is 672 000 €. In addition to the investment of the incinerator the investment for improving the use and recycling of water of 15 000 € is required.

Table 4.11: Characterisation of the Different Solvent Target Values

	Status Quo	**Waterborne Basecoats**	**Thermal Incineration**	**Conden-sation**	**Powder Coating**
Solvents [mgC/m^3]	297.70	171.23	2.98	233.00	0
Investment [€]	0	75 000	687 000	140 000	245 000
Operating Costs [€/a]	45 000	24 200	45 000	29 000	30 000

Compared to thermal incineration, the switch to waterborne basecoats requires only a smaller investment. In case of a switch to waterborne basecoats 30 000 € for the realisation of the heat integration are required, additional 30 000 € for the improved pretreatment section and 15 000 € for new spraying tools and equipment. Consequently, a total of 75 000 € must be invested to change the current coating system to waterborne basecoats. But the lower investment results in significant lower abatement efficiency leaving 171.73 mgC/m^3 in the total waste gas of the coating section.

The change in techniques to powder coatings shows with respect to solvent emissions the highest possible difference to the process integrated or secondary measures discussed so far. Since the powder coatings contain no solvents, a reduction to 0 mgC/m^3 is possible. However, the investment for the introduction of a powder coating system including training and start-up difficulties must be considered. In case of a change to powder coatings the filler application is not required any more due to the inherent thicker coating layers of powder coatings. However, as discussed before, the pre-treatment must be improved in that case. An advantage of the powder coating system is that the powder can be recycled and the high overspray rate of the bicycle coating can be improved. In addition the installation of an automatic coating system with standard industrial robots is suggested. By using robots as an automatic coating tool the overspray can be reduced significantly in comparison to the currently used rotating discs. Thus, four coating robots are required for the two coating lines. Since only standard tasks are required from the robots a used, standard industrial robot is sufficient and can be obtained for 20 000 € per robot. Furthermore, the four coating booths must be reconstructed with a circulating air system for the recycling of the powder. The investment results in 245 000 € considering 35 000 € for the heat integration and 15 000 € for the improved pre-treatment.

4.2.4 Discussion of the Target Values by the Pinch Analysis Approach

In the previous sections target values concerning the energy, water and solvent consumption in a process are approximated and significant factors are determined in a pre-optimisation to identify meaningful savings potentials. Only generic modules calculating the target values are presented emphasising the strength of the pinch analysis approach to determine rough targets. However, a multitude of extensions and specific modules for specific processes have been developed for the pinch analysis approach enforcing a trade-off between on the one hand applicability and intention of the pinch analysis versus on the other hand accurate modelling and detailed results. The major goal of the pinch analysis is to identify optimisation potential by leaving the options for specific designs open and generating new ideas concerning the realisation of the optimisation potential identified. In many cases not a single "best" network can be identified but a range of good ones. Detailed precision is meaningless in the definition of the target values but will be considered in the subsequent design phase [Kemp, 1991].

Here target values for the reference company of the case study are identified and specific unit operations are illustrated discussing the realisation of the savings potentials with respect to the different process design options for the bicycle company. The application of the pinch analysis to a SME shows the concentration of a few relevant streams. However, for the discussion of savings potentials meaningful targets and unit operations are evaluated. By considering several mass- and energy flows a multi-criteria problem is constituted since no single process design is the best alternative in all target values and identified investment and operating costs. Thus, in the following section multi-criteria methods are proposed to discuss the possible combinations of unit operations building up the different options and consolidating the presented data in one single decision table.

In the Section 4.3 two different approaches to evaluate the target values are presented before in the following section, Section 4.4, inter-company applications for the pinch analysis approach are presented for an industry park of several SME.

4.3 Evaluation of the Overall Optimisation Potential

The aim of this section is to illustrate the evaluation of the different savings potentials identified in the last section and to consolidate the different target values determined by the pinch analysis approaches to an overall assessment. First, a relative assessment can be obtained by a simple metric defined as an Euclidean norm modified by weights (cf. Chapter 3.2 on page 63) illustrating the basic relationships between the mass- and energy flows and emphasising the importance of preferential information in multi-criteria analysis. The analysis by the metric is followed by an evaluation using the multi-criteria method PROMETHEE (described in Chapter 3.3 on page 71). In contrast to the metric, which is based on the absolute attribute values characterising a technology combination with respect to the pinch point, PROMETHEE is based on pairwise comparisons of the different alternatives. The application of PROMETHEE and the development of new sensitivity analyses for PROMETHEE to investigate the preferential parameters and data uncertainty is the focus of the analysis.

4.3.1 Evaluation based on a Metric

In the last section different target values are identified by the pinch analysis approaches for energy, water and solvents for the production of bicycles. In addition, each process design option is characterised by reference values for the use of energy, water consumption and solvent emission. In order to determine the overall resource efficiency, all values are consolidated in one table (cf. Table 4.12).

Table 4.12 shows the proposed process design options characterised by the different resource target values. The options *Waterborne Basecoats (T_1)*, *Condensation (T_3)* and *Powder Coating (T_4)* consider a realisation of the proposed heat integration of the waste gas of the drying ovens to pre-heat the drying air. In the case of *Thermal Incineration (T_2)* furnace temperatures of 982 °C have to be reached. Thus, a heat exchanger realising 50 % heat recovery of the overall system is considered and the ratio of the drying ovens is considered in the analysis by the metric. In the *Status Quo (T_0)* no heat integration is considered.

Furthermore, an *ideal alternative S_{pinch}* illustrating the theoretical minimal targets is used as a reference and as the new origin for the determination of a distance measure. Since no preferential information is available from the reference company the weighting of the environmental aspects is taken from a comparable analysis [Schollenberger and Treitz,

Table 4.12: Characterisation of the Different Process Design Options for the Metric

	w_j	S_{pinch}	T_0	T_1	T_2	T_3	T_4
Energy [kWh/h]	0.3	7	76	22	38	22	25
Water [m^3/h]	0.3	0.14	2.56	0.46	0.32	0.32	0.28
Solvents [mgC/m^3]	0.4	0	297.70	171.23	2.98	233.00	0
d_λ^{norm}			0.58	0.24	0.14	0.32	0.08
δ_{MOPA}			0 %	58.32 %	76.56 %	45.02 %	86.25 %

2005]. The exemplary weighting[54] reflects the included mass and energy flows of energy (30 %), water (30 %) and solvents (40 %). The attribute regarding the solvent emissions is slightly more emphasised considering the impact of the coating to the different environmental media. However, the weighting vector must be subject to detailed sensitivity analysis to discuss the robustness of the results (Sections 4.3.2.4 and 4.3.2.5).

Figure 4.15 illustrates the four process design options, the status quo and S_{pinch} as the combination of the individual target values of the different pinch analyses. The technology combination of powder coating and the installation of a thermal incinerator are positioned almost at the bottom of the plane visualising the small solvent emissions.

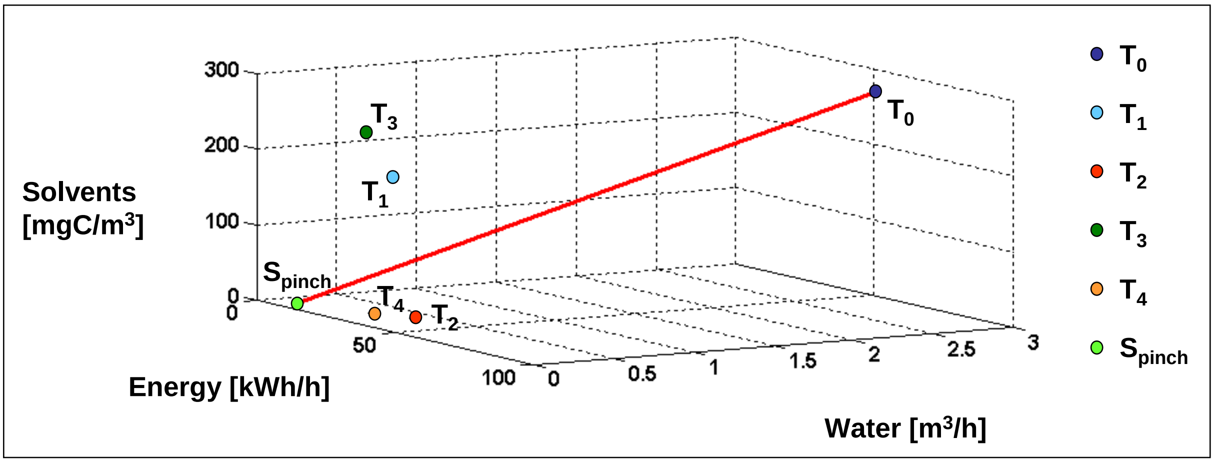

Figure 4.15: Illustration of the Characteristic Values of the Different Process Design Options

[54] It is not the aim of the thesis to provide general weighting vectors, but to illustrate the impact of the weighting and the preferential parameters and how the impact on the result can be analysed by sensitivity analyses.

By applying the metric for resource efficiency (introduced in Chapter 3.2) the overall savings potentials for the different process design options are determined (cf. Table 4.12). The option *Powder Coating* provides the highest savings potential with 86.25 %, followed by the *Thermal Incineration* with 76.56 %. The switch to *Waterborne Basecoats* (58.32 %) and the *Condensation* (45.02 %) are inferior to the first two options. Since T_4 and T_2 realise almost the complete savings potential with respect to the solvent emissions this effect causes the highest contribution to the overall savings potential.

Figure 4.16 shows the Pareto surface of S_0 for the proposed weighting and an equal weighting of all resources visualising the indifference compensation ratios between the different resources.

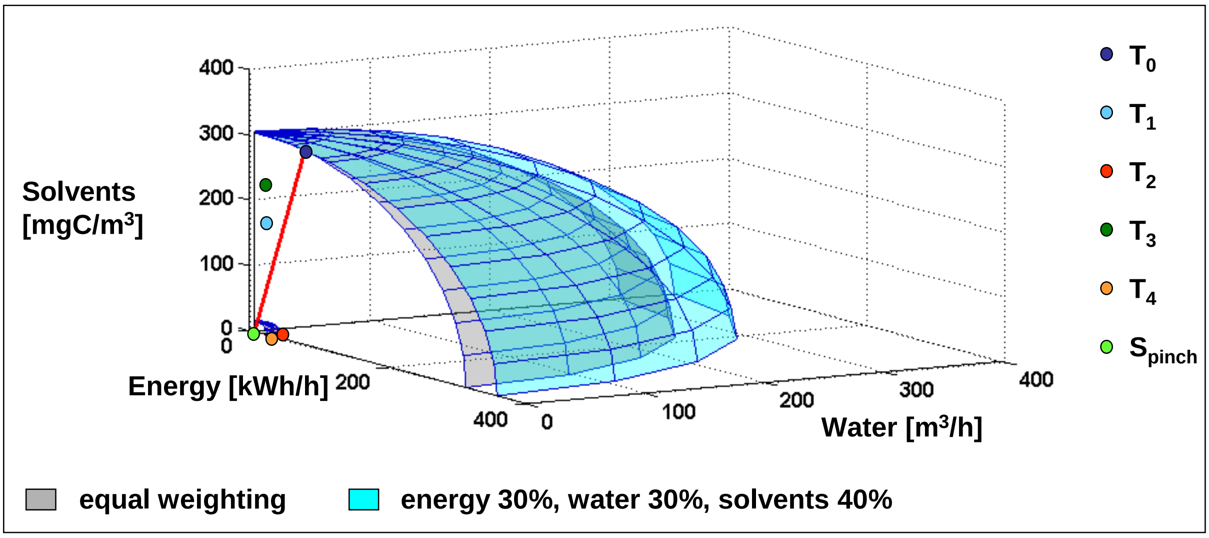

Figure 4.16: Illustration of the Metric for Energy, Water and Solvents

Since all described process design options are characterised by lower values in all criteria than the status quo, a change in the weighting factors does not lead to an exclusion of one option. However, by varying the weighting between the different resources, the determined savings potential changes. For example by focussing on energy efficiency and increasing the weighting factor for energy over 70 % and assuming equal weighting factors of 15 % for water consumption and solvent emissions, the process design option of *Waterborne Basecoats* has the highest savings potential. The Pareto surface of the best option T_4 covers the area closely around S_{pinch} because of the high savings potential and the small solvent emission value.

4.3.2 Evaluation based on PROMETHEE

In addition to the approach presented in the last section a different possibility for the simultaneous consideration of the various criteria is the application of an outranking multi-criteria analysis. For this case study the same set of data is used for the evaluation with the multi-criteria method PROMETHEE [Brans and Mareschal, 2005; Brans et al., 1986]. Table 4.13 shows the decision table for the analysis summarising the findings of the different applications of the pinch analysis in Section 4.2.

Table 4.13: Characterisation of the Different Process Design Options

	Status Quo (T_0)	**Waterborne Basecoats** (T_1)	**Thermal Incineration** (T_2)	**Conden-sation** (T_3)	**Powder Coating** (T_4)
Energy [kWh/h]	76	22	38	22	25
Water [m^3/h]	2.56	0.46	0.32	0.32	0.28
Solvents [mgC/m^3]	297.70	171.23	2.98	233.00	0
Investment [€]	0	75 000	687 000	140 000	245 000
Operating Costs [€/a]	45 000	24 200	45 000	29 000	30 000

In the evaluation using PROMETHEE[55] the same weighting factors[56] are used for all five criteria as in the metric presented in the last section. The weighting reflects economic and environmental aspects each by 50 %. As economic attributes the investment (20 %)

[55] The diploma thesis of Benjamin Schrader focused on the modelling and implementation of the multi-criteria method PROMETHEE ("Strategische Entscheidungsunterstützung: Implementierung und beispielhafte Anwendung eines Software Tools zur Evaluierung von Mehrzielentscheidungsproblemen", Institut für Industriebetriebslehre und Industrielle Produktion, Universität Karlsruhe, 2005)

[56] Using the same weighting factors in a classical and in an outranking approach is problematic and individual weighting factors must be set for each method. However, since no specific preferential information is available for this case study, the same factors have been used for PROMETHEE. By applying sensitivity analysis for the simultaneous change of all weighting factors and applying Monte Carlo Simulation for the preference parameters, the impact of the weighting on the results is discussed. It is not the aim of this thesis to provide general weighting factors.

and the change in operating costs (30 %) are included in the analysis and the mass and energy flows are reflected in the three environmental criteria energy (15 %), water (15 %) and solvents (20 %). As in the weighting within the evaluation based on the metric, the attribute regarding the solvent emissions is slightly more emphasised considering the impact of the coating to the different environmental media.

Furthermore, for all criteria the preference function type VI has been selected using half of the difference between the maximal and the minimal attribute value of each criterion[57] as the inflection point s of the respective Gaussian function. All preferential parameters are stated in Table A.5 in the appendix and sensitivity analyses for the preference type and parameters are provided in the following.

In the next section the results of the analysis are presented applying standard available methods for PROMETHEE and in a subsequent steps the results of the new sensitivity analyses for the preference and data uncertainties for PROMETHEE are shown.

4.3.2.1 Results of the Analysis

On the basis of the decision table and the preferential parameters the switch to *Powder Coating* has the highest $\Phi(a)$ flow compared to the other alternatives and is ranked first. Figure 4.17 shows the aggregated outranking flows of the positive outranking flow $\Phi^+(a)$ (the strength of an alternative), the negative outranking flow $\Phi^-(a)$ (the weakness of an alternative) and the net outranking flow $\Phi(a)$ (overall rating). The small Φ^- for the alternative *Powder Coating* indicates, that it has a strong performance on most criteria, whereas the small Φ^+ of the *Status Quo* is a sign that this alternative is weak in most attribute values.

This result is confirmed by the spider diagram of the single criterion net flows $\Phi_j(a)$ of each criterion (cf. Figure 4.18) which shows that the *Status Quo* is outranked with respect to most criteria and only for the *Investment* criterion outranks the other alternatives. Hence, also a reasonable change of the weights of the different criteria will show the *Status Quo* as the worst alternative, which only ranks first by a weighting of *Investment* of over 92 %. However, as the spider diagram shows, the decision is influenced by conflicting criteria and depending on the preference parameters and the weighting, one or the other alternative is ranked first.

[57] Due to the significant difference of the status quo to the other process design options, the status quo is not considered for the determination of the preference parameters p, q and s.

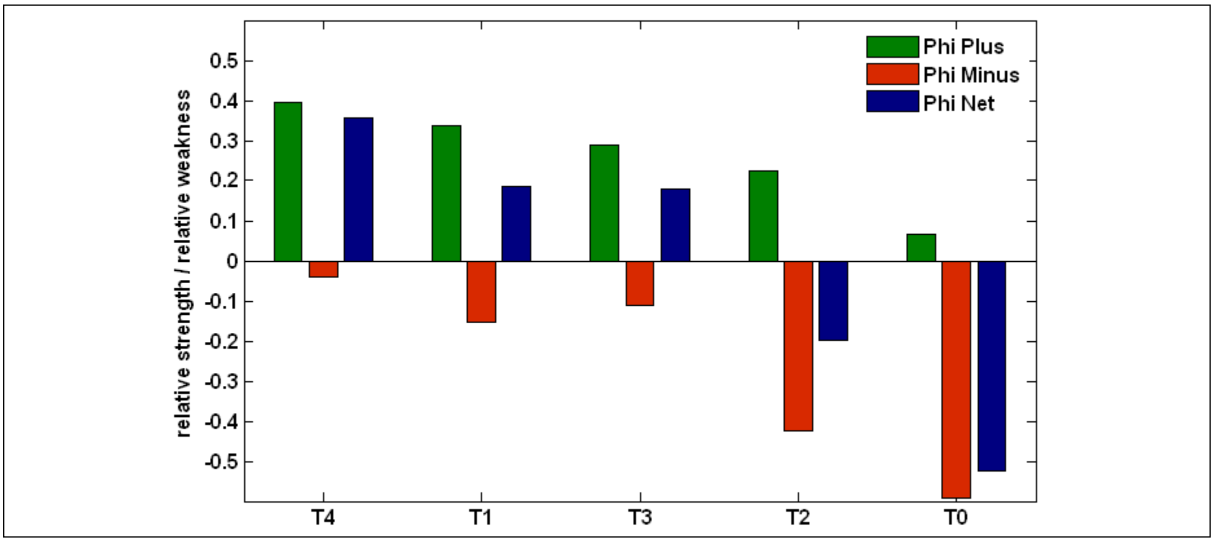

Figure 4.17: Outranking Flows $\Phi^+(a)$, $\Phi^-(a)$ and $\Phi(a)$ of the Process Design Options

All criteria contribute to the differentiation between the considered process design options as the unweighted single criterion net flows in the spider diagram illustrate. The option *Thermal Incineration* is dominated by the option *Powder Coating* since it is outranked in each single criterion. Thus, the line of the alternative *Thermal Incineration* is always inside the polygon of the option *Powder Coating*.

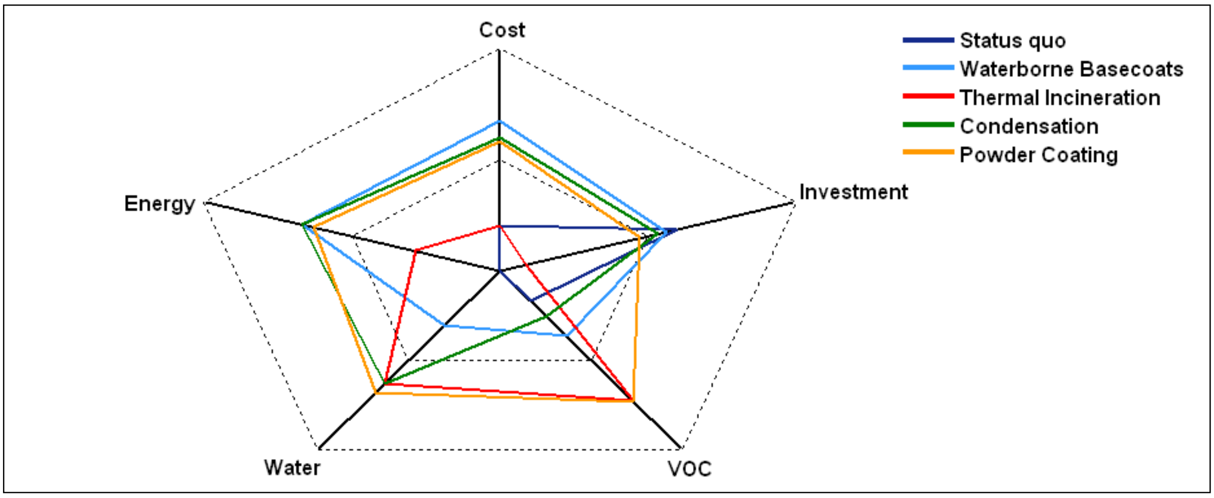

Figure 4.18: Spider Diagram of the Different Process Design Options

From a theoretical point of view the alternative *Thermal Incineration* would not need to be considered further. However, the option is considered in the following since it is an effective technique for the emission reduction of solvents in the waste gas. If a switch in techniques to powder instead of liquid coatings is not favoured, the option of thermal incineration achieves the best emission reduction[58].

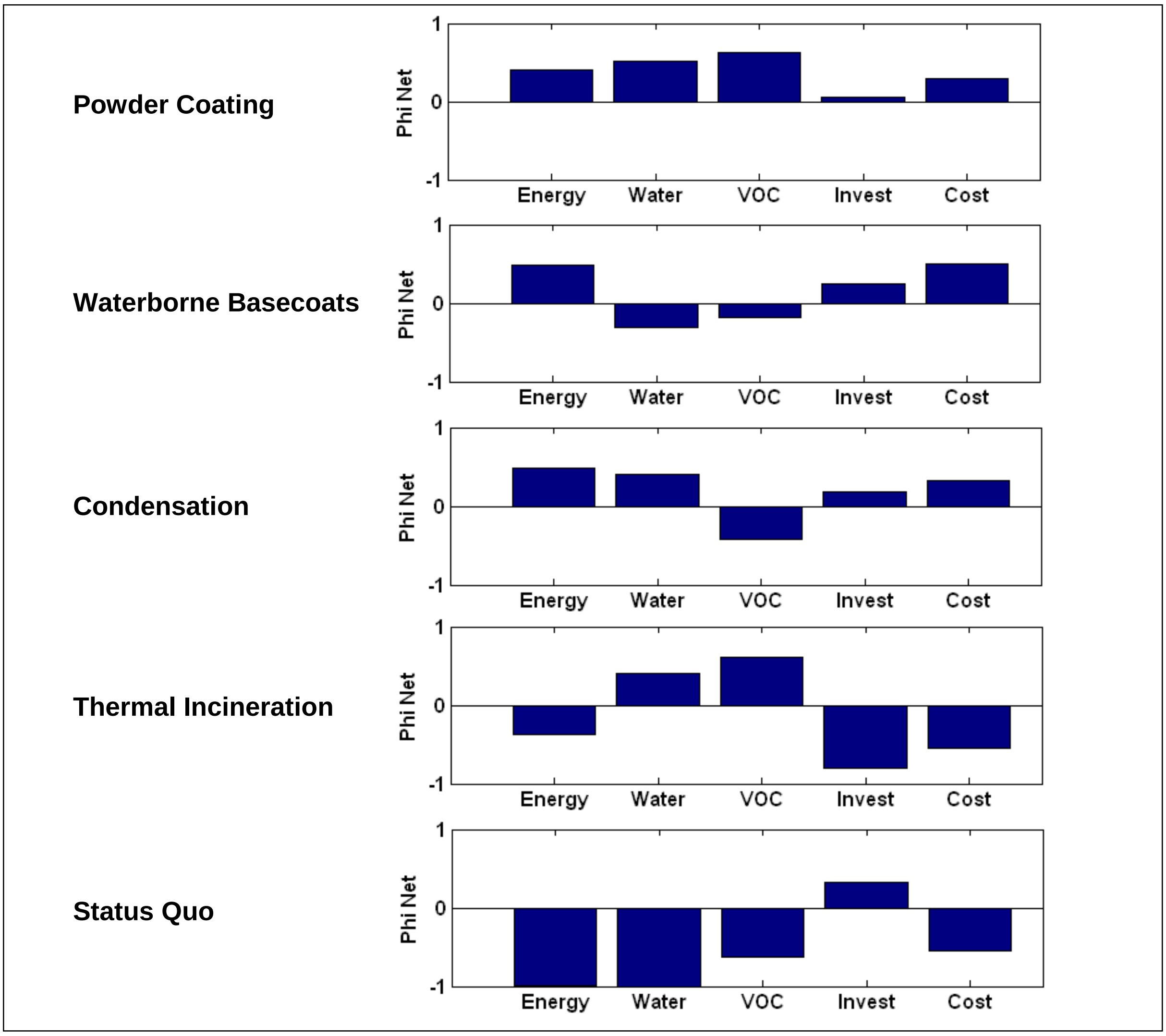

Figure 4.19: Profiles of all Process Design Options

The comparison of the profiles of the alternatives *Waterborne Basecoats* and *Condensation* reveals significant differences in the strengths and weaknesses of the alternatives (cf. Figure 4.19). The bar chart shows the quality of each process design option for each criterion j by the single criterion net flow $\Phi_j(a)$. Whereas the waterborne basecoats are superior in the emission reduction of solvents in the waste gas and slightly better in the initial investment (due to the smaller investment in equipment such as spray guns com-

[58] For a discussion about the selection of criteria and the consideration of further aspects see Section 4.3.2.2 on page 142.

pared to a condensation facility), the condensation option is superior with respect to the fresh water consumption since the waterborne basecoats require additional pre-treatment steps resulting in higher water demand.

The option of a thermal incinerator has its strength in the effective reduction of solvent emissions from the gaseous waste stream. However, due to the high investment this option is outranked by the other alternatives and ranks even behind the switch to waterborne basecoats or a condensation system, which is illustrated in the PROMETHEE I and II ranking (cf. Figures 4.20 and 4.21).

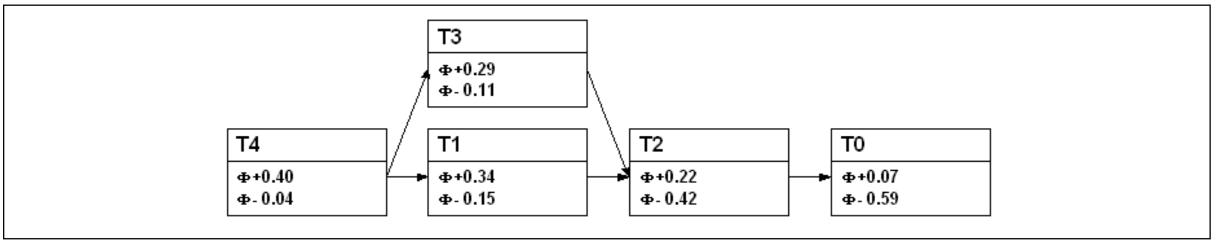

Figure 4.20: PROMETHEE I Ranking of the Process Design Options

Even though it is possible to differentiate between the alternatives in an overall assessment there exist incomparabilities as the PROMETHEE I ranking shows (cf. Figure 4.20). The switch to a powder coating based process is the preferred alternative. The outstanding performance results first from the significant reduction in water consumption since no water curtains are used and second from the elimination of solvent emissions due to the solvent-free coating. However, the alternative *Waterborne Basecoats* and *Condensation* have incomparabilities since a switch to waterborne basecoats provides more advantages, illustrated in the higher positive outranking flow ($\Phi^+_{T_1} = 0.34$ compared to $\Phi^+_{T_3} = 0.29$), but also faces more disadvantages, illustrated in the higher negative flow ($\Phi^+_{T_1} = 0.15$ compared to $\Phi^+_{T_3} = 0.11$).

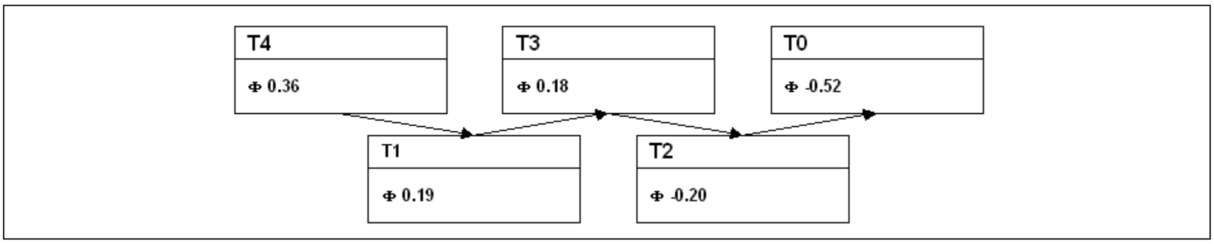

Figure 4.21: PROMETHEE II Ranking of the Process Design Options

Based on the PROMETHEE II ranking the analysis suggests a switch to powder coatings as first option before a switch to waterborne basecoats (T_1) and the installation of a condensation system (T_3). Nevertheless, the difference between the options T_1 and T_3 is very narrow. This is underlined by the fact that there exist incomparabilities between T_1 and T_3 in the partial PROMETHEE I ranking.

4.3.2.2 Principal Component Analysis of the Decision Problem

The *Principal Component Analysis (PCA)* is used used for sensitivity analysis. By projecting the alternatives from the $\mathbb{R}^k$ of k different criteria onto the plane of the first two principal components the so-called GAIA plane for PROMETHEE can be spanned and the decision problem can be visualised as described in Section 3.3.5 on page 85. The purpose of applying a factor-analytic technique is to aggregate the attribute information to present them in an adequate way.

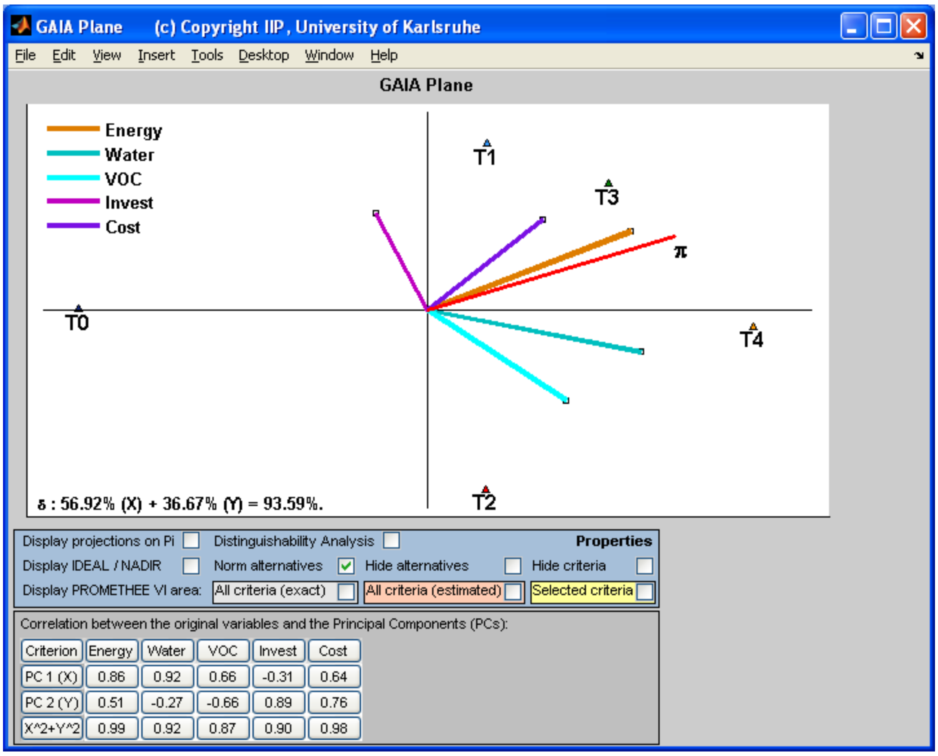

Figure 4.22: Principal Component Analysis of the Decision Problem

In Figure 4.22 the plane of the 1^{st} and 2^{nd} principal component is displayed for all criteria using the preference type VI and the preference parameter s as half the difference of the maximal and minimal attribute values excluding the status quo. Apart from the alternatives and the criteria axes, the unit vector of the weighting vector can be projected on the GAIA plane as the PROMETHEE decision stick π.

The different criteria are shown as axes in the new coordinate system of the first two principal components. Only one half of the plane is covered by the criteria axes. Consequently, the question must be addressed if the chosen criteria adequately reflect the decision problem. Especially, criteria in favour of the status quo are not considered, such as for example availability of the new coating material, additional maintenance of the new installations, or required training for the new installation. Since the question of resource efficiency is the focus of the analysis, it is assumed that all different coatings and installation fulfil technical requirements and security issues since no specific data was available to model these criteria.

Roughly 93 % of the total information is illustrated in the diagram. The correlation between the criteria and the first two principal components is shown in the table at the bottom of Figure 4.22. It shows that the criteria *Energy*, *Water* and *VOC* are mainly represented by the first principal component and *Investment* and *Costs* mainly by the second one. Consequently, the GAIA plot can enhance the comprehension of the given problem, but the loss of information must be considered since two distinct points in the $\mathbb{R}^k$ of k different criteria might be projected on the same point in the plane. Consequently, the projections on the decision stick can intersect, too, even if for this case study no intersections can be observed (cf. Figure 4.23).

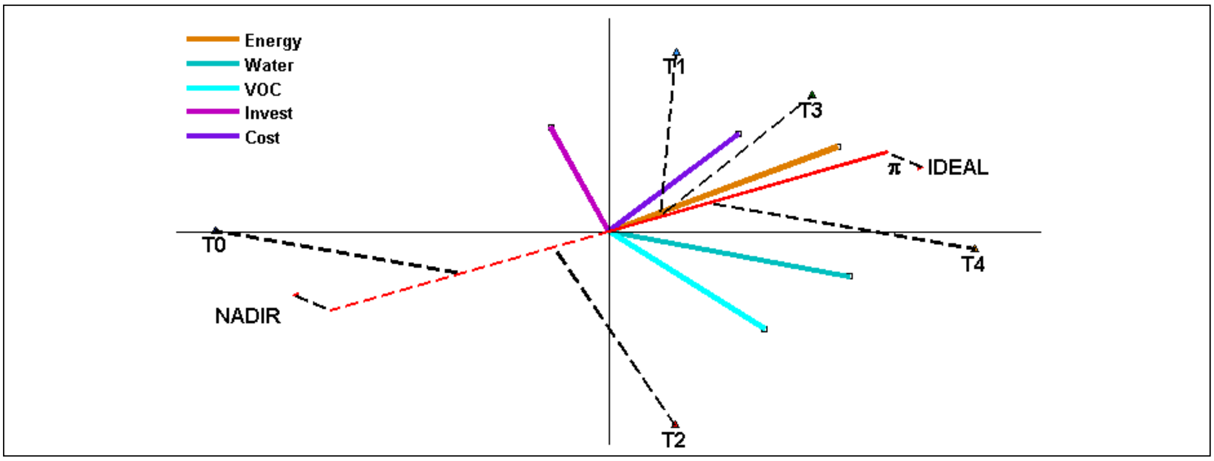

Figure 4.23: Projections on the Decision Stick π

The projections of the alternatives intersect with the decision stick π at the Φ net value of the alternative where the head of π is 1 (the projection of an alternative which has the best performance in all criteria, the so called IDEAL), the origin 0 and the head of the diagonally arranged line to π corresponds to -1 (the projection of the alternative which has the worst performance in all criteria, the so called NADIR) (cf. Figure 4.23).

The ranking of the alternatives can be seen at the order of intersections of the projections with π. Since the switch to waterborne basecoats (T_1) and the installation of a condensation system (T_3) show almost equal performance with respect to Φ, they intersect with π at almost the same position.

4.3.2.3 Sensitivity Analysis with Respect to Data Uncertainty

In Table 4.13 all attribute values are deterministic values but can be characterised by an uncertainty level as a percentage, such as 10 % of the deterministic value. Instead of using deterministic attribute values for each alternative with respect to each attribute, a set of different attribute values is drawn for each alternative with respect to each attribute by Monte Carlo Simulation. Thus, when calculating the relative differences of the attribute values (also called relative *preference differences*), a set of different values is generated for each pairwise comparison instead of only one individual value. Therefore, each alternative is not only represented by one point on the GAIA plane, but as a scatter plot. In this case attribute values are generated using a normal distribution and by assuming an uncertainty level and a normal distribution with 1 000 samples[59]. The uncertainty level can cover a more stringent range, for example ±5 % - ±10 % for more accurate data and a broader range for criteria which are more difficult to quantify such as for example ±10 % - ±50 %.

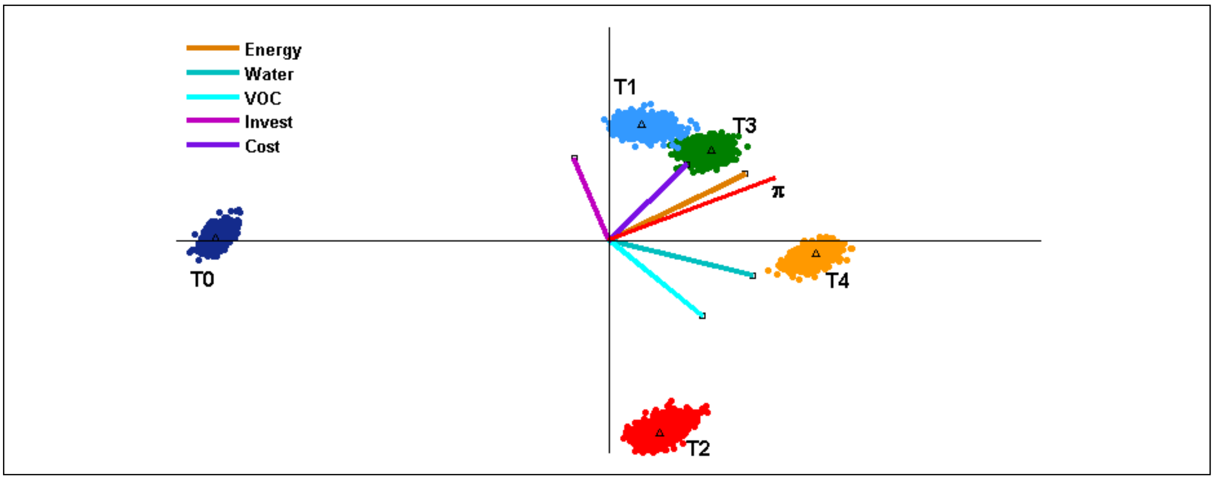

Figure 4.24: Distinguishability Analysis with an Uncertainty Level of ±10 %

[59] For a graphical analysis such as the distinguishability analysis a Monte Carlo Simulation with 1 000 samples is in general considered to be sufficiently large.

With an uncertainty level of ±10 % the different process design options can clearly be distinguished from each other. Even the options *Waterborne Basecoats* and *Condensation*, which are incomparable considering the preferences, can be distinguished since the areas of projections do not overlap.

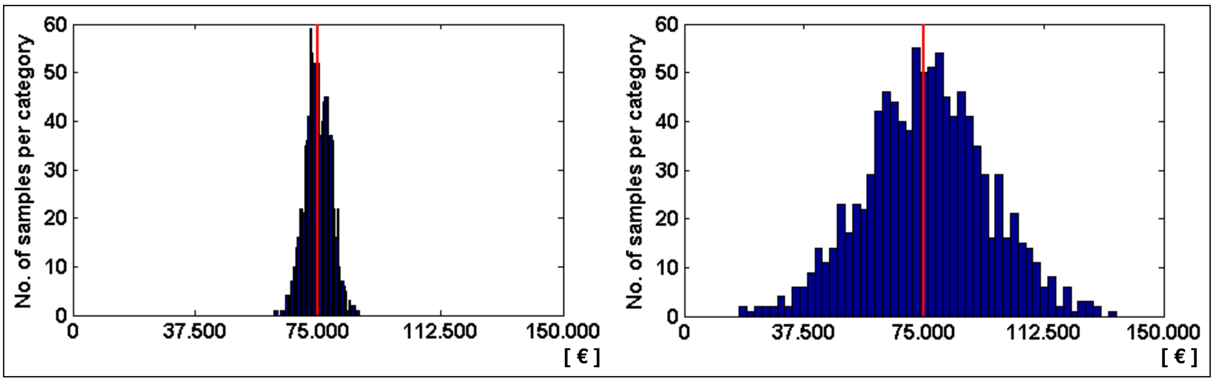

Figure 4.25: Data Distribution of Attribute Value Investment *for Alternative* Waterborne Coatings *with Uncertainty Level of 10 % (left) and 50 % (right)*

In the first distinguishability analysis an uncertainty level of ±10 % is assumed for all attribute values of the alternatives, but in a second analysis ±50 % is taken into account to investigate the sensitivity of the attribute values. Figure 4.25 shows the data distribution for an uncertainty level of 10 % and 50 % of the attribute value *Investment* for the alternative *Waterborne Basecoats*.

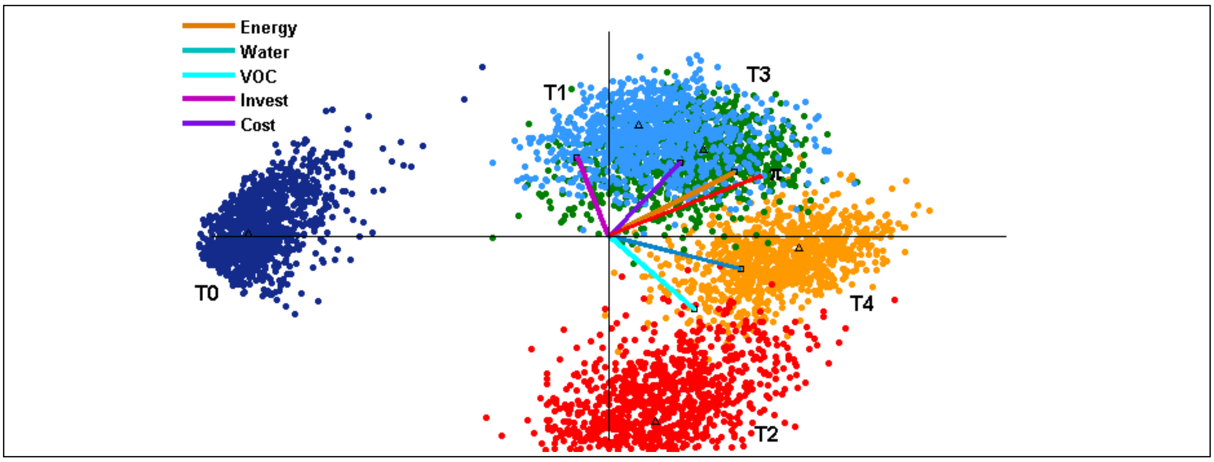

Figure 4.26: Distinguishability Analysis with an Uncertainty Level of ±50 %

As Figure 4.26 shows the different process design options can still be distinguished from each other by an uncertainty level of ±50 %. Only the options *Waterborne Basecoats* and

Condensation do now overlap considerably. Since no design variants are considered in the analysis, such as for example different condensation systems or different thermal incinerators, the various design concepts can be distinguished by their characteristic performance and the different strengths and weaknesses.

4.3.2.4 Evaluation of Preferential Parameters: Weighting

Sensitivity analyses are useful to analyse not only the uncertainty in the underlying data, but also in the modelling of the decision makers' preferences. Therefore, special sensitivity analyses for preferential uncertainties within the outranking approach PROMETHEE are applied to analyse the impact of the preference parameters to the overall result. Various sensitivity analyses (cf. Table 3.3 on page 79) can be used to facilitate modelling and transparent depiction of the decision problem within PROMETHEE. On the one hand the robustness of a decision can be investigated by changing the weighting of one criterion from zero to 100 %. On the other hand the robustness of the parameters q, p, and s of the preference function in PROMETHEE can be investigated by carrying out a Monte Carlo Simulation using specific uncertainty levels (e.g. ±10% or even ±100 %) or by evaluating all possible preference type combinations.

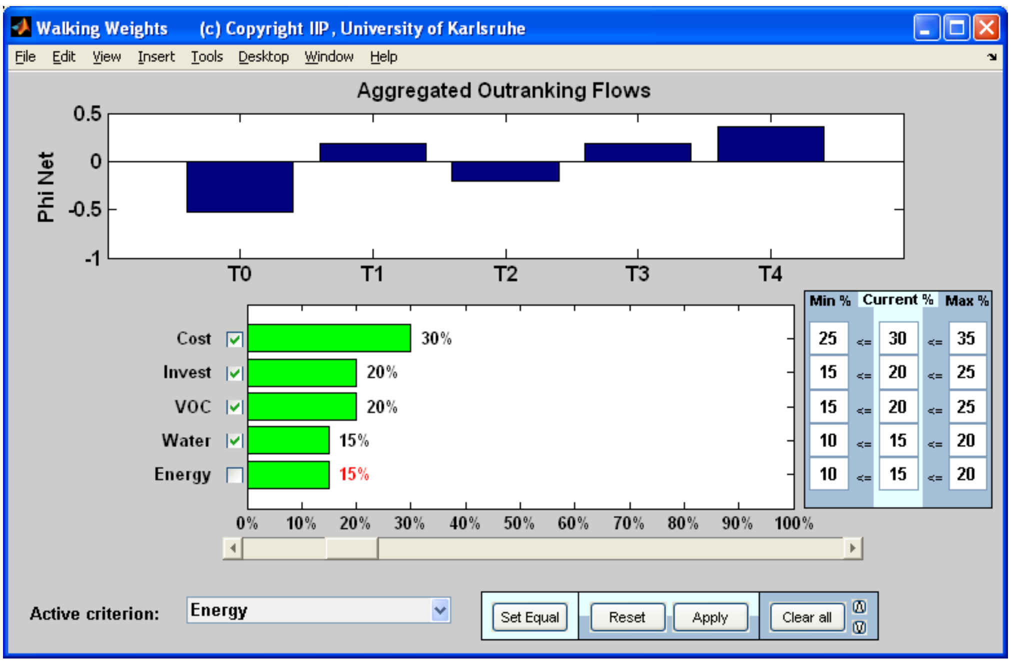

Figure 4.27: Sensitivity Analysis by Walking Weights

Enabled by an interactive decision support methodology it is useful for the decision maker to change the weighting of a selected criterion by a scroll bar and modify the current weighting (i.e. walking weights cf. Figure 4.27). On the one hand by increasing the weight of the considered criterion the required weighting factor can be obtained either from all other criteria or only from selected criteria. This depends on the selection of the decision maker using the check-box right next to each criterion (cf. Figure 4.27). On the other hand by reducing the weight of the considered criterion the spare weight can be reallocated either to all other criteria or only to selected criteria. Not only the weights of each criterion are shown in a bar chart, but simultaneously, the Φ net flows of the considered alternatives are shown in a bar chart and the height of each bar (i.e. Φ) changes with the weighting.

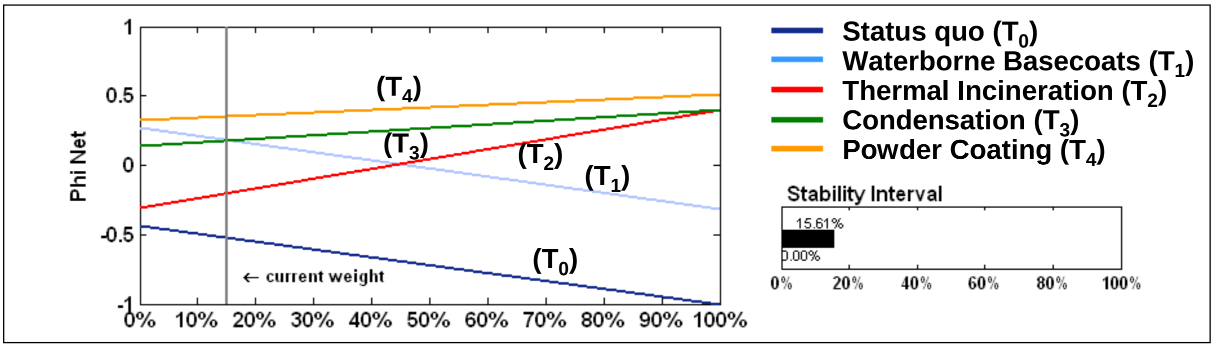

Figure 4.28: Sensitivity Analysis of the Weight for Criterion Water

Figure 4.28 shows the sensitivity analysis for the weight of the criterion *Water*. Each line represents one alternative and the gradient of the lines shows the influence of the selected criterion on the performance of the alternatives. The current weighting is 15 % and the stability interval around this weighting reaches from 0 % to 15.61 %. Thus, the ranking changes directly if the weighting of the water criterion is changed. Even though the powder coating option is the best alternative for any weighting factor of *Water*, right above the upper limit of the stability interval the waterborne basecoats option changes positions with the condensation option. By an weighting of more than 44.6 % the thermal incinceration becomes third and even better than the change to waterborne basecoats.

The stability interval in case of the sensitivity analysis for the criterion *Costs* is [27.81 %, 61.64 %], but the option *Powder Coating* is the best alternative from 0 % - 61.64 %. Above the stability interval the waterborne basecoats are the preferred alternative due to their lower operating cost.

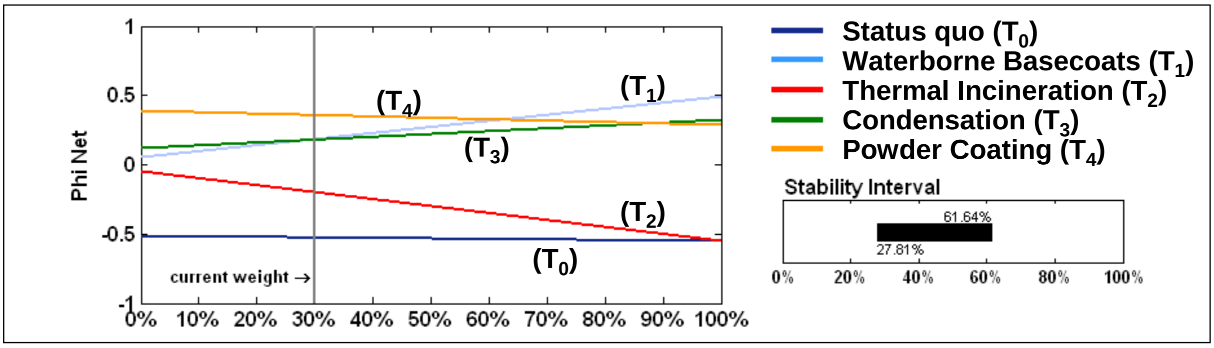

Figure 4.29: Sensitivity Analysis of the Weight for Attribute Costs

The stability interval for the criterion *Energy* is $[0\,\%, 72.1\,\%]$ and for the criterion *Solvents* covers the range of $[18.24\,\%, 41.31\,\%]$. However, the option *Powder Coating* is the best alternative within $[3.79\,\%, 100\,\%]$ and only below $3.79\,\%$ the option *Condensation* would be the best alternative. Concerning the attribute *Investment* the stability interval around the current weighting is $[13.18\,\%, 37.84\,\%]$.

By defining upper and lower bounds for each weight (cf. Figure 4.27) the convex hull of all valid weighting combinations can be projected on the GAIA plane, visualising the range of π, i.e. the PROMETHEE VI area Δ visualises the area to which π is restricted if it stays inside the defined boundaries with an assumed absolute variation, in this case of $\pm 5\,\%$, in the weighting of each criterion simultaneously (cf. Section 3.3.5.4). The PROMETHEE VI area and the decision stick π illustrate the influence of different weights in the GAIA plane, since they are not taken into account in the projections of the criteria and alternatives.

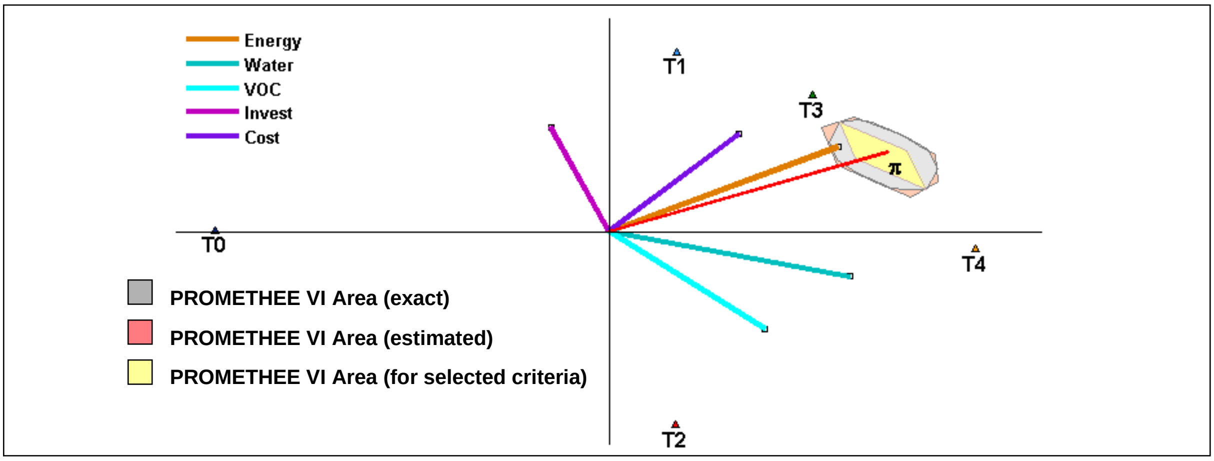

Figure 4.30: PROMETHEE VI Area

As Figure 4.30 illustrates a "soft problem" must be solved (cf. Section 3.3.5.4), since the origin is not part of Δ and therefore good alternatives lie in the general direction of the decision stick. It is assumed, that in case of a soft problem a compromise is easier to find than in a "hard problem", where the origin belongs to Δ and basically all alternatives may possibly be selected. In addition to the exact calculation (grey area) also an estimated PROMETHEE VI area is shown (for a detailed description of the different areas refer to Section 3.3.5.4 on page 90). However, considering the small number of criteria, the areas do not differ considerably and the calculation time is not a problem[60].

4.3.2.5 Evaluation of Preferential Parameters: Preference Function

Considering the difficulties in modelling value judgements it is especially important to carry out sensitivity analyses for the intra-criteria preference function in PROMETHEE. The sensitivity analysis is done for the preference parameters by a Monte Carlo Simulation and for the preference type by an enumeration of all possible preference type combinations.

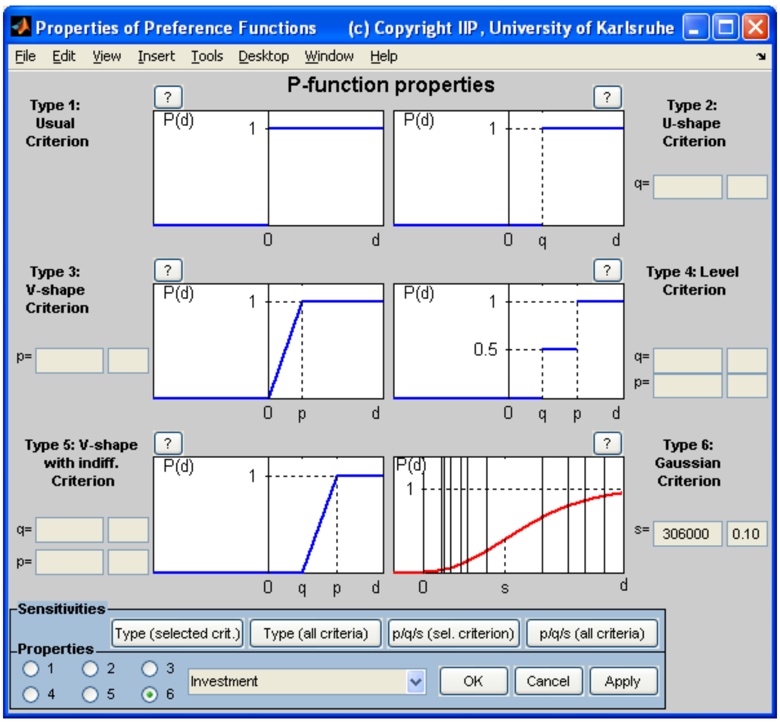

Figure 4.31: Preference Function of Criterion Investment

[60] If more than ten criteria are used, the calculation time slows down considerably. However, it is possible to calculate Δ for an example of the iron and steal industry provided in [Geldermann, 1999] with 21 criteria and 9 alternatives.

For each criterion it is possible to define a preference function by selecting a preference type and defining the appropriate parameters (cf. Figure 4.31). The preference function is based on the differences in attribute values stemming from the pairwise comparisons. Figure 4.31 shows the selection of preference type VI for the criterion *Investment* with an inflection point at 306 000 € and an uncertainty level of 10 %. The Gaussian function illustrates the slope of the preference function and the vertical lines illustrate the existing differences between the attribute values. Thus, it is possible to visually identify the relevant range for the selection of preference parameters.

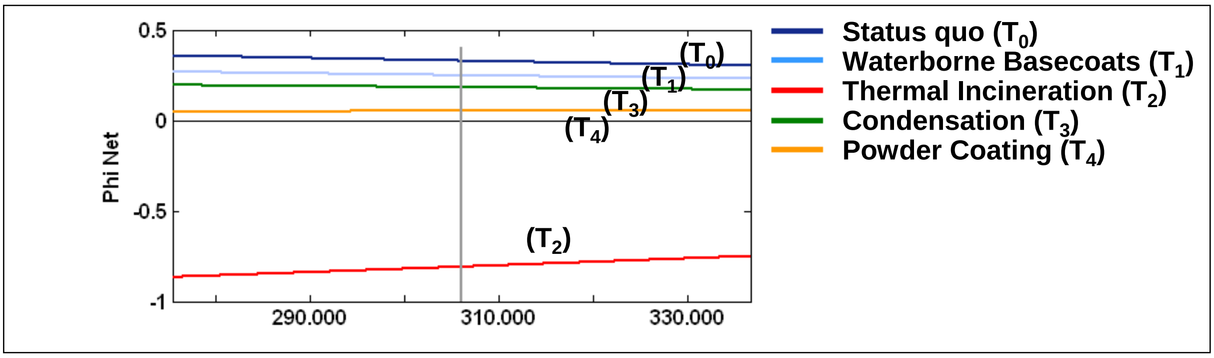

Figure 4.32: Sensitivity Analysis of the Preference Parameter of Criterion Investment

Figure 4.32 shows the sensitivity analysis for the parameter s around the proposed inflection point at 306 000 € for the single criterion net flow $\Phi_j(a)$. The Monte Carlo Simulation for the preference parameter is based on a uniform distribution and an uncertainty level of 10 % with 306 000 € as the mean of the distribution, which is half of the difference between the maximal attribute value (687 000 €) and the minimal attribute value (75 000 €) of the different available design options excluding the status quo.

By varying the inflection point the magnitude of the differentiation between the different investments is modelled. A higher value for s results in more indifference between the different investments whereas a smaller value for s means a higher focus on the differences in the investments and smaller difference results already in more distinct preference values. The *Status Quo* ranks first for any value of s since no investment is considered in this case and *Thermal Incineration* is outranked by all other alternatives since it requires the highest investment.

However, the overall contribution does not significantly change by varying s. Nevertheless, the analysis also shows that by for example increasing the uncertainty level of s for all criteria to 100 % there is a significant effect on the overall results (cf. Figure 4.33).

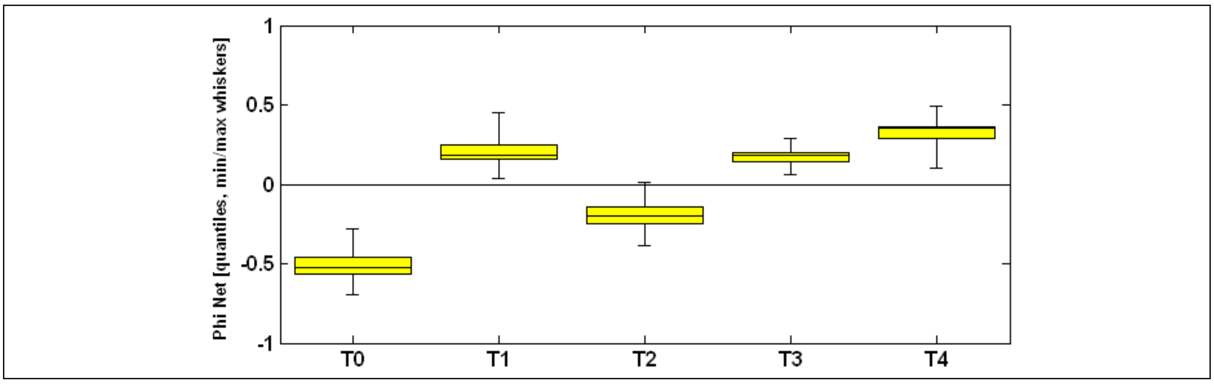

Figure 4.33: Sensitivity Analysis of all Preference Parameter of all Criteria

In case of an uncertainty level of 10 % there exist no overlaps between the process design option *Powder Coating* and the sencond and third ranked options *Waterborne Coatings* and *Condensation*. By increasing the uncertainty level to 100 % shifts exist in the overall ranking of the alternatives nevertheless the alternative *Powder Coating* is still considered the best alternative in 87 % of the cases. The boxplot in Figure 4.33 shows $\Phi(a)$ of all alternatives according to the deterministic value for each alternative as the middle line within the box, and the lower and upper quartiles (25^{th} and 75^{th} percentiles) of the normal distributed values over the defined uncertainty interval as the edges of the boxes. The whiskers visualise the maximal and minimal $\Phi(a)$ net for each alternative within the uncertainty interval.

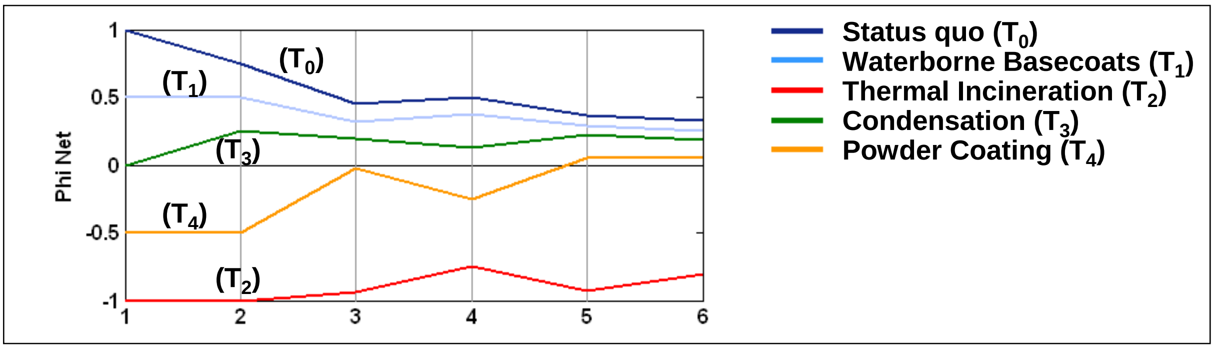

Figure 4.34: Sensitivity Analysis of Preference Function Types of Criterion Investment

Figure 4.34 shows the impact of the selection of a specific preference type for the criterion *Investment*. Since the ranking is based on the absolute differences in attribute values between the alternatives, the ranking of the alternatives does not change by changing the preference type. However, the magnitude of the preference of one alternative compared to another changes as the single criterion net flows $\Phi_j(a)$ illustrate.

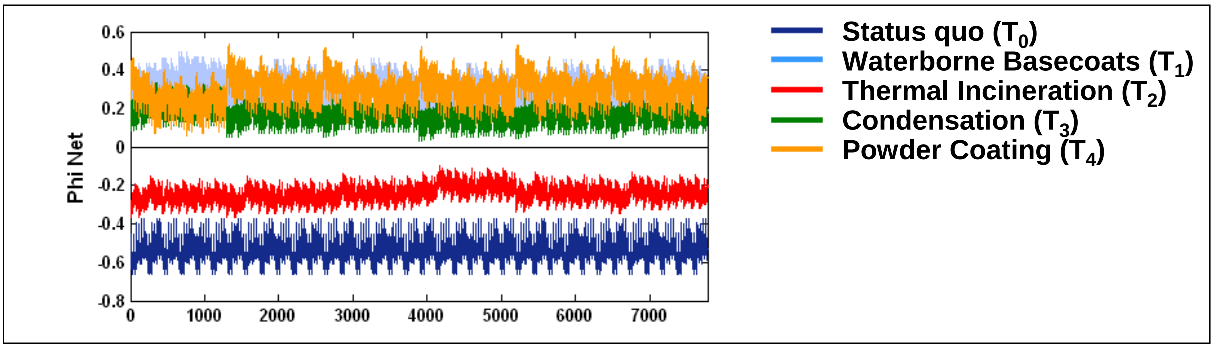

Figure 4.35: Sensitivity Analysis of all Preference Function Types of all Criteria

Further calculations show that in the case of the permutation of all preference types (I - VI) for all 5 criteria, the alternative *Powder Coating* is only the best alternative in 52 % of all $6^5 = 7776$ possible combinations of preference type functions (cf. Figure 4.35). In 48 % the option *Waterborne Basecoats* is ranked first. In this case the weights and the preference parameters are fixed and only the effect on the overall result is analysed by changing the type of preference function for each criterion. Herewith, the low robustness of the decision is demonstrated and emphasises the need of a high transparency of the decision problem to be able to interpret the obtained results in the best possible way. To summarise, the analyses reveal that no clear preference for one alternative is obvious, since the option *Powder Coating* shows the best performance of most criteria, but both the option *Waterborne Basecoats* and *Condensation* of solvents show comparable performances depending on the preference modelling.

4.3.2.6 Recommendations based on the Analysis

This section shows the application of the multi-criteria approach PROMETHEE to the evaluation of process design options for the process of industrial bicycle coating. Four process design modifications (T_1: the switch to waterborne basecoats, T_2: the installation of a thermal incineration system, T_3: application of a condensation system, and T_4: the switch to powder coatings) are discussed and compared to the status quo. The analysis revealed that the result depends highly on the modelling of the preferential parameters. For the assumed preferential parameters the analysis suggests a switch to powder coatings and thereby provides the same result as the metric presented before.

Since powder coatings are solvent-free and particularly suitable for metal parts, such as bicycles, due to the electrostatic application and do not require water curtains to absorb the coating particles in the cabins and provide a low waste generation by using the possible recycling of the coating particles, various technical, economic and environmental aspects give reasons to favour a switch to powder coatings. Especially, the improvement of the application efficiency by using a standard industrial robot and the reduced overall energy demand favour the option T_4 compared to the other alternatives[61].

The general disadvantage of powder coatings is the limited control of the layer thickness [Ondratschek, 2002]. However, by changing from a three to a two layer coating higher film thickness is taken into account and future developments will decrease this limitation. Thus, the switch to powder coatings is a change in techniques and leaving the company well prepared for future challenges.

The switch to waterborne basecoats is the simplest way to achieve a reduction in the solvent emissions[62]. Even though the reduction is only based on a switch in the basecoat application, since no waterborne clearcoats are currently available for this application, the measure is quite effective considering the small required investment. The option of a condensation system turned out to be incomparable to the switch to waterborne basecoats[63]. As shown in the economic evaluation of the condensation system the operating costs highly depend on the value of the recovered solvents. If the recovered solvents can be used directly in the same process by a closed loop recycling the condensation is a noteworthy option for the waste gas cleaning of industrial bicycle coating. Since the concentration of the solvents in the waste gas determines the investment in heat exchanger a concentration unit by a zeolite wheel is suggested leading to a higher concentration of the solvents in a reduced air flow. However, if the solvents cannot be reused the operating costs of a condensation system does not justify the achieved solvent emission reduction.

The option of a thermal incineration turned out to be too expensive as a waste gas cleaning technique. Even if only the waste gas of the drying ovens is considered and a

[61] In the case study only the heat integration of the waste gas of the drying ovens of the powder coating system is considered resulting in a higher energy demand as the status quo because of the higher drying temperatures. However, a reduction of operating costs is considered due to a changeover from conventional three layer coating processes to a two layer powder coating installation.

[62] The implementation of solvent emission reduction measure, such as for example the switch to waterborne basecoats results in an exemption of the emission threshold limits with respect to the European Solvents Directive [EC 99/13].

[63] The installation of a condensation system would be considered as a secondary measure with respect to the European Solvents Directive [EC 99/13] and in this case an emission threshold of 150 mgC/m^3 must be complied with. However, in the case study an overall emission limit by installation of a condensation system of 233 mgC/m^3 was determined.

considerably lower gaseous waste stream must be treated, this results in an investment of 201 000 € compared to 687 000 € for the installation of an incinerator for the total waste air. However, the overall emission reduction efficiency is considerably lower[64] and the option of thermal incineration only for the waste gas of the drying ovens (referred to as option T_5) is incomparable to the thermal incineration of the total waste gas stream, but still outranked by the option *Waterborne Basecoats* and *Condensation*[65]. This result differs from the analysis by the metric presented before. Since no cost parameters are considered, the effective overall reduction in the solvent emissions provides a significant contribution to the overall good performance according to the metric.

The application of several sensitivity analyses for the underlying data and value judgement uncertainty proves that the results highly depend on the modelling of the preferential parameters and consequently a transparent modelling of the decision problem furthers the communication of preferential information and a compromise solution. The data uncertainty has only a limited effect on the distinguishability since the different concepts can well be differentiated. Even though the weighting, i.e. inter-criteria preferences, of the different criteria has a considerable impact on the overall results the influence of the intra-criteria preferences, such as the preference type and the parameter of the preference function, may be more relevant in this case than the impact of the uncertainty of the weighting factors. By applying the simulation techniques an evaluation of the robustness of the decision is enabled and an adjustment of the model is possible.

4.3.3 Discussion of the Results

This section shows the methodology for an evaluation of the overall optimisation potential for a case study of industrial coating of bicycles. In the previous section target values and characteristic figures describing different process design options are identified and economic operating parameters of certain technology combinations, such as for example the condensation of solvents, are evaluated and consolidated in this section. The results of the analysis of target values for mass- and energy flows are aggregated to a distance measure which can be used for the comparison of the investigated process design options. The metric provides a simple, illustrative method to discuss trade-offs and compensation

[64] In Europe the installation of a thermal waste gas treatment, like a thermal incinerator, results in an overall emission limit of 20 mgC/m^3 with respect to the European Solvents Directive [EC 99/13].

[65] The aggregated outranking flows (cf. Figure A.1), the PROMETHEE I ranking (cf. Figure A.2) and a distinguishability analysis (cf. Figure A.3) including T_5 are provided in the appendix (starting from page 199).

ratios in the context of mass- and energy flow management and consequently provides a useful tool for discussion the influence of value judgements in the multi-criteria analysis.

Furthermore, the single parameters can be investigated by a multi-criteria analysis using PROMETHEE offering the possibility of carrying out several sensitivity analyses. The sensitivity analyses provide a good understanding of the effects of the different modelling parameters and the application of the Monte Carlo Simulation offers the possibility of an analysis including of several parameters simultaneously. Consequently, the application of the Monte Carlo Simulation in combination with a Principal Component Analysis can help to understand the impact of the uncertainties of the raw data on the overall results. Additionally, decision makers should be aware of the influence of the selected criteria and the chosen weighting factors as demonstrated by the effect of different preference function parameters or weighting vectors.

4.4 Implications for a Strategic Planning

Not only inter-company networks and supply chain management have gained increased importance by concentrating on core competences and realising synergies, but also eco-industrial networks provide significant optimisation potential by closing material and energy flow loops by utilising by-products or by reusing waste of industrial sites as a valuable input within the network (cf. Section 4.4.1).

By applying the production pinch analysis (cf. Section 2.1.3.2 on page 26) intra- and inter-company production networks on the basis of product streams can be analysed and options for capacity planning as part of the strategic planning of the company or future options for cooperation within an industry park or through the supply chain can be evaluated. Especially, questions concerning the capacity adjustment in seasonal and dynamic markets can be addressed by applying the production pinch analysis (cf. Section 4.4.2).

Consequently, two general alternatives to apply the methodology to different process design options in the context of a strategic advancement of the business planning are presented in the following. First, on a basis of process streams in the setting of an inter-company network and second on a basis of product streams for capacity planning in seasonal and dynamic markets in an intra-company setting [see also e.g. Geldermann et al., 2007b].

4.4.1 Optimisation of Inter-Company Networks

An analysis of an inter-company energy network in Karlsruhe shows that a positive ecological and economic impact results from different regional energy supply strategies [Frank, 2003]. In the analysis future options of a subsequent inter-connection for example by pipelines and the utilisation of waste heat in neighbour companies are discussed as well as the construction of a new, more efficient power generating facility. Cost savings potentials of up to 20 %/a and emission reductions of 20 % - 30 % of CO_2, NO_x and SO_2 emissions are identified. The analysis of a common solid waste system of a supplier park for an automotive company [Tietze-Stöckinger, 2005] reveals the effect on economies of scale and the utilisation of large scale technology for SME by a longterm cooperation of the companies on site. A reduction of the overall cost was mainly accomplished by a significant reduction of the required transports. In addition an analysis of regional networks is possible as shown by a study on recycling networks in the building and construction industry [Schultmann, 2003]. By modelling the transport infrastructure the locations of waste generation and the locations of the recycling facilities using *Petri Nets* with information from a *Geographical Information System (GIS)* regarding the impacts on costs and emissions. However, even though the inter-company analysis may provide significant savings potentials, the realisation provides additional technical and organisational restrictions in contrast to one intra-company production network.

4.4.1.1 Model of an Industry Park

Starting already in the early 1980s and especially since 2003 within the "Accelerating Small and Medium Enterprise Development Law of PRC" industry parks are planned and extended to further the development of the 2.6 million SME in China [Geldermann, 2006b; Geldermann et al., a,b]. The environmental management of industry parks challenges the cooperation between companies of different sectors. Whereas in Europe the majority of industry parks has a focal company, such as for example an automotive company, organising its affiliated supplier park, in China quite frequently SME of about the same size are pooled in one industry park. Nevertheless, the establishment of an eco-industry park is seen as a marketing instrument to attract foreign investment and certification as eco-industry park increasingly attracts attention [Zeng et al., 2005].

In the following the model of an industry park as shown in Figure 4.36 is assumed to discuss the application of the pinch analysis to inter-company networks[66]. Thus, only the

[66] The model of the industrial park was developed in a series of discussions with Prof. Lu, College of Environmental Science and Engineering, Tongji University

mass and energy flows relevant for heat integration are discussed and other product or solid waste streams, such as for example packaging scrap, are neglected. Aim of the analysis is to exemplarily present the application of the thermal pinch analysis to an inter-company network based on a selection out of several case studies [Geldermann et al., 2006c] from Chile and China[67]. There are four individual companies settled in the industry park:

- *Bicycle 1* is the bicycle producing company introduced in the preceding sections (cf. Chapter 4.1 - 4.3) producing approx. 1 million bicycles per year.
- *Bicycle 2* produces on a smaller scale (< 100 000 bicycles per year). The production process is similar to the one of the reference company *Bicycle 1*. There exists a continuous pre-treatment section and frequently two-colour coatings are applied as a basecoat[68]. Furthermore, the company faces even larger seasonal changes than *Bicycle 1* and thus bed frames are welded and coated in the same facilities. A detailed analysis including the calculation of target values by the pinch analysis approach and the evaluation of the overall savings potential by multi-criteria analysis is provided in [Schollenberger and Treitz, 2005].
- *Fishery Nets* repairs, cleans and impregnates fishery nets used for salmon cultivation. The nets must be changed every four month. Because of the growing algae and mussels they become more and more heavy. In addition, fouling may be the source for bacteria or other illnesses for the salmon. After cleaning the nets with high pressure cleaners and large-scale washing machines, the nets are repaired and impregnated. The impregnation is achieved by a dip coating containing conventional solvent-based coatings. In a last step the nets are dried in a drying tower. A detailed analysis about this case study is provided in [Ludwig et al., 2006].
- *Alcohol Distillery* is an agricultural cooperative producing Pisco, a brandy-like spirit, from a wine distillation process[69]. In the harvest season several distributed

[67] The PepOn project used a series of case studies with on-site investigations in Chile and China and data and process characteristics were acquired. However, it turned out to be difficult to find individual industry parks in which every single company was willing to cooperate. Thus, an model of an industry park is presented comprising companies from Chile and China to illustrate the application of the methodology to inter-company networks

[68] Within the PepOn project several diploma thesis were carried out in Chile in cooperation with the Unidad de Desarrollo Tecnológico (UDT) in Concepción and local companies. The diploma thesis of Alexander Hercher focused on solvent emission reduction measures ("Technische und wirtschaftliche Möglichkeiten der Minderung von Lösemittelemissionen am Beispiel eines industriellen Lackierbetriebes in Chile", Institut für Industriebetriebslehre und Industrielle Produktion, Universität Karlsruhe, 2005)

[69] Within the PepOn project several diploma thesis were carried out in Chile in cooperation with the Unidad de Desarrollo Tecnológico (UDT) in Concepción and local companies. The diploma thesis of

facilities collect the grapes from the affiliated winegrowers and after removing the peduncles and maceration, the must is fermented and stored. In a second step throughout the whole year the wine is continuously distilled. The distiller's wash is the major source of emissions and is treated in an organic wastewater treatment system. A detailed analysis is provided in [Ludwig et al., 2006] and a similar study has been done for a case study in China [Guo et al., 2005].

Figure 4.36 shows a map with assumed distances and locations of the different case studies.

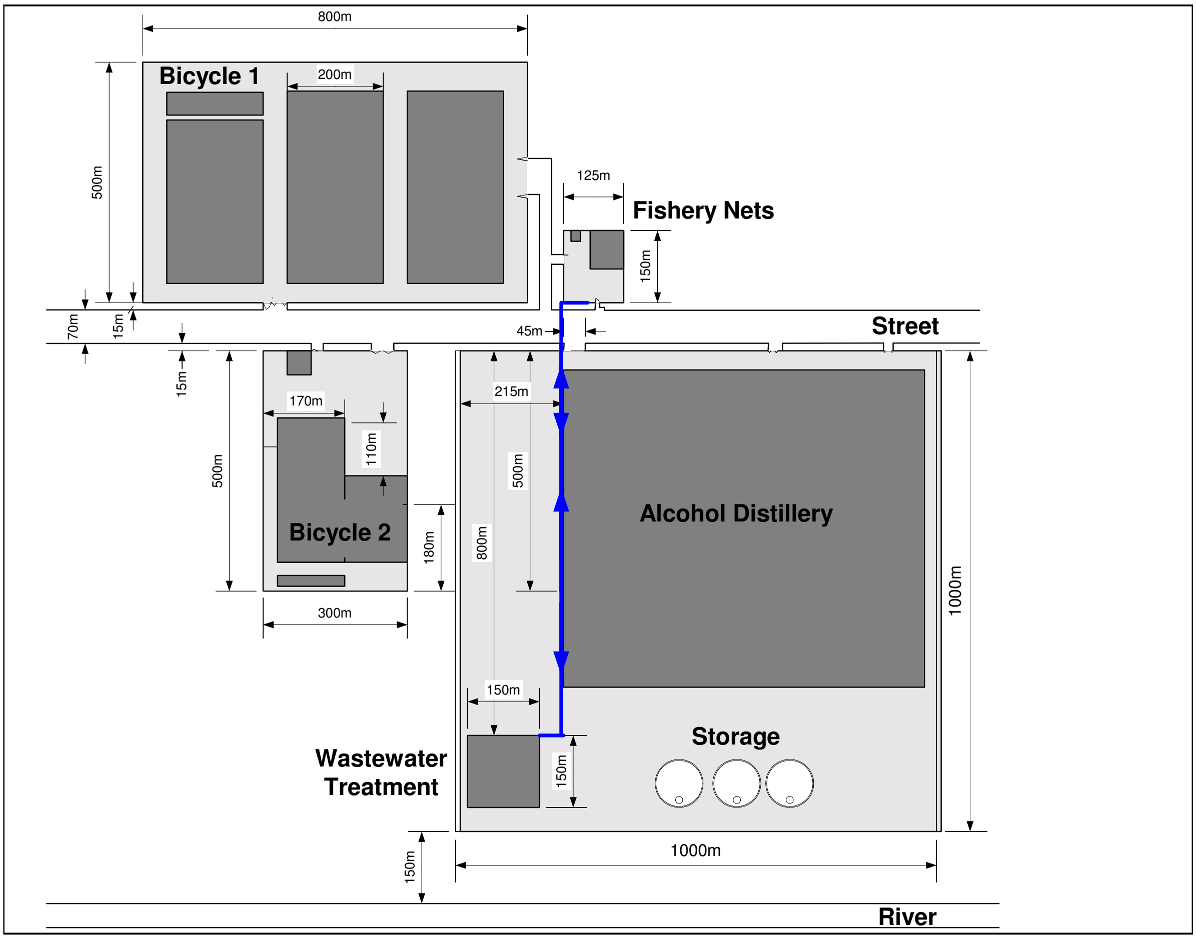

Figure 4.36: Required Piping of Inter-Company Heat Exchange within an Industry Park

Carl Richers focused on mass- and energy flow management in the alcohol production ("Optimierung der Energie- und Stoffströme in der chilenischen Pisco Produktion", Institut für Industriebetriebslehre und Industrielle Produktion, Universität Karlsruhe, 2005)

4.4.1.2 Application of the Thermal Pinch Analysis for the Industry Park

By compiling all the heating and cooling requirements of the different companies in one single analysis an overall hot and cold composite curve for the industry park can be constructed (cf. Figure 4.37). The composite curves show a limited range of overlap resulting in only limited heat integration possibilities. In total a minimum cooling requirement by cold utilities of 2 260 MJ/h exists, compared to a minimum heating requirement by hot utilities of around 2 050 MJ/h. The overlapping range constitutes 939 MJ/h (=260 kWh/h). Major heat source is the distiller's wash of the alcohol distillery of 104 kWh/h, which is available at 92.5 °C, but which cannot be used internally due to quality restrictions of the Pisco production. In the analysis a ΔT_{min} of 20 °C is assumed.

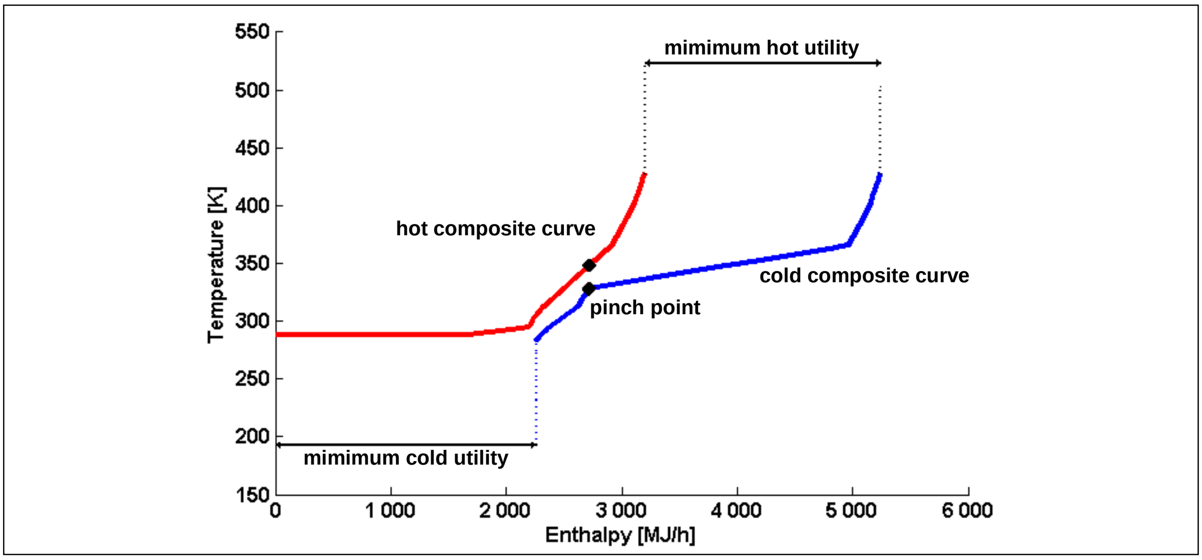

Figure 4.37: Hot and Cold Composite Curves of the Industry Park

Since the heat is available at a relatively low temperature level the integration possibilities are limited. But the heat is available from a liquid stream, the transportation in insulated piping is possible without significant heat loss within the short distances of the considered industry park. Because of the wide stretching road a culvert as an underpass of the street is necessary increasing the costs for this option significantly.

One unit operation for the realisation of identified savings potentials is the heating of the drying air of the fishery net company. The nets are dried in a drying tower which has a temperature of 40 °C at the bottom and as low as 20 °C at the top of the drying tower using an air flow of 6 000 Nm^3/h requiring 52 kWh/h. Assuming a fixed heat capacity of

4.5 kJ/kgK for the distiller's wash and no heat losses a total of approx. 1.5 m^3/h of the distiller's wash are required to reach the necessary temperature. Thus, a fluid-gas heat exchanger (with finned tube and shell) of 60 kW is suggested. By considering the cost for the heat exchanger of around 15 000 €, the cost for the rotary pump of around 1 000 € and the piping[70] of around 160 000 € the integration provides no economic advantage to the current process layout of a simple gas burning heat supply considering savings of approx. 15 000 €/a (cf. Figure 4.36). However, if no culvert would be required assuming the fishery net company at the same side of the road the piping costs would some up to only around 60 000 € . Thus, with rising energy prices the option of interconnecting the process stream may provide a good investment.

4.4.1.3 Discussion of the Application of the Pinch Analysis to Inter-Company Networks

An application of the thermal pinch analysis to a model of an industry park are shown and the difficulties of applying the pinch analysis to an inter-company network of SME are discussed. Not only lack of information regarding the potential partners and insufficient trust concerning the dependency on the partners, but also the high degree of uncertainty concerning the benefits and costs of inter-company concepts and the risk of introducing new bottlenecks in the processes build the obstacles to inter-company networks.

Nevertheless, by using the pinch analysis approach a rapid overall assessment of the possibilities of resource integration is possible supporting the discussion about further cooperation by technical data. However, this integrated approach requires a tight coupling of mass, energy, economic and ecological assessment approaches based on a detailed analysis of the case at hand. Using the pinch analysis as an adequate planning tool, technical solutions are identified and an economic and ecological evaluation of inter-company concepts is enabled. The analysis shows that a close spatial proximity of the various SME and an integration of flexibility or backup capacities is essential for building inter-company networks. Ultimately, a fair distribution of costs and revenues of the inter-company concept is required among the cooperating firms.

[70] Considering a water flow of 1.5 m^3/h, an $40 - 50$ mm pipe with insulation is required. Already in this small scale environment the piping costs prevent an economic use of the available heat. Considering the pipe, mountings, insulation and a culvert, the piping costs sum up to 100 000 € with additional 60 000 € of labour costs for the installation

4.4.2 Production Pinch Analysis

Since the demand of bicycles varies throughout the year, the question arises how the level of production should be chosen to address seasonal changes and by considering dynamic growth the problem must be addressed how to adjust the production accordingly. There are several options available for the reference company: One possibility could be the production of a second product requiring similar operations as the welding, coating and assembly of bicycles. An example would be the welding and coating of bed frames constituting a similar product without seasonal changes as a case study of a Chilean bicycle company shows [Schollenberger and Treitz, 2005]. A second option would be to produce bicycles for different markets with shifted seasons. For example the Chinese bicycle company produces bicycles in the summer (June, July, August), the low season of the US, European and Chinese market, for the Chilean market. Assuming that the shipment takes one to two month the bicycles are available at peak times in spring in the southern hemisphere (October, November, December) especially before Christmas.

4.4.2.1 Discussion of Production Strategies for Seasonal Markets

Different production strategies to supply the required amount of products can be compared. The production planning pinch analysis is based on material balances. In translation of the original thermal pinch analysis the problem is described by first a quantity parameter, such as the temperature level T at which a certain energy flow is available or required, and second a quantity parameter, such as the enthalpy ΔH. The quality parameter in the production planning pinch is the time of production, similar to the *time average models* in the modelling of batch processes. The quantity parameter is the demand of units to a certain time.

In addition to the original production pinch approach strategies for capacity adjustments can be analysed. Thus, different options for the level of production are discussed based on costs, such as investment dependent costs, labour costs, material costs, inventory costs, stock-out penalty costs and costs for capacity adjustments. The assumption is based on the original production pinch analysis [Singhvi and Shenoy, 2002] that an increase of capacity requires a larger workforce and hence results in hiring costs (for example the costs of one man month per worker) and an decrease of production results in lay-off costs (for example the costs of two man month per worker). Hence, the adjustment of the level of production depends on the magnitude on the adjustment.

Similar to the modelling of re-use and re-generation processes in the water pinch analysis reducing the overall fresh water flow rate but generating costs, the adjustment of the production level at the production pinch point reduces the overall level of production resulting in a steeper slope of the production composite curve. Based on the different options in the thermal and water pinch analysis several strategies for the evaluation of the production planning of an production network can be formulated (cf. Table 4.14).

The first three strategies illustrate different ways based on flexibility and costs to comply with the demand composite curve and to supply the required aggregated demand. The *Average Production* strategy and the *Max-Zero* strategy are used benchmarks for the evaluation of the trade-off of the penalty for stock-outs on the one hand to the inventory costs on the other.

Table 4.14: Available Strategies in the Production Pinch Analysis

No.	**Strategy**	**Number Pinch Points**	**Number Capacity Adjustments**	**Possibility Stock-Out**
1	Fixed Production Level with one Pinch Point	1	0	no
2	Variable Production Level with one Pinch Point	1	1	no
3	Variable Production Level with multiple Pinch Points	var.	var.	no
4	Average Production	0	0	yes
5	Max-Zero Strategy	0	1	no

Challenge for the analysis is the determination of the starting time interval for the analysis. In contrast to the thermal pinch analysis in which all heating and cooling requirements are sorted according to their quality parameter temperature and resulting in a theoretical minimal utility target, the sorting of the demand in the production pinch analysis is infeasible. Consequently, the analysis can result in sub-optimal solutions and the results significantly alter depending on the selected starting interval. Here, the beginning of the peak season, which means the highest growth rates, is taken as the starting point of the evaluation.

In the following the bicycle production of the reference company is taken into account and a distribution of the demand for bicycles throughout the year is assumed according to Table 4.15. The five basic strategies for production planning are discussed for the bicycles company (cf. Table 4.14). Since the seasonal increase of demand starts in October it is the starting month of the evaluation. All the assumed cost parameters are provided in the appendix (cf. Table A.6 on page 199).

Table 4.15: Assumption of Distribution of Bicycle Demand in 2004/2005

Month	Units	Month	Units
October 2004	90 000	April 2005	80 000
November 2004	90 000	May 2005	60 000
December 2004	110 000	June 2005	50 000
January 2005	130 000	July 2005	50 000
February 2005	120 000	August 2005	60 000
March 2005	90 000	September 2005	70 000

Figure 4.38 shows the demand composite curve of the production pinch analysis illustrating the aggregated demand in accordance to the months of 2004/2005 starting with October 2004. Furthermore, both strategies with one single pinch point (Strategies 1 and 2) and the average production rate (Strategy 4) are shown.

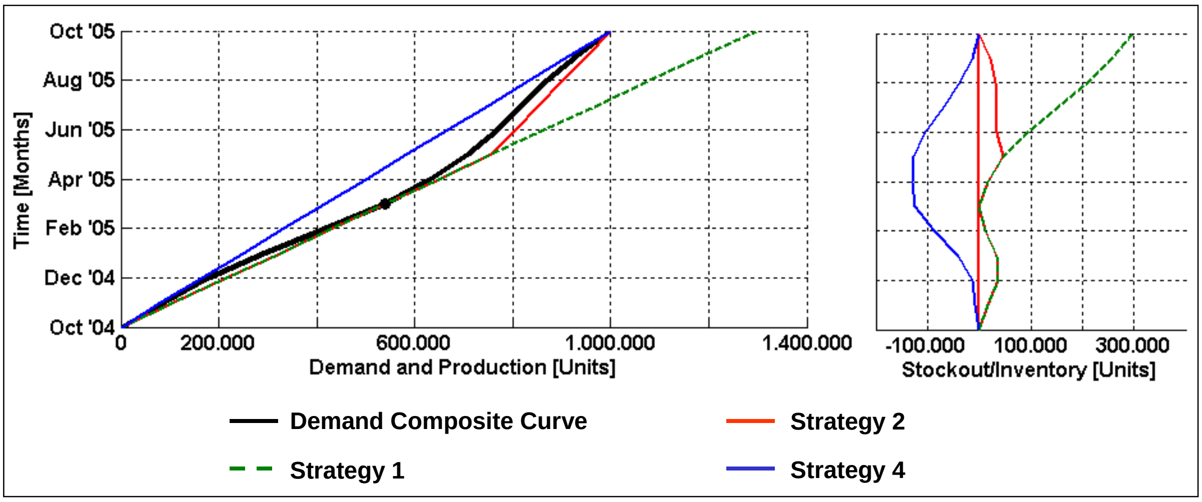

Figure 4.38: Composite and Grand Composite Curves of the Production Pinch with Strategies 1, 2 and 4

Strategy 1 with a fixed level of production requires a production rate of monthly 108 000 bicycles to prevent any stock-outs and total costs of 30.9 million € arise. In Strategy 2 with one capacity adjustment a production rate of 108 000 is suggested in the peak season from October to March and a production rate of 48 000 in the low season from March to September. In this case Strategy 2 generates costs of 22.7 million € and is preferred to Strategy 1 based on the total annual cost for production including the cost for storage and capacity adjustments, i.e. hiring or layoff cost. However, based on the analysis the costs differ significantly due to the high number of units stored in Strategy 1. In addition Strategy 4 is illustrated as an average production rate of 83 334 bicycles per month to fulfil the annual demand of 1 million bicycles. In this case stock-outs are allowed, but are valued as lost business. In this case less equipment is required but due to lost business the overall cost accumulates to 23.5 million € and ultimately this strategy is more expensive in the long run than Strategy 2 distinguishing between high and low season.

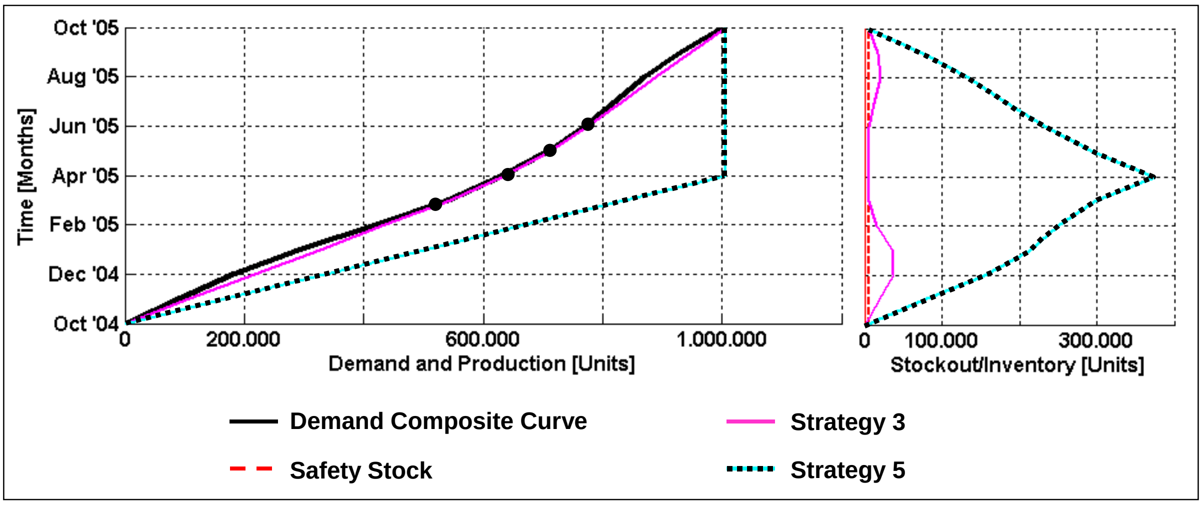

Figure 4.39: Composite and Grand Composite Curves of the Production Pinch with Strategies 3 and 5

Strategy 3 and 5 are shown in Figure 4.39 taking into account a safety stock ΔI_{min} of 5 000 units. In Strategy 3 multiple capacity adjustments are allowed compared to Strategy 2 with only one capacity adjustment. As Figure 4.39 illustrates the production curve closely follows the demand curve by identifying four pinch points. Thus, as in Strategy 2 in Strategy 3 the production rate would be 108 000 bicycles per month from October to March. However, starting in March the production rate would decrease continuously until the start of the new peak season (March: 90 000, April: 80 000, May: 60 000 and June to September 57.500 bicycles per month). Strategy 3 would generate costs of 22.1 million €. As a sensitivity analysis Strategy 5 does not only differ between high and low season, but selects only between full or zero production for each month. Consequently, in Strategy 5 the production rate in the first half of the analysis period per month is 166 667 bicycles from October to April and zero in the second half.

However, the determination of the starting time interval of the evaluation highly influences the results of the analysis[71]. This aspect is roughly discussed in Section 2.1.3.2 on page 26. For the analysis the beginning of the peak season is proposed as the starting interval of the analysis. However, more comprehensive research concerning the time-variance of the results is necessary.

4.4.2.2 Discussion of Production Strategies for Dynamic Markets

The application of the pinch analysis methodology to production planning provides a simple but effective tool for analysing production strategies. By using estimated growths rates and including several periods the analysis supports the aggregated capacity planning of a company in a dynamic market.

Based on the cost parameters the different production strategies can be evaluated. For the analysis minimal and maximal production capacities can be set. For example the bicycle company has a maximal production capacity of 150 000 bicycles per month. Following Strategy 2 with two different production rates, one for the peak and one for the low season, in 2008 the maximal capacity is reached in the peak season, assuming an effective production of 90 % of the maximal capacity. In this case the production rate in the low season can be increased, the production rate of the peak season can be extended by one month, or a capacity extension requiring investment can be realised. By including outsourced production the existing capacity may be sufficient if there exists uncertainty concerning the stability of the growth rates in the comming years.

4.5 Discussion and Conclusions of the Case Study

This case study applies the multi-criteria decision support method for process design and evaluates the overall optimization potential by applying the new methodology to a bicycle company in China. Bicycle production is an important industry sector in China and for the determination of available savings potentials, target values for the bicycle company

[71] An detailed analysis about the starting time interval of the production pinch analysis and the application of the production pinch analysis to different case studies is provided in a diploma thesis by Prisca Borsi ("Supply Chain Management by the Pinch Analysis Approach", Institut für Industriebetriebslehre und Industrielle Produktion, Universität Karlsruhe, 2006)

are identified by the pinch analysis approaches and an overall performance evaluation is demonstrated.

With the advent of more advanced process models and computational power, process integration technologies have gained in importance. The advantage of the pinch analysis can be seen in the determination of the theoretical optimum for a given set of heat and material streams. In the case study, target values were identified for heat integration, water management and solvents recovery using the pinch analysis approach. In addition, the analysis showed how the identified theoretical target values can partly be realised by taking into account basic unit operations. For example, in the case of heat integration a specific heat exchanger is suggested to use the waste heat of the drying ovens to pre-heat the fresh air flow of the drying process of the coating section of the bicycle production. In the case of the water pinch analysis, an ion exchanger or a filter is suggested to regenerate the water of the pre-treatment steps of the bicycle coating. The recovery of the solvents used in the coating application from the gaseous waste stream is evaluated by thermal condensation following the pinch analysis procedure. An detailed economic analysis of the condensation system showed, that an installation highly depends on the possibility to recycle the recovered solvents. For the economic analysis the pinch analysis approach provides figures characterising the fundamental dependencies based on the heat exchanger surface. In a subsequent step a more accurate economic evaluation can be achieved by applying flowsheeting and simulation techniques for the single unit operation. For example, the effect of different temperature gradients within the heat exchanger can be evaluated in more detail. Consequently, by including material properties and unit operations in the analysis of the total system's performance the economic analysis is based on the characteristic mass and energy flows of the system providing an adequate level of detail to inform the selection of a preferred option.

Multi-criteria analysis facilitates the selection of a preferred option by combining the different target values and investigating the overall optimisation potential of different process design options. In addition, the multi-criteria analysis supports the transparent modelling of the decision process by explicitly including preferential information. By clearly visualising the different technology combinations and their relative positions it is possible to evaluate trade-offs and the effect of different environmental priorities. For the case study the analysis by the metric and by PROMETHEE suggests a switch to powder coating instead of the existing solvent-based liquid coating process. In addition to eliminating the solvent emissions in the coating step, the material efficiency can also be improved significantly by recycling the coating powder and using a circulating air system. Because of the geometry of a bicycle frame, large amounts of overspray are generated by using high rotating discs as occurs for the status quo. By using a standard industrial robot the material efficiency can be improved significantly and the manual touch-up is not required any more.

Even though the results of the metric are insensitive to changes of the weighting factor by considering the environmental aspects only, the sensitivity analyses in PROMETHEE reveal that there does not exists a robust solution. The realisation of a specific process design depends in this case highly on the preferential parameters. To evaluate the impact of the different modelling parameters and the uncertainty with respect to the data and even more with respect to the value judgements of the decision maker various new sensitivity analysis have been executed using Monte Carlo Simulation for the preference parameter and an enumeration of all possible preference type combinations of the preference function.

A further advantage of the methodology developed in this thesis stems from the capability to embrace additional considerations as the case study shows. Depending on the special focus of the analysis new elements can be integrated as for example specialised modules for modelling mass transfer processes by the pinch analysis approach or to integrate the capacity or production planning in the assessment. In this way individual technology combinations can be compared based on the results of the pinch analysis approaches and in addition different types of data and preferential uncertainties are addressed in the framework of a multi-criteria analysis.

Chapter 5

Conclusions and Outlook

Improving the resource efficiency of a production network based on detailed process characteristics has a long tradition in chemical process engineering. The required simultaneous consideration of different mass and energy flows such as for example for heat, water and solvents leads to a multi-criteria process design problem which must solved.

One approach to support the analysis of resource efficiency of the underlying process system is the pinch analysis. Originally developed for studies on heat integration it can also be applied to water and wastewater networks, to the recovery of solvents or to analysing product streams for production planning. Using pinch analysis, theoretical consumption target values for the process streams under consideration can be calculated based on the maximal heat, water and solvent reuse. In addition, unit operations are discussed with respect to the realisation of savings potentials.

Combining pinch analyses with different objectives, a Multi Objective Pinch Analysis (MOPA) is applied that takes into consideration economic, environmental and technical process details to identify a resource efficient production method including the development of a process model, the determination of characteristic figures by applying pinch analysis and a subsequent evaluation. For the comparison of different technological options, a metric for resource efficiency is developed to determine a measure for the possible savings potential. Together with other criteria the outranking multi-criteria analysis method PROMETHEE is applied and new sensitivity analyses are introduced. By using Monte Carlo Simulation together with Principal Component Analysis, the uncertainty associated with the decision can be evaluated in a comprehensive sensitivity analysis.

The developed multi-criteria decision support model is applied to a case study of a bicycle producing company. The case study begins by investigating the serial coating of bicycles in China. The main question to be answered is if it is worthwhile to modify the paint application process in order to increase the resource efficiency. Additionally, the context of the company within an industry park is investigated. In a model of an industry park the optimal reuse of mass and energy flows into an integrated approach is assessed with special focus on the applicability for smaller production processes. By applying the developed methodology to a series of case studies[72], the applicability to support practical research questions is demonstrated.

5.1 Conclusions of the Pinch Analysis Methodology

The field of process integration aims at assessing entire production processes with an integrated approach to the analysis, synthesis, and retrofit of process plants by integrating mass and energy flows that minimise both costs and waste. Pinch analysis is a mature design and optimisation approach within process integration based on mass and energy flows. The characteristic principle of the approach is to view a production network as one interconnected system of unit operations which aims at optimising the overall performance by including new unit operations, introducing new connections between streams and closing material cycles. Thus, it is possible to define theoretical optimal target values based on physical laws and chemical engineering principles.

The details of process designs that would realise the established performance targets are however addressed by the pinch analysis approach only to a limited extent. The pinch analysis is useful for conceptual process evaluation and for definition of performance targets before the next step of more detailed analysis using flowsheeting and simulation. Only through flowsheeting and simulation it is possible to consider process specifics in detail and evaluate the performance, operability and flexibility of techniques based on different process designs. Whilst specific extensions to the original pinch analysis are available to consider the special requirements of certain operations (for example mixing and interception of water and wastewater process streams or the scheduling of batch processes) the strength of the pinch analysis is to leave the specific design and thus determine theoretical target values.

[72] In the context of this thesis only a selection of different case studies which are analysed in the framework of the PepOn project are presented. Further case studies from Chile and China and applications to inter-company networks can be found in the final report of the PepOn project [Geldermann et al., 2006c]

Besides the application of the pinch analysis to production planning, there exist several applications of the pinch analysis methodology to mass and energy flows. Three different major applications are identified:

- *Thermal Pinch Analysis:* The basic idea of the thermal pinch analysis is a systematic approach to the minimisation of lost energy in order to come as close as possible to a reversible system. In its first step the pinch analysis yields the best possible heat recovery at the thermodynamic optimum. Further recovery can only be achieved by changing conditions or structures of the investigated system. Thus, the pinch analysis requires the combination of hot and cold process streams to composite curves and the description of the respective temperature-enthalpy relationships. Additionally, a minimum temperature gradient ΔT_{min} must be set representing the driving force of the heat transfer. The result of the pinch analysis is the energy savings potential for the considered set of processes.

- *Water Pinch Analysis:* Furthermore, pinch analysis can also be applied to calculate water and wastewater savings. Instead of considering temperature-enthalpy relationships the water pinch regards concentration-mass load curves. All streams of the investigated system are combined to a limiting composite curve describing the "worst" water quality acceptable. The freshwater curve describes the water supply of the system. The slope of the curve is a measure for the flow rate. The water supply and limiting curve match at the pinch point and the resulting slope defines the minimum water flow rate needed.

- *Solvents Pinch Analysis:* Besides heat exchange and water management, another application of the pinch analysis is for solvents or multi-component solvents since their separation from waste gas is usually carried out via thermal condensation. This permits a translation of organic solvent reclamation into a heat exchange problem. By using phase diagrams the targeted VOC concentration can be described by temperatures of the gaseous waste stream. The application of solvents pinch analysis is used to find the most cost-effective solution for the condensation of solvents from gaseous emissions.

The key question, however, is the realisation of the identified target values. The catalogue of Best Available Techniques (BAT) provides a pool of available unit operations and technology combinations to suggest unit operations to realise the identified savings potentials or emission reductions. These descriptions comprise key figures on energy and material consumption, as well as information about the caused impact. Additionally, economic aspects, for example operating costs and investment, have to be taken into account considering country-specific parameters and pay-off periods.

The presented pinch analyses are applied to individual energy and material flows in large technical production facilities of the process industry, without simultaneous optimisation of material and energy flows. Thus, the extension of these methods for inter-company mass and energy flow networks for small to medium sized companies as described in this thesis expands the field of application of the pinch analysis. In particular, the pinch analysis provides insights in the growing number of industry parks especially for developing and industrialising countries. By combining the three pinch analysis approaches with multi-criteria analysis design recommendations for intra- and inter-company production networks can be systematically evaluated, negative environmental effects can be reduced permanently and critical points in the production network can be identified.

The case study on industrial bicycle coating in China demonstrates the application of the methodology. Individual target values for the use of energy, consumption of water and recovery of solvents are determined based on the pinch analysis and different unit operations are discussed concerning the realisation of the individual savings potentials. In this way different process design options are characterised by several criteria, such as for example the available possibilities for heat integration or water reuse for the different options.

5.2 Conclusions of the Multi-Criteria Approach

One of the main challenges following the determination of the target values is the evaluation of alternative techniques taking into account strengths and weaknesses according to their environmental and economic performance. However, since no single alternative may be the best in all criteria there exist incomparabilities. In this context multi-criteria analysis aims at identifying efficient alternatives and reducing incomparabilities, since a comprehensive evaluation of different technological options requires the simultaneous consideration of different mass and energy flows and economic performance.

The definition of resource efficiency from an applicability point of view is complex because various parameters must be considered and representative ones must be selected. This is especially true for environmental resources, in which the market prices do not reflect full costs. Therefore, the idea is to understand waste not as material to be discarded, but as a potential future resource. Thus, the material properties and available processing and recycling technologies determine the value of a resource.

Resource efficiency as the overall objective for the assessment is broken down into a multi attribute optimisation problem for energy-, water- and solvent-process streams. The target values for these resources are identified using pinch analyses and the weighting parameters for the resources are chosen according to the decision maker's preferences. Consequently, various aspects of the definition of value judgements in a multi-criteria analysis must be discussed.

A relative efficiency measurement by multi-criteria analysis is used in this thesis to resolve incomparabilities and to compare different techniques in an integrated technique assessment. Two different multi-criteria methods are applied:

- *Metric:* A metric is introduced as a multi-criteria assessment tool to illustrate trade-offs and compensation ratios where incomparabilities are resolved by a distance measure and weighting factors. The metric for resource efficiency provides a performance measure for the possible savings potential and for the savings ultimately realised. A set of optimal solutions is delivered by the pinch analysis approach, which spans a domain of to be considered technology combinations relative to the current status. The specific technologies implemented in the subsequent process design eventually define the savings being realised. As a distance measure a modified Euclidean norm is incorporated considering the weights for the different resources. Other norms can be included to evaluate the basic modelling parameters.

- *PROMETHEE:* The outranking approach PROMETHEE is applied for an integrated technique assessment and preferential information is modelled by weighting factors and preference functions based on pairwise comparisons. PROMETHEE is applied to discuss the ranking of the alternatives and the relative strengths and weaknesses of the alternatives reflected in their profiles. Furthermore, comprehensive sensitivity analyses for preferential and data uncertainties are the major contribution of the Multi Objective Pinch Analysis.

The potentials and driving forces, i.e. gradients, in the material and energy system are taken into account, and the decision support system helps to transparently model the attribute data for the comparison and the involved subjective preferences of policy makers or business managers. There is always a subjective element in the decision, which especially becomes obvious not only with respect to the weighting factors, both in the application of the metric and of PROMETHEE, but also in the definition of the norm in the metric or the definition of a preference function in PROMETHEE. This thesis concentrates on the production processes, in preference to the personal / psychological side of decision making in SME as investigated in organisational theory. The influence of the uncertainty in the preferential parameter on the results is investigated by comprehensive sensitivity analyses.

Parametric sensitivity analyses are used to investigate the influence of the preferential parameters of PROMETHEE to the overall results and Monte Carlo Simulation (MCS) is used to investigate simultaneous changes in all parameters. The Principal Component Analysis is expanded by MCS, in order to investigate uncertainties in all attributes. However, the analysis of the principal components not only furthers the evaluation of the current decision problem and helps to assess if the selection of criteria sufficiently describes the decision problem, but furthermore supports a technology management by illustrating potentials for unit operations or gaps in available technologies. Like in the concept of ecological product development a design for environment is stipulated for process innovation by multi-criteria analysis.

This thesis shows the application of Multi Objective Pinch Analysis to different mass and energy flows. Target values are determined by applying the pinch analyses with a special focus on economic parameters. The different target values are combined with a multi-criteria analysis for the identification of a resource efficient process design option. This is demonstrated by a case study of industrial bicycle coating. Several new sensitivity analyses are applied for preferential and data uncertainties.

5.3 Outlook

The topics of sustainability, resource efficiency and cleaner production are currently receiving increasing attention. Reaching further than just pollution prevention, they aim for a holistic approach. Therefore, a multi-scale, consistent and systematic approach is necessary to analyse industrial production networks. In this thesis an approach combining pinch analyses with multi-criteria analysis is developed and applied to a case study. Since Multi Objective Pinch Analysis is a novel approach to a systematic assessment of production networks, many potential fields for future research are opened:

The fundamental idea of the pinch analysis approach is to identify target values in a system's assessment. New fields of application for the methodology based on the engineering principles to other fields of research will further the interdisciplinary research. The economic and environmental evaluation of techniques is highly complex and systematic tools are required. Thus, the pinch analysis can provide the base for incorporating different fields of expertise thereby generating new insights.

It is necessary to overlay the approach of process integration and network design with the multi-criteria assessment to gain sustainable improvements and to understand environmental dynamics in an intra- and inter-company production network in a systematic way. Improved computational modelling will enable this progress and information will be available to the entire enterprise for the resource planning. The performance of a process is modelled and simulated by indicators and the design alternatives are evaluated by a number of different criteria. In this field new attributes can be included, such as flexibility of the process design, labour utilisation or risk minimisation in order to reflect various aspects of a cleaner production strategy.

Furthermore, aspects addressing the organisation of inter-company production networks within industry parks must be included in the analysis taking into account the planning horizons of the individual companies.

In addition the aggregation procedure in multi-criteria analyses can be further evaluated based on the impact of different norms on the performance indication of different alternatives and by incorporating additional sensitivity analyses concerning rank stability regarding limit values for value functions or the uncertainty level for the distinguishability analysis. For example, it would be useful to know up to which uncertainty level the alternatives can be distinguished from each other and which criterion is the most sensitive with respect to data uncertainty and requires more accurate data. Furthermore, aspects concerning group decision making must be addressed in the context of process design and how a common understanding can be enhanced in an inter-company setting.

Cleaner production and resource efficiency are key elements of global environmental policy and the question must be addressed how economic growth and environmental performance can be harmonised. Based on the experiences from the case studies in China and Chile an understanding of the problems encountered in emerging and developing industrial nations is achieved and as a result, specific suggestions for the modification or further development of Best Available Techniques for utilisation in the other countries can be implemented.

The methodology developed in this work is robust to encompass the application of the pinch analysis approach to different mass- and energy flows and to identify meaningful targets characterising a production system and enabling its assessment by a multi-criteria analysis considering data and preferential uncertainties.

Chapter 6

Summary

In order to improve the performance of a production process, a detailed mapping of the mass and energy flows is necessary and it is important to understand which process characteristics of the design are the main drivers of its impact on the resource efficiency. Therefore, a quantification of effects and a consistent, systematic approach to optimise the overall system's performance are necessary to support the decisions in process design striving for the best utilisation of process streams considering multiple criteria. The aim of multi-criteria decision support for process design is to identify savings potentials and to create innovative process designs by considering techno-economic relationships and by addressing questions concerning environmental and safety standards in their country-specific context and priorities.

Process integration is proposed as the systematic approach for characterising process design options (*Chapter 2*). Specifically, pinch analysis is used to identify theoretical targets prior to the development of a specific design. By applying the classical thermal pinch analysis, theoretical thermodynamic minimal target values for heating and cooling utilities are determined. The theoretical minimum target depends on the minimal temperature gradient ΔT_{min} between the cold and hot process streams and defines the possible savings potential with respect to energy. However, there exists a trade-off between the savings in operating costs for the utilities and the investment in the heat exchanger requiring an economic analysis.

The pinch analysis approach has also been successfully applied in the field of water and wastewater management because its principles can be transferred to the analysis of water consumption. The goal of the water pinch analysis is to reuse water as efficiently as possible, while adhering to the requirements of the process steps. Target values can be identified based on minimum fresh water consumption by analysing mass load vs.

concentration relationships. Since unit operations with an unchanging mass load of the water stream, for example a cooling operation, can only be mapped with difficulty by the concentration vs. mass load, different approaches coexist. For example the analysis on concentration vs. flow rate diagrams takes the water quantity as the general basis to identify the water savings potential or as another example the analysis based on stream mapping diagrams focuses on identifying different recycling possibilities of single streams rather than constructing composite curves. The fundamental difference between the thermal pinch analysis and the water pinch analysis lies in the definition of the quality of a stream since the single quality parameter in a heat integration analysis is the temperature, whereas in a water pinch analysis the water quality is characterised by several parameters. Thus, single and multi parameter approaches have been developed for the water pinch analysis. However, as in the thermal pinch analysis, a trade-off between the water consumption and the investment in water regeneration installations or water recycling techniques exists.

In addition, the pinch analysis can be applied in the field of gaseous emissions containing organic solvents by thermal condensation. By using concentration-temperature relationships it is possible to translate the target concentration of the solvents in the waste gas into a required endpoint temperature of condensation to which the waste gas must be cooled down. The theoretical target value with respect to the solvent emission is zero. Consequently, an economic analysis is necessary for evaluating characteristic figures for the reclamation of organic solvents using thermal condensation. A trade-off between operating costs for the cooling, the value of the solvents recovered and the required investment can be observed.

The conclusion of Chapter 2 is that it is the strength of the pinch analysis to determine target values for individual process designs by focussing on the entire system's performance in a systematic and consistent way by applying process engineering principles. This allows each alternate process design to be compared to the theoretically best target. The economic selection of an appropriate technology is based on the technical requirements. Therefore, a process-based, integrated methodology which considers the different available unit operations is developed. The approach is used to assess the techno-economic-environmental optimisation potential in chemical processes based on interdependencies of process streams.

Since unit operations interact in complex ways and have a major impact on the overall system's performance, the question must be addressed how to combine the individual target values for the use of energy, consumption of water, and recovery of solvents in one overall approach (*Chapter 3*). The techno-economic assessment on the basis of detailed process characteristics requires the simultaneous consideration of different mass and energy flows which thus leads to a multi-criteria problem. A multi-criteria approach is used to integrate and compare several techniques of the identified optimisation potential in chemical process design. The newly developed Multi Objective Pinch Analysis (MOPA) consolidates the different individual targets into one overall assessment of resource efficiency of process design.

First, a metric for resource efficiency is developed providing a distance measure for a relative efficiency assessment of different process design options. By incorporating an Euclidean norm modified by weighting factors, the impact of different priorities with respect to the different mass and energy flows can be analysed. Consequently, the impact of preferential parameters on the overall results become apparent.

Second, the outranking approach PROMETHEE is applied as a different possibility for the simultaneous consideration of the various criteria. Outranking approaches are based on relative differences in the individual performance characteristics with respect to the different criteria. Since the complexity of multi-criteria decisions requires comprehensive analyses to show the impact of the decision makers' modelling various new sensitivity analyses for PROMETHEE are presented and discussed to evaluate preference and data uncertainty. Therefore, Monte Carlo Simulation and Principal Component Analysis are combined.

The developed Multi Objective Pinch Analysis is applied to a case study, which demonstrates the features of the preceding chapters and the potential of the methodology *(Chapter 4)*. The use of energy, the consumption of water, and the generated solvent emissions are the major relevant mass and energy flows in the coating step of the bicycle production. There is a special focus on the application of the methodology to intra- and inter-company production networks of small and medium sized enterprises.

The case study shows for example that there exists a demand of hot utility for drying the coating of the bicycle frames. By reusing the hot waste heat of the drying ovens to pre-heat the fresh air for the drying process the total demand of hot utility can be reduced by heat integration. In comparison to the theoretical thermodynamic minimum the optimal economic target is determined.

In the bicycle production the water consumption can be almost solely traced back to the pre-treatment and the coating application. But the analysis showed that it is difficult to find a common key contaminant required by a single parameter analysis. The conductance of the water is selected as the quality parameter of the water pinch analysis for the pre-treatment steps of the bicycle coating in the case study. By including regeneration and recycling processes the theoretical water target value can be determined and different characteristic values can be identified for different process design options.

The solvents pinch analysis is applied for the gaseous emissions containing organic solvents by thermal condensation. Since the theoretical target value with respect to the solvent emissions is zero the economic analysis is the focus of the solvents pinch analysis. As the economic analysis for the case study of the bicycle company shows, the results depend highly on the value of the recovered solvents. If the recovered solvents from the waste gas of the drying process by thermal condensation can be reused directly in the coating application, the installation of a condensation system provides economic advantages. Nevertheless, in the case study the reuse of the recovered solvents is limited and due to the low solvent concentration low temperatures must be reached. The case study showed that the solvent emissions of the status quo can be considerably reduced by including a condensation system.

A multi-criteria approach is used to integrate the three target values determined by pinch analyses and to compare several process design options by MOPA. Four different technique combinations are discussed with respect to the coating application of the bicycle in comparison with the status quo: *(1)* switch of the coating material to coatings with lower solvent content, such as waterborne basecoats, *(2)* installation of a thermal incinerator, *(3)* condensation system and *(4)* switch to powder coating. Besides the quantitative and qualitative data, preferences have to be taken into account in order to rank the different options.

By applying the resource efficiency metric, a relative efficiency assessment illustrates the impact of different priorities with respect to the different mass and energy flows. The analysis with the metric suggests a switch to powder coating based on the highest resource savings potential of 86 % realised followed by the installation of a thermal incineration system with 77 %. A switch to waterborne basecoats realises 58 % and a condensation system 45 %. However, the savings ultimately realised are determined after the implementation and start-up of the modified process.

The analysis of the different mass and energy flows including operating costs and investment with PROMETHEE also suggests a switch to powder coating. A switch to waterborne basecoats and the installation of a condensation system are found to be incomparable based on the inherent strengths and weaknesses of the two technique combinations. The installation of a thermal incinerator is effective in the reduction of solvent emissions in the waste gas. By including the operating costs and the investment in the analysis all other options are preferred because of the high required investment for a thermal incinerator. In addition, the analysis supports the modelling of preferential parameters for the selection of a process design option. By sensitivity analyses the impact on the result is evaluated with respect to the inter-criteria preferences, i.e. the priorities between the different criteria, and of the intra-criteria preferences, i.e. the value judgement of the decision maker with respect to differences in the process characteristics regarding only one criterion. The sensitivity analysis for the intra-criteria preferences illustrate that the ranking of the different process design options depends highly on the modelling parameters for this case study and provides decision support for the determination of the preference parameter modelling.

Furthermore, the pinch analysis approach can be used not only within a single company, but also in inter-company networks of several small and medium sized companies. Implications from a technical point of view for the application of the pinch analysis to an industry park include considering the costs for piping, insulation and the definition of process requirements to enable an interconnection of process streams. The case study shows the installation of a heat exchanger to reuse the waste heat of one company in another one. By applying the pinch analysis to inter-company networks, potentials for future collaboration can be identified and target values can be determined. In addition, the pinch analysis can be applied to product streams for the evaluation of seasonal markets, such as for example the bicycle production. This production pinch analysis can then be used to evaluate the trade-off between inventory costs, stock-out costs, production costs and investment. Different production strategies can be compared, for example for the bicycle company a lower production rate in the low season and a higher production rate in the peak season.

Techno-economic and environmental assessment of process design for various targets by pinch analyses including country specific economic parameters and perceptions is achieved in the multi-criteria evaluation. By incorporating multi-criteria analysis in the early process design stage it is possible to bring together interdisciplinary knowledge from various fields of expertise. The development of innovative concepts requires the support of the different departments involved and the transparency and communication of technical process data and preferential information is enabled by decision support through multi-criteria models. Thus, the subjectivity to certain aspects is addressed openly, such as for example the time until an investment must be paid off or the selection of considered criteria for evaluation. This results in a consistent approach for process optimisation to reduce both energy and material loss in the production process.

This thesis shows the application of different pinch analyses combined with a multi-criteria analysis to the identification of an appropriate process design option for industrial bicycle coating. Multi Objective Pinch Analysis (MOPA) consolidates the different individual targets into one overall assessment of resource efficiency. Therefore, the target values can be combined to one formalised savings potential using a metric for resource efficiency or can be compared in an outranking multi-criteria approach. By applying new sensitivity analyses for preferential and data uncertainties using a combination of Monte Carlo Simulation and the Principal Component Analysis, the evaluation of process design options allows a deeper understanding of the effects of the different modelling parameters on the overall results.

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Appendix A

Data of the Case Study

Table A.1: Coefficients of Heat Capacity (Gas)

solvent name	A_g	B_g	C_g	D_g	E_g
m-Xylene	$-1.26 \cdot 10^{01}$	$5.66 \cdot 10^{-01}$	$-2.80 \cdot 10^{-04}$	$2.03 \cdot 10^{-08}$	$1.72 \cdot 10^{-11}$
Ethyl Acetate	$7.24 \cdot 10^{00}$	$4.07 \cdot 10^{-01}$	$-2.09 \cdot 10^{-04}$	$2.85 \cdot 10^{-08}$	0
Toluene	$-2.05 \cdot 10^{01}$	$4.80 \cdot 10^{-01}$	$-1.64 \cdot 10^{-04}$	$-8.87 \cdot 10^{-08}$	$5.44 \cdot 10^{-11}$
Benzene	$-6.07 \cdot 10^{01}$	$6.33 \cdot 10^{-01}$	$5.80 \cdot 10^{-04}$	$2.80 \cdot 10^{-07}$	$-5.49 \cdot 10^{-11}$

Table A.2: Coefficients of Heat Capacity (Liquid)

solvent name	A_l	B_l	C_l	D_l
m-Xylene	$-2.00 \cdot 10^{02}$	$3.06 \cdot 10^{00}$	$-8.26 \cdot 10^{-03}$	$7.93 \cdot 10^{-06}$
Toluene	$-5.63 \cdot 10^{01}$	$1.77 \cdot 10^{00}$	$-5.19 \cdot 10^{-03}$	$5.49 \cdot 10^{-06}$

Table A.3: Coefficients of Vapour Pressure Curve

Solvent Name	**A**	**B**	**C**	**D**
m-Xylene	$-1.01 \cdot 10^{01}$	$-7.95 \cdot 10^{03}$	$8.33 \cdot 10^{01}$	$5.94 \cdot 10^{-06}$
Toluene	$-8.80 \cdot 10^{00}$	$-6.92 \cdot 10^{03}$	$7.41 \cdot 10^{01}$	$5.75 \cdot 10^{-06}$

Table A.4: General Process and Model Parameters for the Solvents Pinch Analysis

Variable	**Value**	**Remarks**
lower bound of temperature range	150 K	end point for the calculation of concentration diagram etc.
upper bound of temperature range	321 K	equivalent to the supply temperature of the waste gas stream
approximation temperature interval	0.1 K	control parameter for linearisation
system pressure	0.1 kPa	required for the calculation of saturated concentrations
flow rate	0.1 Nm^3/h	used for the calculation of energy flows per unit time
minimum ΔT_{min}	2 K	minimal driving force for heat exchange
maximum ΔT_{min}	20 K	maximal driving force for heat exchange
T_{humid}	278 K	end temperature for the dehumidification
VOC-emission	1 kgC/Nm^3	threshold of VOC emission (upper bound of condensation temperature)
T_{sysmin}	278 K	minimal operating temperature of the whole system

Table A.5: Preferential Parameters Multi-Criteria Analysis (Uncertainty Level: ? Columns)

Criterion	w_j^-	w_j	w_j^+	**t**	**p**	**?**	**q**	**?**	**s**	**?**
Energy	10 %	15 %	20 %	6	17.47	10 %	3.86	10 %	8	10 %
Water	10 %	15 %	20 %	6	0.19	10 %	0.05	10 %	0.09	10 %
Solvents	15 %	20 %	25 %	6	237.83	10 %	51.42	10 %	116.50	10 %
Investment	15 %	20 %	25 %	6	563 635	10 %	81 698	10 %	306 000	10 %
Costs	25 %	30 %	35 %	6	18 337	10 %	2 809	10 %	10 406	10 %

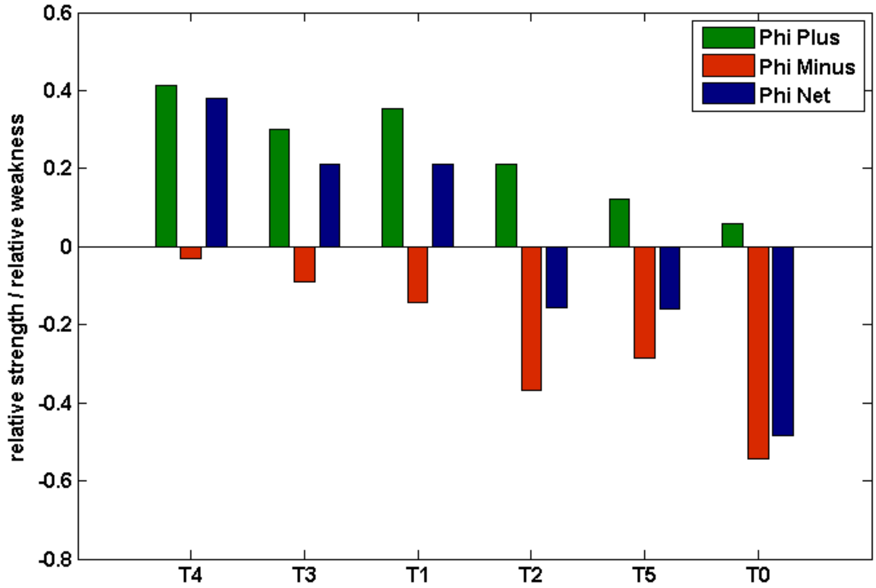

Figure A.1: Aggregated Outranking Flows with Additional Alternative Thermal Incinceration T_5

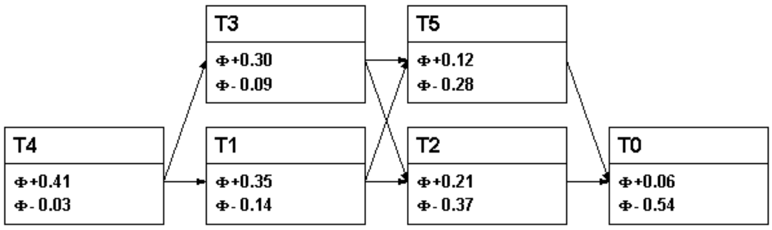

Figure A.2: PROMETHEE I Ranking with Additional Alternative Thermal Incineration (T_5)

Table A.6: Parameters Economic Evaluation Production Pinch Analysis (data partly from [Singhvi et al., 2004]

Variable	**Value**
production time per bicycle	1.03 h/unit
labour costs	435 €/month
material costs	9.50 €/unit
production costs	27 €/unit
stock-keeping cost rate	20 %
selling price	33 €/unit
hiring costs	206 €/worker
layoff costs	340 €/worker

Table A.6: Parameter Economic Evaluation Production Pinch Analysis (cont.)

Variable	**Value**
capital demand	450 €/unit
ratio investment depended costs	17 %

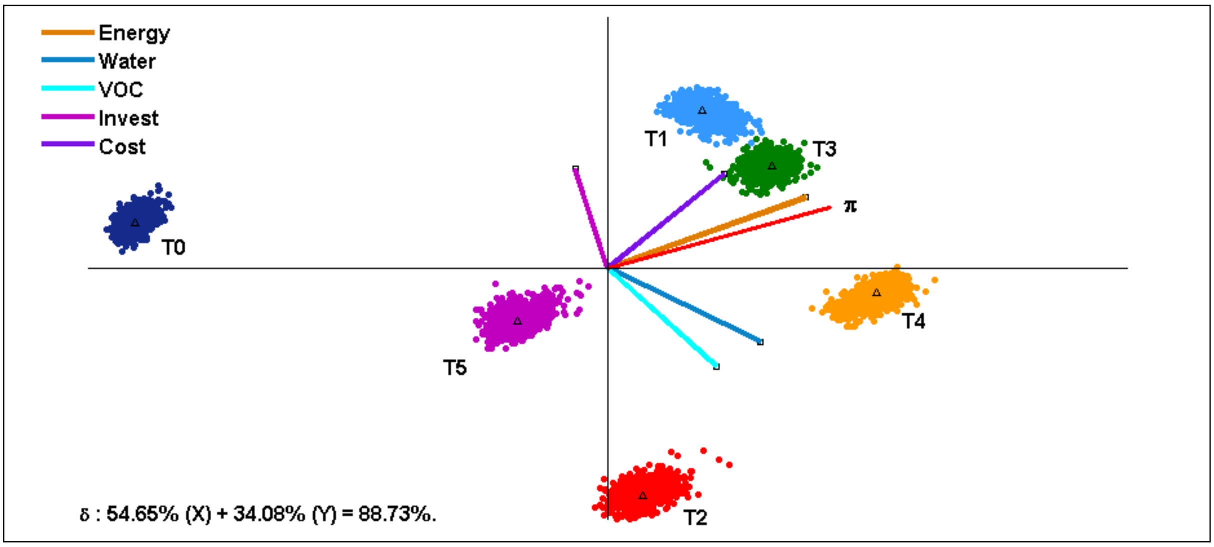

Figure A.3: Distinguishability Analysis with Additional Alternative Thermal Incineration T_5

Intra- and inter-company production networks have gained increased importance in developed and industrialising countries. By reusing waste of industrial sites as a valuable input within the production network, material cycles can be closed and resource efficiency can be improved.

In order to improve the performance of a production process, a detailed mapping of the mass and energy flows is the basis to understand which process characteristics are the main drivers for resource efficiency. Therefore, a quantification of effects and a consistent, systematic approach to optimise the overall system's performance are necessary to support the decisions in process design striving for the best utilisation of process streams considering multiple criteria.

Thus, the objective of this dissertation is to develop an integrated multi-criteria decision support model for production process design.

The developed methodology is applied to a case study of the industrial bicycle coating, which demonstrates the features and the potential of the method. The use of energy, the consumption of water, and the generated solvent emissions are the major relevant mass and energy flows in the coating step of the bicycle production. Therefore, the target values including operating costs and investment are combined to one formalised savings potential using a metric for resource efficiency and are compared using an outranking multi-criteria approach.

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