

**SUSTAINABLE CHEMICAL
PROCESSES AND PRODUCTS**

SUSTAINABLE CHEMICAL PROCESSES AND PRODUCTS

NEW DESIGN METHODOLOGY AND DESIGN TOOLS

Proefschrift

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Voor mijn ouders

לִיהוָה הָאָרֶץ וּמְלוֹאָהּ תִּבְּל וְיֹשְׁבֵי בָּהּ

De aarde en haar volledige inhoud is van de Heere God
Van Hem is de bewoonde wereld en al haar inwoners
(Vrij naar Psalm 24)

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Chapter 1

INTRODUCTION

Summary *The main question dealt with in this thesis is: how can a trained chemical engineer develop a conceptual design of a chemical process plant in such a way that the final result clearly contributes to sustainable development. While reading this question, two main subjects come in mind: a) what is a conceptual design of a chemical process plant and what is the task of the chemical engineer in this kind of design, and b) what is sustainable development and how can the contribution to sustainable development be expressed and measured. In this Chapter, these questions are elaborated to hypotheses, and the structure of this thesis is described.*

1.1 Importance of the subject

The point of departure of this thesis is the conviction that the current chemical industry, as well as society in general, is not sustainable. Innovations and developments of processes are still too often hazardous to the environment, or they are only focused on economic growth. In addition to posing hazards, these innovations are themselves vulnerable to societal changes and demands (e.g. rapid changes in legislation). It really is a challenge to implement inherently environmentally friendly and sustainability considerations during the current process design practice.

In this thesis the incorporation of sustainable development into the chemical engineering practice is discussed. This leads to the following main question of this thesis: *how can a trained chemical engineer design a chemical process plant or a chemical product in such a way that the final result contributes to sustainable development*. While reading this question, two main subjects come in mind: a) how can the design of chemical process plants and chemical products be described and what is the task of the chemical engineer in that, and b) what is sustainable development and how can an engineering contribution to sustainable development be stimulated and evaluated.

1.1.1 The need for sustainable development

From the early 1960s it became clear that human society can have an irreversibly disturbing effect on the environment and that fast economic growth of mainly richer societies can obstruct the necessary increases in welfare of mainly poorer societies. Many problems that have occurred during the last 40 years would seem to have been avoidable. But they did occur because lack of management or lack of knowledge initiated adverse developments, while blocking other desirable developments.

This perception led to discussion about a kind of development that is not only focused on economic growth, but also on the development of a better society that maintains itself in balance with nature. Such a kind of development is defined as *sustainable development*. Firstly defined by a UN-report *Our Common Future* (World Commission on Environment and Development 1987), but later elaborated upon by an enormous number of publications from almost every societal actor. In this thesis, this whole amount of opinions, visions, and discussions is called *the sustainability debate*. Chapter 2 deals with the main items of this debate and structures its relevance to the chemical process industry.

1.1.2 The role of the chemical engineering discipline

The field of chemical engineering plays an important role in the debate on sustainable development. Mainly for two reasons: 1) the production of chemical process plants contributes greatly to the national income and their products are absolutely essential to a modern society; thus, the development of society is dependent on the development of the chemical process industry and *vice versa*. 2) Many known environmental problems can be linked directly to the operation of

chemical processes or the use of chemical products and resulting waste streams to soil, water, and air. Also the analysis of such waste streams and their avoidance belongs to the field of chemical engineering.

Sustainable development has to do with large scales and integral approaches, which involves the character of process design methodologies. Nowadays no general integrative design methodology exists for chemical process design, and there is no clear overview of engineering criteria for sustainability. To order to be able to apply the concept of sustainable development in practice, it is necessary to influence innovation in the chemical engineering field.

1.1.3 *Scientific challenge of this research*

The scientific challenges of this research are formulated as follows: i) only little is known about structured methodologically designing of chemical processes, thus the development of a general design methodology for the conceptual process design phase is indeed relevant, ii) practical cases are elaborated, which can be useful for industry in that they illustrate the use of the above-mentioned methodology, iii) translation of vague and broad societal consideration into concretely defined engineering criteria, guidelines or principles, is necessary; this can also useful for other engineering disciplines, iv) the combination of concrete criteria describing sustainable development and the to be developed methodology will deliver an onset for a design methodology, in which the optimal solution is a sustainable chemical process.

In the remaining part of this Chapter these statements are made more explicit by the formulation of hypotheses and the presentation of a plan of approach.

1.2 **Goal and demarcation**

The goal of this research is the development of a methodology to implement the theme of sustainability in the conceptual process design phase of chemical process innovation. From this goal description, it can be said that this Ph.D.-research consists of five parts, see also Figure 1.1: I) description and application of the theme of sustainability, II) study of design methodologies, III) integration of I and II by translating social issues into technological problems, IV) validation of the model by case studies, V) presentation results in a dissertation, articles, on conferences, etc.

This research takes place within the discipline of chemical engineering and, more specifically, in the field of *process systems engineering*. This field is characterized by a scientific approach to the design of chemical processes. From a technological viewpoint, this research is focused on *design tools* that can combine energy and mass in a sustainable way to produce a sustainable product. More philosophically, it deals with the development of a *general design methodology* that enables and improves the relation between technology and societal development. The latter is the focal point of this research.

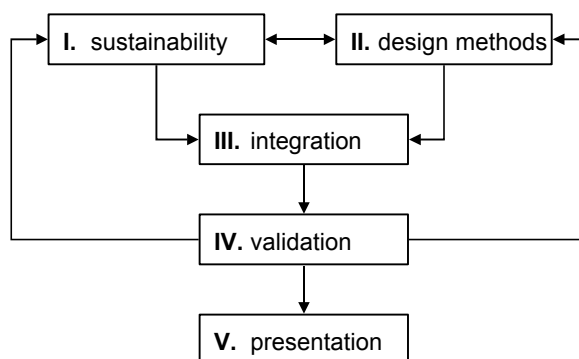


FIGURE 1.1 OVERVIEW OF THE RESEARCH STEPS

1.2.1 Restrictions to the debate on sustainability

The goal and scope of this research is very broad, especially since it is related to the sustainability debate. So a demarcation is very important, and the following restrictions are considered: i) this research considers the sustainable development debate in general; this makes it possible to advance general remarks on the debate, but it is not the goal and scope of this research to contribute directly to this debate, ii) this research deals with the sustainable development of chemical engineering in particular; this is important in order to keep the technological suggestions in a single discipline. Other engineering disciplines, like mechanical engineering, industrial design, architecture etc. are not taken into account directly. Although multi-disciplinary work is essential for the achievement of sustainable development, only the professional background of the author, chemical engineering, is considered, iii) many disciplines are essential for any research on sustainable development, like policy, economics, environmental sciences, social sciences, etc. In this research, their relations to technology or working principles are not considered. Only valuable results from other disciplines are introduced if necessary for the consistence of this research. This is elaborated below.

From experiences during this research, it appears that it is very important to be aware of the pitfalls accompanying this kind of research on sustainability and engineering. Those pitfalls are related to *policy*, *rebound-effect*, and *radical sustainability*

- *Policy pitfall*; many solutions in the field of sustainable development have a societal, political or economic character. Although integration of different disciplines is very important in reaching sustainability, in this thesis a strict distinction is made between technological and political research. This thesis is about the role of engineers and their design skills; it is not about the management that can guide them.
- *The rebound-effect*; the rebound-effect relates to the phenomenon that by making a product or process more sustainable it becomes more attractive or more useful, with the net result that it causes more rather than less environmental damage. Some people state that sustainable development is

development that is not hindered by natural limits and thus allows unlimited growth. In that case it can easily be seen that the net effect of sustainable technological development on the environment would be harmful. It is probably very difficult to create principles that ensure benefit to the environment, society and technology and also ensure prevention of negative effects, but this very goal is one of the starting points of this research.

- *No deep and no radical sustainability*; it is not possible at this moment to speak of a real sustainable chemical process; every contribution followed from the results of this thesis can at best be seen as a more sustainable technology. Although the author also has his ideals and future dreams, he does not want to throw away what already has been gained. So the vision on sustainability presented in this thesis is very moderate and at all times aims at reaching win-win situations, this means that deep or radical sustainability visions are avoided.

1.2.2 *Limited context of conceptual process design*

The main focus of this thesis is the introduction of sustainable development in the stage of *conceptual process design* (CPD); a review of the *status quo* of this design stage is given in Chapter 3. This is a rather broad stage in the start of chemical process innovation; therefore the next restrictions are made for the actors context of the conceptual process design phase, see Figure 1.2, related to *management*, *research and development*, *process flow diagram*, and *stakeholders*. In Chapter 3, an engineering context is described.

Management is a strong facilitator of the conceptual process design (CPD). Management assigns the design and determines the output of the process (a certain amount of a chemical per given time). This management is influenced by the product life span of the product (influenced by consumers and suppliers), by the business strategy (portfolio, etc.), and the current place in the market. All these issues, which influence management, are in turn strongly dependent on the stakeholders (e.g. customers, government, NGOs, local residents, etc.). The general discussion about business policy, market mechanism, supply chain management, etc. is not considered in this research.

The CPD depends also on the knowledge available or achievable within the company. This is the reason that *Research and Development* (R&D) is also a facilitator of the CPD. The R&D department usually cannot order a CPD to be carried out, but R&D's knowledge and innovation are indispensable for the development of new processes. However, during this research no experimental results in the area of R&D are obtained.

The CPD delivers a *process flow diagram* or *flowsheet* consisting of a sequence of various types of equipment carrying out chemical and physical operations (unit operations) at given conditions (e.g. pressure and temperature), a mass and energy balance, and an economic evaluation. From the viewpoint of sustainability, it is necessary that the mass balance proves that, if possible, renewable sources are used and that the process is done in an efficient way regarding the material and energy flows. The energy balance shows the possible use of sustainable energy resources and the efficiency of the heat/energy integration. The economic evaluation

demonstrates the profitability of the process, both for the short and the long term. The focus of this thesis is also on the delivering of a proper process flow diagram, including all necessary data to evaluate on sustainability and profitability. It is essential that *stakeholders'* demands are sufficiently taken into account during the design of a chemical process. Therefore in the final stage of the design procedure, the public must be confronted with the design and an open forum discussion carried out. The engineer is thus forced to defend the design also in non-technological terms, and through this forum discussion possible restrictions imposed by society are taken into consideration already in an early stage of the process development.

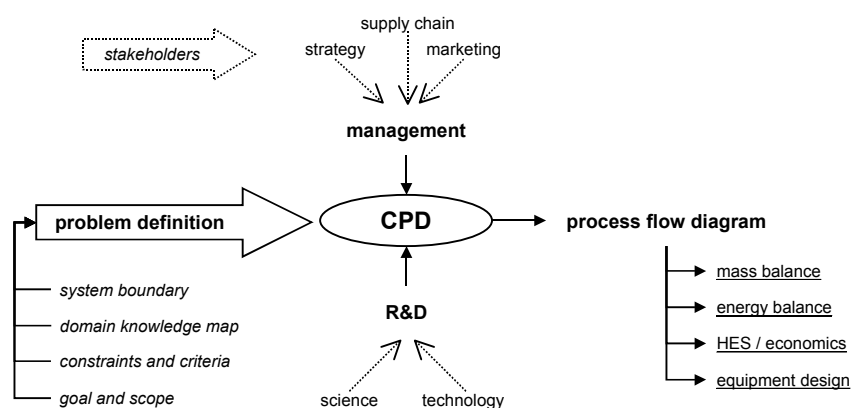


FIGURE 1.2 *ACTORS' CONTEXT OF THE CONCEPTUAL PROCESS DESIGN*

1.2.3 *Points of departure*

In this section, some points of departure are given, which give insight into the position of this research. The next two Chapters elaborate more on this by providing a literature review of the *sustainability debate* (Chapter 2) and the status quo of the *conceptual process design* of chemical processes. For the detailed description of those two issues, see these Chapters.

One of the major actors in achieving sustainable development is the chemical industry, since it is highly resource-intensive and produces large amounts of waste. Although the chemical industry has put an enormous amount of effort in dealing with safety, health, and environmental issues, integrating sustainable development into design and operation is still in its early stages. Therefore this research is focused on trained engineers that design chemical processes and products and have the mission to do that in a sustainable way. Industry is seen in this thesis as willing and motivated to incorporate sustainability during the design phase.

An important question in the sustainability debate is whether sustainable technological development should be seen as a separate discipline or not. The point of departure in this research is that sustainability is a specialty at this moment. So the discussion is focused on how to incorporate the specialized knowledge of the

sustainability field into the field of chemical engineering. In the long term this thesis can perhaps contribute to the discussion on how training of process engineers can be organized in such a way that the integration of sustainability becomes a way to reach the *best practice*.

This project has a strong relation with the project about design for *controllability* by Michiel Meeuse (Meeuse 2002), see also Chapter 3, and design for *safety* by Bastiaan Schupp (thesis not yet published). This relation is established by the Delft Interfaculty Research Center called *Mastering the Molecules by Manufacturing*.

1.3 Hypotheses

The direct motive for this research is the following question:

why do current design methods for the conceptual process design of chemical plants not structurally avoid the problem of unsustainability?

Three reasons are observed: the *absence of integrative design approaches*, the *absence of specific design tools*, and the *gap between chemical process and product design*.

- The absence of an integrative and general design approach inhibits the incorporation of societal issues in the design process. Of course, the chemical engineering field has already a century of experience in dealing with plant design, but a really general methodology on how to design a chemical plant considering all types of external factors does not exist.
- The absence of specific design tools for covering the main issues of the sustainability debate. During the design process, decisions must be made, criteria have to be deliberated, calculations are done, and many more types of activities must also be carried out effectively and efficiently. To perform these kinds of activities as they explicitly relate to sustainability, new design tools have to be developed, as present design tools simply do not exist or are inadequate to deal with sustainability.
- The gap, present between chemical process and product design, leads to confusion. A chemical process is a means to produce a given chemical product, and therefore it would seem very logical that the development of chemical process and chemical product occur concurrently. In practice, however, there is a large difference between the field of chemical product development and the field of chemical process design. Bridging this gap will stimulate sustainable development.

These three above-mentioned points are not mentioned very explicitly in discussions about sustainable design. Many discussions about sustainability and design are focused merely on the question of how a certain problem can be solved, rather than how *in general* sustainability demands should be considered by designers. Not only the content, but also the structure has to be changed in order to meet the above-mentioned three demands. Thus, reasoning from these three points, three hypotheses are formulated as the basis of this thesis.

1.3.1 Hypothesis 1; integral design methodology

Sustainable development of chemical processes and products can best be realized by an integral design methodology that 1) clearly locates the

various design tools that are available or are to be developed and that 2) forces the designer to define the problem, to propose and analyze creative solutions, and to evaluate the design in a consistent and structured way.

The sustainability debate requires a more societal-focused attitude within the current process engineering practice. The design of sustainable processes has to be done amidst a large set of societal, economical and environmental constraints. To reach a real integration of this various disciplines, it is necessary to work with a framework that enables the designer to choose the right tools, criteria, calculation methods, etc. etc. In this way decisions can be made carefully and structurally. This hypothesis is elaborated in the following way:

- The concept of sustainable development can best be integrated when the design team itself formulates its own design criteria. The background knowledge of these criteria is provided by the methodology. The designers have to be confronted with the main principles and problems of the sustainability debate and have sufficient knowledge and insight so that they can formulate specific criteria for their own project that effectively takes sustainability into account. This point is also important in view of the fact that the debate on sustainable development is still very much ongoing. Therefore to presently consider sustainability as if it were some fixed concept would be quite erroneous.
- The decision-making process of a design methodology is strongly dependent on the character of the design project. Therefore a design methodology cannot prescribe the working procedure completely, but has to be flexible so that it can meet specific demands of specific cases.

1.3.2 Hypothesis 2; novel design methods

The incorporation of sustainable development in the design of chemical products and processes requires specific skills and tools. The design methodology should contain enough tools to cover the whole area from need to plant. If tools are newly developed their location in the design methodology should be identified.

The background of this hypothesis is the observation that chemical engineers do not seem very familiar with dealing with the main concepts of the sustainability debate. Solving this problem requires the translation of sustainability concepts into engineering tools. Engineering tools are tools for the basic cycle of decision-making steps: *problem definition, generation of alternatives, analysis of alternatives, and evaluation of results* (those steps are discussed in more detail from Chapter 3 and further). The tools that have to be developed contribute to these different steps in the sense that they help the engineer to incorporate sustainability into design in a concrete way.

This hypothesis is elaborated in the following way:

- For all stages of the basic cycle of decision-making, tools have to be developed to incorporate sustainability into problem definition, the generation of alternatives, the analysis of alternatives and the evaluation of results.

- To show the relevance of the interaction between the general design methodology (hypothesis 1) and the proposed design tools (hypothesis 2), several case studies are elaborated in which the design steps and the results of these tools are assessed and evaluated.

1.3.3 Hypothesis 3; useful for process and product design

A general design methodology, like proposed in hypothesis 1, together with the tools from hypothesis 2, is applicable for both chemical processes and chemical products.

In the opinion of the author, the gap between chemists and chemical engineers is a serious problem and large deficit in the current chemical engineering field. Mainly chemists are involved in doing research and development and in the development of novel chemical products. Chemical engineers are mainly involved in chemical plant innovation. Although both groups work on the application of the chemical science to the development of technologies, the two groups work in different worlds. From the viewpoint of sustainability, it seems necessary that products and processes be developed together. This thesis tries to contribute to this viewpoint by applying the result of the process design methodology to the development of chemical products. The hypothesis is elaborated in the following way:

- The design methodology is developed exclusively for chemical processes and then applied to chemical products. Although it would be advantageous to develop a process and product design methodology concurrently, from a practical and scientific viewpoint this would not be recommended.
- The design methodology is applied to industrial cases in a company that exclusively works on chemical product development. Designing chemical products is not the expertise of the author or the group in which he is participating. However, his lack of experience is compensated by the extensive product development experience in the company in which the new product design methodology shall be applied.

1.4 Plan of approach and the structure of this thesis

The hypotheses and more specifically the sub-hypotheses presented, provide the framework for the plan of approach. The contents overview of this research is presented now in two parts: the *general methodology* and its *design tools*.

- The main goal of this thesis is the development of a new *general design methodology* that enables the incorporation of issues from the sustainability debate into the design practice of the chemical engineering field. An elaborated design methodology for the chemical engineering field does not exist as such, so design knowledge is taken from other engineering disciplines and applied to the conceptual process design of chemical plants. In summary this part of the thesis consists in the following points: i) the integration of various design disciplines to a design methodology for the chemical industry; this design methodology delivers a structure for tools, criteria, guidelines and heuristics, ii) the translation of the main topics of the sustainability debate to technological guidelines, criteria and their metrics;

this is based on literature reviews, experiences in industrial cases and the use of existing tools

- The proposed new *design tools* in this thesis are a result of all the experience gathered during this research combined with scientific insight. These tools and their case studies function as illustrations of how the general design methodology is applied. Besides that the tools show partially how the contents of the sustainability debate can be incorporated in the early stages of chemical process design. The tools are in still in a conceptual stage and it is not pretended that they exclusively deliver contributions to sustainable development.

The development of the general design methodology is the basis of the first part; Chapters 1-4. Chapter 4 gives the description of this general design methodology and also presents the framework for the remaining part of the thesis. The development of various new design tools for process development is the second part of the thesis; Chapters 5-8. In this second part the various steps of the process design methodology are elaborated and illustrated by case studies. The third part of the thesis illustrates the application of the proposed design methodology to the development of chemical products; Chapter 9. Finally, conclusions and recommendations are given in Chapter 10.

Chapter 2

SUSTAINABLE DEVELOPMENT OF THE CHEMICAL INDUSTRY

Summary *In this thesis the main question is how the contents of the sustainability debate can be incorporated into the practice of the chemical conceptual process and product design. This Chapter gives an overview of the sustainability debate, the history of the debate is sketched and the most influential visions on sustainable development are discussed. In many descriptions of sustainable development, a division is made in social, ecological, and economic sustainable development. This Chapter also uses this division and applies it to the chemical process and product development. Finally, specific principles and challenges for the chemical engineering field are derived from the general debate on sustainability. These criteria are the basis for the remaining part of this thesis and they are presented as a comprehensive overview of the sustainability debate and a point of departure for the incorporation of sustainability in the chemical engineering practice.*

2.1 Introduction to this Chapter

Environmental consciousness is growing and has already become important in all kinds of decision-making. Significant progress in reducing the impact of society and industry on the environment was made in the last decades of the past century. Improving the environment is, however, not enough, and this awareness has led to the formulation of the concepts of sustainability and sustainable development. But what sustainability and sustainable development mean and their exact definition are still being debated.

In this Chapter the focal points of the societal debate on sustainable development are derived, based on various documents and opinions. It is not the goal of this thesis to give a contribution to the sustainability debate in general, but the thesis aims at a specific contribution to the incorporation of sustainable development in the field of chemical engineering design.

The goal of this Chapter is to give an overview of the sustainability debate; doing this two questions are kept in mind: i) which visions are most influential and why, ii) how can criteria for sustainable process and product design be derived.

The main idea behind this overview and the accompanying questions is to develop the design methodology flexible to future changes of the sustainability debate. It should be possible that newer insights on sustainable development can be incorporated in the design methodology, or that particular interest of the users of the methodology can be considered, without changing the methodology drastically.

2.2 Historical overview of the sustainability debate

In this section an overview is given of the societal debate on sustainable development. The focus is on all kinds of viewpoints and definitions that are relevant for dealing with the sustainable development of the chemical industry.

2.2.1 *The environmental movement*

Humankind has always used the natural surroundings for its own benefit, so natural resources are converted into useful products and services. In this section, the radical change is discussed that occurred in the attitude of many people towards the environment. The growth of human population, of affluence, or all kinds of technological processes and products lead to large disturbances of the living environment. Disturbances that could be seen easily, like the formation of smog or the extinction of animals. It became clear that the impact of the humans on the environment can be irreversible and that man has to care for earth, instead of exploit it without limits. This all was the start of the environmental movement.

The situation before 1970

Since the beginning of the Industrial Revolution in the 19th century, the scale of the use of natural products by human processes has increased dramatically (Meadows, Meadows, and Randers 1992). For a long time, it seemed that the living environment easily could absorb all the human impacts.

The disturbance of several natural ecological cycles became a problem some decades after the start of the Industrial Revolution in the 19th century. The benefits

of this revolution for the well being of humanity are evident, for example to the development of medicines or the development of modern communication technologies. In general, it can be stated that in the beginning of the 20th century the belief in the improvement of society by the development of science and technology was still very strong. After World War II, the first comments were made about the drawbacks of this development, firstly on the issue of health, but later more and more on the issue of the living environment.

The change in the beginning of the seventies

The environmental movement, started as a sort of anti-technological movement, integrates many ideas and worldviews that are critical towards modern development. Upon the appearance of environmental problems, many societal groups started to disseminate the message that unlimited growth could not be the way that humankind should deal with nature. This led to the publication of books like *Silent Spring* (Carson 1962), *The economics of the Coming Spaceship Earth* (Boulding 1966), *Strategy of Ecosystem development* (Odum 1969), and *The Population Bomb* (Ehrlich 1971) to name a few.

The publication of the report *Limits to growth* (Meadows, Meadows, and Randers 1972) by the Club of Rome had a major impact on the thinking about the environmental impact of the cultural development. According to this report, the five basis elements, *population, food production, industrialization, pollution, and the use of non-renewable resources* all increase exponentially. This exponential growth, if unchanged, would lead to enormous problems, because of counter-intuitive behavior of the interdependent social-environmental system.

Although, mainly the conclusions of this report are outdated, the value of the discussion it started is still visible. In general, natural resources and the environment are no longer regarded as inexhaustible reservoirs and services. On the contrary, it is now recognized that natural resources are limited, that the natural environment has a limited capacity and that these limitations have consequences for the human actions. This increased consciousness has led to various changes in the production and consumption behavior and in the policy-making of countries and companies.

On the other hand, the publication of the Club of Rome's report caused an explosion of counter-reactions. Books with very meaningful titles were presented, like *The Doomsday Syndrome* (Maddox 1972), *The Computer that Printed Out Wolf* (Kaysen 1972), *Is Growth Obsolete?* (Nordhaus and Tobin 1972), *Is the End of the World at Hand?* (Solow 1973), *Models of Doom* (Cole 1973) *In Defence of Economic Growth* (Beckerman 1974), *The Age of Substitutability* (Goeller 1975), *The Ultimate Resource* (Simon 1981), *The Resourceful Earth* (Simon and Kahn 1984).

As shown already, the origin of the environmental movement is an emotional reaction on blindly focusing on economic growth as the blessing of modern development. The same holds for the counter-movement, here represented by the nine books above, that presents the environmental movement as shortsighted and too reactionary. Nowadays, thirty years after all those heated discussions, it is an important lesson that working on environmental improvement, or sustainable

development, asks for a scientific approach, but can not be seen unattached to worldviews.

Sustainability: development of an idea

The environmental movement has reached a lot. Many studies show that in the richer regions of the world (e.g. OESE countries) emissions of pollutants that played an important role in the discussions of the sixties and seventies have been greatly reduced and in some cases even brought back to low levels. However, is this enough? The answer to this question is very difficult to give, and the easiest way out is to state that a detailed discussion on the current situation of the earth is not the focus of this thesis. On the other hand, it is relevant to present some information on the *unsustainability* of the world because this is necessary for getting some insight into the problems that are important in this whole discussion.

At the time the first influential publications concerning the limiting possibilities of the planet were published, the prevailing way of producing and consuming was regarded as being *unsustainable*. However, the consensus on the point of '*unsustainability*' does not imply that there is also consensus about the exact meaning of the term '*sustainability*'. This is not very difficult to imagine. One's perception of a sustainable society is dependent on one's personal ethics and beliefs.

Epistemological and ethical issues

From the Brundtland report and other publications on sustainable development, it is obvious that, in addition to environmental aspects, sustainable development strongly relates to social and economic factors, like eliminating poverty and thus establishing a more equitable society. As such the concept of sustainable development does not relate only to scientific matters (e.g. relation between CO₂ concentration increase and possible climate change), but also to normative or ethical factors, like a fair distribution of wealth.

This implies that no discussion about sustainable development can omit the two basic philosophical questions: 1) what is true (the epistemological question, regarding the reliability of knowledge), 2) what is good (the ethical question concerning behavior of people) (Lemkowitz, Harmsen, and Lameris 1999; Lemkowitz, Harmsen, and Nugteren 1999; Lemkowitz, Korevaar, Harmsen, et al. 2001). Concerning the sustainable development of the physical world, like for example the changes in the concentration of stratospheric ozone the first question falls within the realm of science. However, many environmental issues, and most certainly questions like sustainable development, are highly controversial. Such issues involve various societal actors with large and often conflicting interests. As Allenby (Allenby 1999) stresses, it is essential to try to distinguish the epistemological questions from ethical ones. Separating these two processes is, however, often extremely difficult.

Etymological intermezzo

The etymology of the verb *sustain* links it to the Latin words *sub* (which means *under* or *toward*) and *tenere* (which means *to hold*). The best two descriptions can

be said as *to give support to* or, more related to the subject, *to keep going continuously* (found in the Encyclopedia Britannica On-line). The word sustain dates from the 18th century. The first occurrence of the modern concept sustainability is in the so-called *Blueprint for Survival* by Edward Goldsmith in 1972 (Achterberg 1994):

The principle defect of the industrial way of life with its ethos of expansion is that it is not sustainable. This expansion leads to a) either famines, epidemics, social crises, and wars (no change), b) or a sustainable society (revolution).

The definition of a sustainable society is then given as:

a sustainable society consists of decentralized, self-sufficient communities in which people work near their homes, and have the responsibility of governing themselves.

2.2.2 *Unsustainable state of the world*

In the remainder part of this Chapter, many different views are presented on sustainable development. But firstly, the unsustainable state of the world is discussed.

During the last decades, much has been published describing the current state of Western society and the state of humanity overall. The general conclusion is that the attitude of the society towards nature and the general way of development has to be changed. Societal optimistic to pessimistic visions about the future shows changes of the present attitude towards nature. All these publications are summarized as parts of a description of ‘unsustainability’, which means that in the background thinking of all those people, some future vision is present that describes a future world more lasting than the current world.

From a decision-making perspective, the concept of *unsustainability* is more useful than concept of *sustainability*. Unsustainability, by definition, is viewed as an aspect of *current* reality, while *sustainability* can pertain many possible views of the future. Therefore, agreement about the meaning of *unsustainability* has the potential to drive change in society, and it provides the context in which decisions must be made (Tibbs 1999).

Environmental issues differ spatial scales, this is illustrated by the keywords in Figure 2.1 (Langeweg 1988). The knowledge about the environmental impact of human activities has increased greatly during the last decades. Mainly, those impacts are about the direct living environment of people and strongly related to modern technological actions.

Another important development occurring during roughly the last 10-15 years is the increasing public and political perception of problems manifesting themselves on a new scale. These are problems that are not local or even national, but truly global in scale. For the first time in the history of the human species, humankind’s activities are quite literally affecting the entire planet. Basic causes are the extraordinarily rapid increase in population combined with continuously increasing levels of per capita consumption, resource use and emissions of pollutants. Changes occurring at a global level caused by human activities include: i) increases of concentrations of ‘greenhouse’ gases in the atmosphere occurring at rates and to levels higher than

those ever reached during the last thousands of years, ii) massive deforestation occurring faster than at any time in human history, iii) species extinction and loss of bio-diversity at high rates, iv) ozone layer depletion, v) clean water and food scarcity, vi) depletion of scarce resources, vii) deterioration of eco-systems, viii) growing inequity both within and between nations.

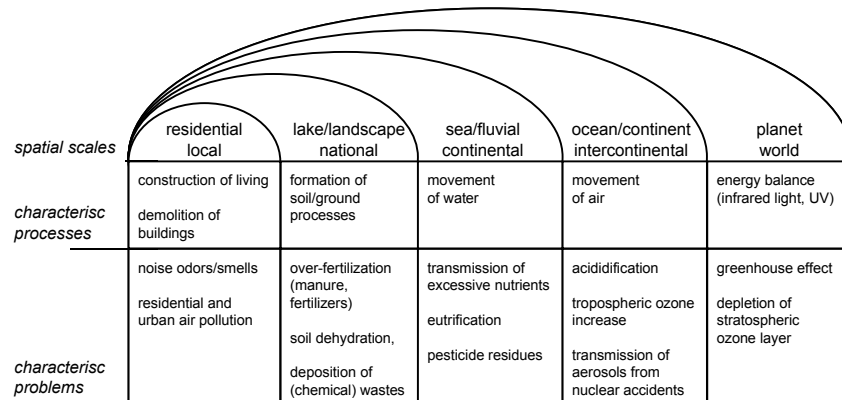


FIGURE 2.1 MAIN ENVIRONMENTAL PROBLEMS

It is beyond the scope of this thesis to give an extended overview of the totality and reliability of the vast amount of data relating to the sustainability debate. Therefore, here a simple framework is provided for illustrating the basic problems of unsustainability by using the so-called Master-Equation. The Master-Equation (also called the Ehrlich-Equation, or the IPAT-Equation) equates the environmental impact (I) of the society to the product of: i) the size of the population in a society (P), ii) the prosperity of that society, or affluence (A), iii) the technology that reaches that affluence (T).

This all is summarized in the equation below, in which the A (based on the *Gross Domestic Product*) and T are given entities (Allenby 1999). For engineers an importance of the IPAT-equation is that it clearly shows that increasingly efficient and clean technology can compensate for increases in population and/or affluence.

$$I = P \times A \times T \quad \text{Equation 2.1}$$

Because of its clarity and simplicity, the IPAT or Masters equation is often used to explain goals for sustainable technological development. The factor 20 reduction of technological impact for the coming 50 years is often used for that purpose. It is defined as follows: if the population growth is assumed to be a factor 2 and the prosperity growth is a factor 5, then future technology must be 10 times cleaner and more efficient than present technology in order to obtain a future environmental impact that is equal to the present one. If the goal is to halve the total environmental impact, then the future technology must reduce its impact on the environment by a factor 20 (Jansen and Vergragt 1993). The same calculation can be done in a less drastically way; if technology becomes twice as efficient and the goal is to use only

the half for the same function, then a factor 4 is reached (von Weizsäcker, Lovins, and Lovins 1998).

Estimations based on the IPAT-equation strongly suggests that it is needed to look further for more sustainable technologies that can reduce the impact of increasing population and affluence, while still fulfilling the needs of society. It should not be forgotten that large numbers of people exist, especially in developing countries, which do not get even their basic needs met. Population and affluence will grow in the future, but even at present earth's natural resources are used at an alarming rate. This raises the question what a *need* really is. Who decides what people need, or what they think they need? This ethical question is not considered in the Master-Equation, but is absolutely essential to any discussion of sustainability and sustainable development.

The issue of inequity

In addition to adverse changes to world environment, economic and societal differences between rich and poor are increasing (decreasing 'equity'), both within nations and between nations. Indeed, the differences between the richest and the poorest countries increase with time (Reid 1995). The Gross Domestic Product (GDP) per capita stays more or less at the same low level for the poorest countries for many decades already, but for rich countries, it grows with very high speed. The richest fifth of the world population enjoys a far greater share of world wealth than the poorest fifth.

Environmental degradation and poverty are causes of war and extensive illegal immigration of the poor to the richer parts of the world. The inequity debate is also a part of *unsustainability*, because it blocks possibilities towards worldwide co-operation. It also limits a real growth of intrinsic quality of life, which is wanted by every human being thinking about his or her and their children's future. Additionally, it is not only unfairness that is important for the issue of equity. The growing consumption of the Western world causes damaging emissions and wastes that already exceed the natural capacity of the ecosystem. If the developing world would have the same growth in the same way as the Western world, the effect on nature would be irreversible and catastrophic.

2.2.3 Definitions of sustainable development

According to Achterberg (Achterberg 1994), the UN-World Commission on Environment and Development, chaired by the former prime-minister of Norway, Gro Harlem Brundtland, really brought the idea of *sustainable development* into the minds of people worldwide. After years of discussion within an intercultural and international workgroup, the so-called Brundtland-Commission agreed upon the following definition, which is the most well known part of their book *Our Common Future*:

*Sustainable development is not a fixed state of harmony, but a process of change in which the exploitation of resources, the direction of investments, the orientation of technological development and institutional change are made consistent with future as well as present needs. **Sustainable development is development that meets the needs of the present generation***

without compromising the ability of future generations to meet their own needs. It contains within two key concepts: 1) The concept of 'needs', in particular the essential needs of the world's poor, to which overriding priority should be given; and 2) The idea of limitations imposed by the state of technology and social organization on the environment's ability to meet present and future needs.

(World Commission on Environment and Development 1987)

To understand clearly what the Commission meant by this definition it is necessary to read the whole book, because a lot of discussion occurred within the Commission about poverty and affluence, distribution of wealth, knowledge, power, and information, the right of the northern part of the world to live more affluently than the southern part, the right to develop, etc. The most admirable aspect of this report is the attempt to bring the two largest world problems, *unlimited exploitation of nature* and *growing inequity within and among nations*, together into one concept that everyone from government to citizen can work on.

Brundtland definition – what can be learnt

Two very important remarks have to be made about the definition of the Brundtland Commission. Firstly, the definition makes clear that development of new technologies, social structures, or whatever, has to take into account economic and social issues (present generations) and long-term and large-scale environmental issues (future generations). Thus developments that have to lead to sustainability are limited and have to consider the idea that every human being must be able to fulfill needs in a more or less equal way. Secondly, it is important to define the concept *development*. This concept is the focus of the Brundtland-Report.

A distinction can be made between two different kinds of development: one that leads to technological innovation (e.g. as used in the term *Research and Development*), and one that is about improving the welfare or social structure of a society (e.g. as used in the term *developing countries*). This distinction is very important, because it makes clear that sustainable development has different meanings in different countries. In a rich country, sustainable development concerns establishing and meeting criteria (e.g. environmental) relating to new and innovative technologies, usually for increasing affluence. In poor countries, however, sustainable development has to do with helping the population simply to *survive* and, if possible, to *thrive*.

It is important to realize that the description of sustainable development in the Brundtland report can be seen not as a detailed plan, but as a framework for working towards a new and better (international) society. The description of sustainable development thus needs further elaboration. The idea of sustainability and a sustainable society worked out in the mentioned report is one possible vision. In this thesis, the vision of the Brundtland report is the starting point. This does not imply that other visions are of less importance, but it is impossible to cover all the many themes of the sustainability debate in one comprehensive definition.

In summary, some aspects can be seen in the Brundtland-Definition that characterizes sustainability: the *focus on human being*, their *needs*, the extended

time-scale (future generations), and the extended geographical scale (the whole world):

- *Sustainable Development is anthropocentric.* Sustainable development gives priority to the needs of the human beings. Although the whole planet's welfare is also considered, in terms of vitality of eco-systems and biodiversity, this is mainly to conserve the planet as a supplier of raw materials and as a place to live in for humans. To put it bluntly, most other species on the planet would probably be better off if mankind would become extinct, but this is not what sustainable development is about.
- *'Needs' are the starting point.* The most important aspect of sustainability is the meeting of needs. This includes the needs of everybody in the world, especially the poor. It is clear that every person in the world has a number of basic needs that should at least be fulfilled in a sustainable world. Examples of such basic needs are shelter, food, access to clean water, medical care, education, etc. But beyond these basic needs, what people really need is difficult to define. This is one of the things that make sustainability a complex subject to work with, because it should be based on a societal debate.
- *The time scale.* Sustainability does not only take into account the way the world is now, but also the longer term; i.e. future generations. It is important that in every sustainability debate the time scale is defined explicitly.
- *The geographical scale.* Although in many parts of the world people live in luxury, in other parts of the world there are still people who do not even have access to clean drinking water, proper schooling, or nutritious food. If the desired event could be reached that all the earth's people could have access to similar luxuries as the developed world is enjoying now, the earth's natural resources would never be sufficient to supply the required resources. Besides that, sustainable development discusses the global impacts of emissions, technologies, economics etc.

Various other definitions of sustainable development

The definition and vision of the Brundtland Report are described more practically by three other United Nations Commissions, the International Union for Conservation of Nature and Natural Resources (IUCN), the United Nations Environment Program (UNEP) and the World Wide Fund For Nature (WWF), called *Caring for Earth, a strategy for sustainable living* (IUCN, UNEP, WWF, 1991). This report defines sustainable development as: *Improving the quality of human life while living within the carrying capacity of supporting ecosystems.*

The *Caring for Earth* - report contains nine Chapters, with the following titles, that also can be seen as nine issues of sustainable development:

- Respecting and caring for the community of life
- Improving the quality of human life
- Conserving the Earth's vitality and diversity
- Minimizing the depletion of non-renewable resources
- Keeping within the Earth's carrying capacity
- Changing personal attitudes and practices

- Enabling communities to care for their own environments
- Providing a national framework for integrating development and conservation
- Creating a global alliance

To illustrate the broadness of sustainability, here some more definitions are given, found in declarations of firms and governments (main source: International Institute for Sustainable Development, www.iisd.ca) or in scientific literature.

In their opinion, sustainable development means:

- a growing economy that provides equitable opportunities for satisfying livelihoods and a safe, healthy, high quality of life for current and future generations
(The President's Council on Sustainable Development, USA)
- achieving a balance between the desire for economic growth with the necessity for environmental awareness and protection
(Earth Pledge Foundation, New York, USA)
- managing economic systems in such a way as to guarantee future generations the opportunity to enjoy a level of well being equivalent to or better than that experienced by the those now alive
(Lawrence Berkeley National Laboratory, Berkeley, USA)
- to respect basic human rights, to realize fairness in human society
(Global Industrial and Social Progress Research, Japan)
- economic growth that does not deplete irreplaceable resources, does not destroy ecological systems, and helps reduce some of the world's gross social inequalities
(J. Roger Hirl, OxyChem, USA)
- the ability of human society and Nature to develop in harmony now and in the future
(Reid 1995)
- Sustainability is a relationship between dynamic human economic systems and larger dynamic, but normally slower-changing ecological systems, in which: (1) human life can continue indefinitely, (2) human individuals can flourish, and (3) human cultures can develop; but in which effects of human activities remain within bounds, so as not to destroy the diversity, complexity and function of the ecological life support system
(Upham 2000)

It becomes obvious that in the vision of some people sustainability has to do with *durability* and maintaining or improving the current situation. The feeling is growing that if the limitations of nature are reached, nature will start to hinder the progress of human development in a hard way; thus other paths have to be found to enable the economy to grow. Another vision is to see the societal development from an evolutionary principle, which states that every development of humanity's possibilities has to be in agreement with its surrounding nature.

Attitude of the western society towards nature; some worldviews

Visions on sustainable development have a lot to do with worldviews, and the relation of this worldview to technology, nature, and society. To explain three

important views in Western society, three relations are distinguished: the relation technology-nature (I), technology-society (II) and nature-society (III). Table 2.1 summarizes this, partially based on (Achterberg 1994) and (Lemkowitz, Harmsen, and Nugteren 1998). The vision on these different relations varies depending on the worldviews involved: 1) an *ecocentric* worldview sets nature (*eco-* comes from ecology) central and this implies a marginal role for man. Man is only one of the enormous number of living organisms, and therefore he should not have a too large impact on nature, 2) in the *Judeo-Christian* view, nature is created by God, and the Creator has given to humanity the moral capacity to deal at best with Nature. In this vision, the human being is the most important creature, but his actions are restricted by God-given rules, 3) in an *anthropocentric* worldview, humanity (*anthropo-* comes from the Greek word for human) has the central place, and nature is not more than a resource.

TABLE 2.1 THE ATTITUDES OF VARIOUS WORLDVIEWS

	Ecocentric	Theocentric	Anthropocentric
Technology - Nature (I)	Technology fits into and depends on nature. Natural resources should not be depleted.	Technology improves human life and is also an instrument in caring for nature.	Maximum development of technology within natural limits. Nature could be replaced by human actions.
Technology - Society (II)	Technology has to provide only basic needs.	Results of moral issues determine the role of technology.	All technological development is centered on fulfilling human needs.
Nature - Society (III)	Nature has an intrinsic value. All that can harm any kind of life should be avoided; precaution is essential.	Stewardship for the Creation is an obligatory mandate. Respectful and responsible use of Nature is necessary.	Nature is resource for human purposes. However, next generations must have the same chances.

Of course, it is not possible within the scope of this thesis to distinguish profoundly between these three worldviews. The table is only given to illustrate several key attitudes and to emphasize the importance of keeping these in mind when carrying on a dialogue with the different stakeholders affected by and related to the design. Being conscious of worldviews, of oneself and of other actors, greatly improves discussion between different actors.

Above, the Brundtland definition is discussed. The worldviews presented here show that there are other voices, which have a different view of sustainable development and even criticize the Brundtland description. The general comment of such dissenting groups is that the Brundtland description stems from an anthropocentric worldview, which places man too much at the center.

Compared to profit-driven development, which essentially sees no limit to development (thanks to mankind's ingenuity) central to Sustainable Development is

the existence of inherent limitations. Nature is one such limitation, and therefore it would be better to speak also of the needs of Nature instead of only the needs of humans. A possible way to provide for the *needs of Nature* can be found by recognizing the *intrinsic value* of the natural system. In other words, nature has an inherent value, completely independent of mankind. This obviously is a non-anthropogenic value statement. However, it is rather difficult to decide which part of nature has an intrinsic value, or if this holds for the entire natural system or not. Which part of Nature humans can manipulate and which part cannot? From a theocentric vision, man has a clear surplus value in the natural system. In the theocentric view humans have the responsibility for guarding nature and for being steward of nature. This results in a moderate viewpoint between anthropocentrism and eco-centrism.

Actors and systems

In achieving sustainable development, different actors will play different roles; it is important that each actor knows its responsibilities and is able to reflect these responsibilities in the role it plays in stimulating achieving sustainable development. In a short overview Stainer (Stainer, Ghobadian, and Stainer 1999) gives some guidelines for the different actors in a technology-based culture: i) *engineers*; be aware of the implications for society and environment, ii) *non-scientists*; understand applied science, iii) *companies*; sustainable growth is allied to risk management, iv) *politicians*; develop the skills for sustainable policy, v) *all groups*; recognize the need for communication.

Sustainable development requires a broad understanding and a broad approach. Following Allenby (Allenby 1999) and Lemkowitz (Lemkowitz, Korevaar, Harmsen, et al. 2001), sustainable development must be approached from three general areas: natural systems, technology, and human culture (Figure 2.2). Engineering design concerning sustainable development thus requires a comprehensive approach in which the humanities and the physical sciences are integrated.

The remarks in this paragraph make clear that defining sustainable technology has much to do with the vision of nature, society, and technology and that achieving sustainable development requires combining knowledge from a wide variety of fields. If done wisely, integrating all those different factors results in a technology that can make the society more sustainable. On the other hand, it should be emphasized that the same reasoning can be used for arguing a strongly technocratic system. Therefore, it is very important to state that the debate on sustainable development has to go on and that engineering practice, like the development of design methodology, should be open towards new societal insights. It would be highly unwelcome if the scientific or engineering world would generate the rules for society.

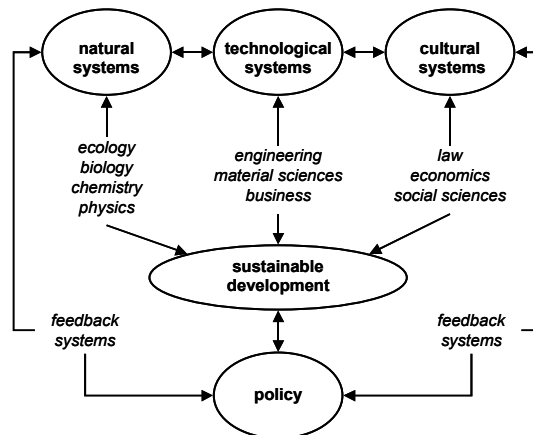


FIGURE 2.2 SUSTAINABILITY REQUIRES THREE SYSTEMS AND POLICY

From the sustainability debate to engineering criteria

Until now, this Chapter gave an overview of the main topics in the sustainability debate. This can be seen as background of all the work presented in the remainder part of this thesis. From the sustainability debate, engineering criteria are defined which are presented in the next section.

2.3 Sustainable engineering criteria

So far, different definitions and principles are presented that describe the ideas of sustainable development. Now, it is time to come to a translation of the concepts from the sustainability debate to engineering criteria. From the discussion above, the following definition is given for sustainable development:

sustainable development is the integration of social issues with environmental considerations into a lasting and profitable long-term development.

This definition has the following essential aspects:

- Development should provide in the needs of people. If the choice must be made between man and nature, then the well being of man is more important (under clear deliberation of the next remark). In this thesis the time span of sustainable development is at maximum 50 years, i.e. ca. two generations.
- Development should not irreversibly endanger the non-anthropogenic part of nature, because nature has an intrinsic value. It can be that a plant or animal has no visible influence on the well being of people, however no living organisms should be threatened by extinction, as this is irreversible harm.
- As much as possible, development should not harm any human beings; in particular, irreversible harm should be avoided. When harm does occur, it should be fairly compensated.
- Development should not have an unexpected or uncontrollable impact on the environment of now and the future. The status quo of the environment is a

reference point. Changes in the environmental situation get the disadvantage of the doubt according to the precautionary principle.

The sustainable development of chemical plants is a very broad issue. Not only the engineering issues, like the construction of the plants, the choice of the raw materials and energy resources, the catalyst regeneration, etc., influence the final sustainability, but also external factors, like the final use of the product, the trends the product actuates, in fact the whole societal structure.

In this section, criteria are given for embedding sustainable development into design. Sustainability is about long-term and large-scale development at all levels (end-use, product, process). That is the reason that later this Chapter also deals with the issue of system levels, to get some insight in the whole system and to define the boundaries of the chemical engineering discipline.

The so-called *triple-bottom-line* will be discussed first, because it delivers a simple and effective framework for discussion of sustainable development. The triple-bottom-line is a concept defined in the financial and business world. Some define it as *Social, Ecological and Economic Sustainability*; others translated it into a catch phrase: *People, Planet, and Profit* (van Dieren 1995). Here, the summary of the World-Bank is used (Serageldin, Munasinghe, Steer, et al. 1994): 1) *Social-Cultural Sustainability*; key concepts: empowerment, participation, social mobility, social cohesion, cultural identity, institutional development, 2) *Environmental Sustainability*; key concepts: ecosystem integrity, carrying capacity, biodiversity, global issues, 3) *Economic Sustainability*; key concepts: growth, equity, efficiency. In the remainder part of this section, these issues are elaborated more and their relevance is discussed for the chemical industry.

2.3.1 *Social-cultural sustainable development*

Mainly, development is focused on economic improvement only. However, a development that meets the present and the future needs of people has a clear social component. The social structures in and within nations have to be changed, before one can speak of real *sustainable* development. It is mainly the incorporation of societal issues that makes the difference between *greenness* (i.e. taking the environment into consideration) and *sustainability* (taking both the environment and the present and future needs of humanity into account). In this thesis there are two arguments that underline the central importance of societal issues.

Firstly, designers should become aware of the importance of social issues. They will, however, usually need some guidance in learning how to treat these issues in their work. Examples of social issues are: equity, openness, precaution, image, etc. Still, many technological developments are banned out after some time, because of the changing societal insights or the underestimated influence of societal action groups. This means that active societal participation during technological change is very important and that the creation of new technological trends has to be done with caution. One way of doing this is by the involvement of the societal stakeholders during the process design. This can be done by interviews, forum discussions etc, with questions on a larger scale and a broader and more conceptual level.

Secondly, all people are equally entitled to benefit from modern technologies that improve the quality of life. This can be defined by the so-called Equity-Principle: *a*

fair distribution of wealth, power and knowledge among the increasing world population. As a consequence, the demand for resources and the pressure on the environment will increase strongly in the 21st century.

From a business perspective the emphasis on social issues is twofold. One is the connection with trends in the society, which ensures the robustness of the business management. The other is the avoidance of negative image of the company, which can have a very strong negative influence on the profitability and stability of the business. This implies that social indicators for sustainable development should contain measures to value the *preference* by the society. To avoid limitations due to the poor-rich division and the increasing population, the technology being developed should be *available* to everyone. In other words what is the resource of knowledge, in the sense that everyone can do it, without harming culture and ecology.

Figure 2.3 shows that there are two basic needs of local people: i) the production of chemicals should not produce unacceptable risk *to their well being*; ii) and it should improve their *quality of life*.

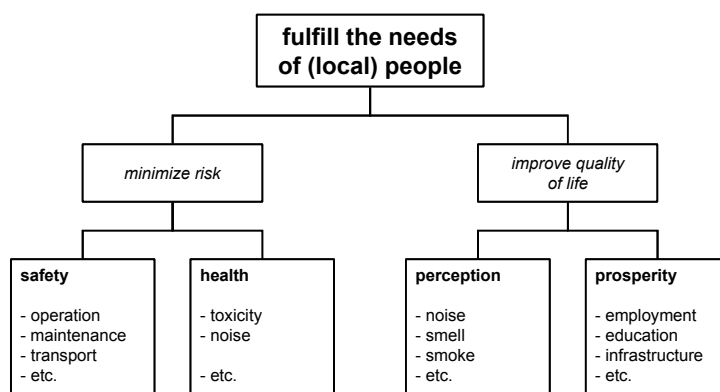


FIGURE 2.3 CHEMICAL PROCESS AND ITS SOCIAL ENVIRONMENT

2.3.2 *Environmental sustainable development*

The diversity and quality of all life on earth is threatened by changes in the global climate, by pollution of water, land, and air, and so on. In the last few decades much attention has been given to solving *environmental* problems, and in this field much progress has been made, particularly in the developed countries. However, the knowledge about the environmental system is still one of the main items in the sustainability debate.

The ecological part has to do with the impact of human action on the environment. Mainly this means all the known environmental problems and processes that disrupt the ecosystems. In a sustainable world, all these known problems must be minimized or avoided. In addition, as far as possible, sustainable development must have the power to avoid creating new problems. These considerations lead to a

twofold question: how large is the irreversible effect of human acting on the environmental system, and how can this effect be measured?

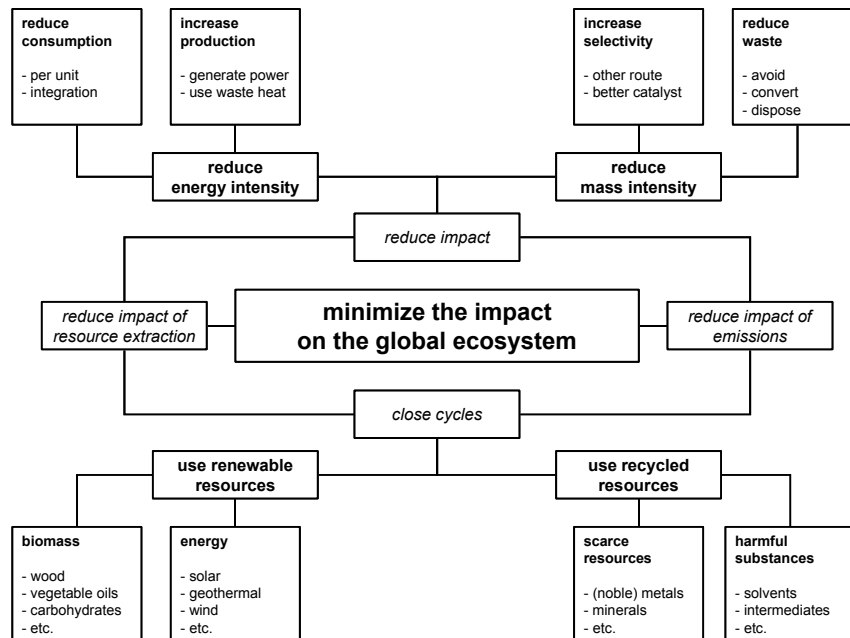


FIGURE 2.4 MINIMIZING THE IMPACT ON THE GLOBAL ECOSYSTEM

Compared to conventional environmental considerations, from the point of view of sustainable development, the scale (both temporal and spatial) to be considered is larger and the intrinsic value of nature is more important. Therefore, designing a sustainable process requires that designers be aware of the effects of the process on the surroundings from a large temporal and spatial perspective. The *precautionary principle* can provide a framework by stating that harmful and uncontrollable effects can occur beyond the system boundaries.

The consideration of a larger life span of the product and process, preferably the total life cycle, can improve environmental performance. Such consideration includes the impact of the various steps in the life cycle and the indirect effects of the activities around the life cycle. Also the resources for the processing steps have to be considered and are important in the whole of the processing performance. In assessing total performance, the carrying capacity of the surroundings plays an essential role; such assessment is part of the collective responsibility of the plant management.

The global ecosystem is a very complex system with many processes, which are all interdependent. Figure 2.4 shows that the impact on the global ecosystem has two origins from an industrial perspective: the *extraction of resources* and the *emission of wastes*.

2.3.3 *Economic sustainable development*

It is obvious that if scarce non-renewable resources like fossil fuels or rich metal ores are going to be depleted, prices will increase, and therefore economics is a very important discipline in the achievement of sustainable development of the chemical industry. However, more arguments can be given for a detailed discussion on economics in the sustainability debate. Here, three are given:

- The economic aspect determines the success of any new technology invented, so the feasibility of sustainable concepts is strongly dependent on how well they can be translated into realistic economic evaluation. On the other hand, the introduction of a product that is successful economically may eventually prove to be unsustainable, as the success of the product can lead to a rebound effect. From a sustainability perspective, not only short term profits are considered, but also long term economic threats have to be foreseen, which point to unsustainability, like the rising costs of non-renewable feedstocks, more stringent legislation that enforces expensive waste treatments, possible higher future taxes, etc.
- Continued economic development is needed to improve quality of life throughout the world. In the current societal situation, zero growth is not an option. This is also in accordance with the wish that under-developed countries also can fulfill their needs in a more equitable way.
- In the long term, additional costs of using renewable resources must be taken into account. In order to provide a sustainable basis for growth, it is often argued that *external costs* should be incorporated in calculating true cost price. External costs comprise all potential environmental and health costs not considered by the market, but passed on to society to be paid later and/or at some other place. Examples are the costs of restoring damaged ecological systems, damage to peoples' health caused by pollution, damage to structures caused by corrosive pollutants, etc. Additionally, not only, the direct production costs must be taken into account, but also the costs that are incurred by the rest of the life cycle of products and by-products. For example, the price of fossil fuels depends not only on the exploration costs, but also the costs incurred by the production of the greenhouse gas CO₂ and resultant adverse climatic effects, whose costs will be many trillions of dollars.

The internalization of external costs is very important in relation to sustainable development. A main cause of unsustainability is that the current modern technology is too cheap in the sense that it does not incorporate the real costs of energy sources and feedstocks. If external costs are internalized, unsustainable processes and products will disappear from the market. However, it is also a main problem that no exclusive solution can be given to the calculation of the level of external costs, like the economic value of nature or the costs of biodiversity loss. In any discussion about economic development, it is of course essential to define the term 'profitability'. From the viewpoint of sustainable development, if *external costs* are taken into account, sustainable technology will be more profitable in the long-term than conventional technology. For this it is necessary that prices are calculated for many external factors, like societal impact of the technology, the

cultural changes, the long-term effects of emissions, etc. In this thesis this is not further elaborated. In Figure 2.5 the major drivers that determine the profitability of a chemical process are sketched.

The figure shows that the economic benefit or profitability can be maximized through *reducing the costs* and/or through *increasing the revenues*. Every of the mentioned costs has a sustainability part. This implies that sustainable development of the chemical industry is not only a purely economic development, but must consist of an integration of all the other factors.

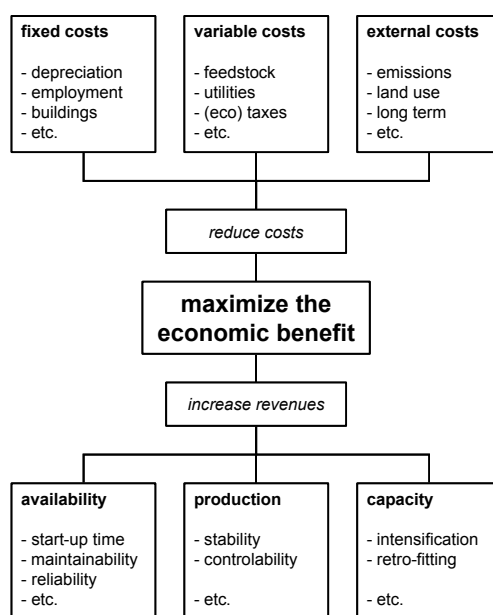


FIGURE 2.5 ECONOMIC SUSTAINABLE DEVELOPMENT

2.4 Sustainable development and chemical industry

It is beyond discussion that industry, and especially the chemical industry, is of essential importance to the modern society. Without technology-based industry, there is simply no way in which present populations can be provided with modern medical care (e.g. antibiotics, vaccines, pain relievers), sufficient food, safe drinking water and sanitation, and the services typical of the high standard of living (e.g. wide varieties of foods, mass worldwide transportation and tourism, electronic communication, etc.).

In spite of these benefits, it should be considered also that important environmental problems originate from the chemical industry. On the other hand, it must be recognized that this branch also has a lot of knowledge to solve such environmental problems. Speaking about sustainable chemical engineering has to do with awareness of the dependence of society on chemical engineering and its influence

on the environment, of maximizing benefit and minimizing risk – both over long time and spatial scales.

2.4.1 *Relevant unsustainability problems*

From the first part of this Chapter, it becomes clear that sustainable development of societies or industries requires solutions to the following problems: i) depletion of scarce resources (ecological and economic importance), ii) widening gap between rich/poor (social and economic issues), iii) technological development without sufficient precaution concerning possible adverse effects (technological issue), iv) clean water and food scarcity (social and economic importance), v) biodiversity reduction (ecological problem).

Chemical Engineering can play a vital role in solving all of these problems. In the following paragraphs, some basic thoughts are presented, which further support the hypothesis that new design methodologies are required.

2.4.2 *Sustainability, safety, health, and environment*

A methodology for sustainable chemical plants can learn very much from all the work that has been published on implementing safety and environmental considerations into design. Figure 2.6 (Lemkowitz, Harmsen, and Nugteren 1999; Lemkowitz, Korevaar, Harmsen, et al. 2001; Lemkowitz, Pasman, and Harmsen 1999) illustrates the inter-relationship between the concepts of *safety*, *health*, *environmental* and *sustainability* in terms of time and distance scales. In the next Chapter, also other external factors are introduced, that play a role in chemical engineering.

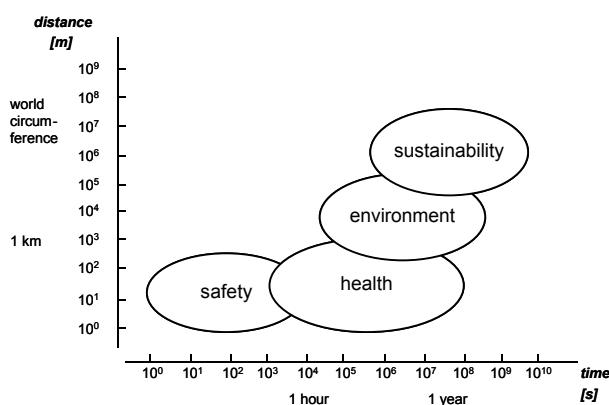


FIGURE 2.6 INTERRELATIONSHIP OF SUSTAINABILITY AND SHE

From the point of scale, *safety* is the most limited of the four concepts. This is so because safety relates to a limited time and spatial scale and concern only human beings and property. For the chemical industry, safety issues typically concern events like fire, explosion, and toxic releases. These, and their effects, occur

relatively quickly and generally affect only people and property in the direct vicinity of the location where the incident occurs.

Health issues concern workers and the public, but not the non-human environment. The time scale includes both short-term exposure and acute effects due to chronic exposure leading to adverse effects lasting a whole lifetime. The spatial scale for worker health is limited to the plant itself, while public health issues (e.g. particulates, acidification) may include local or even a national distance scale.

Environmental risks can refer to acute events, like a sudden discharge of toxic compounds into a river causing massive poisoning of fish. Usually, however, environmental risk refers to relatively low-level exposure of people, nature and property to environmental pollutants over long-term periods. Environmental exposure does not relate just to human beings, but also to all forms of life and also to the complex inter-relationships between species in a biological system (ecosystems).

The four concepts are strongly interrelated. The chemical industry already uses methods to implement SHE-issues into the engineering of new plants, and in some ways the considerations of sustainable development are an addition to this approach. To a certain extent, sustainability covers the whole area of safety, health and environment (SHE), but in practice it is useful to distinguish sustainability from SHE, because of the different levels of detailed knowledge required and the differences in practical applicability. Thus, considering sustainability of chemical plants implies that those plants are safe, profitable, environmentally benign, etc. regarding current standards.

2.4.3 *Existing green engineering tools*

Taking nature into account is not something exclusive to the sustainability debate. Since the 1970s many theories and methods have been developed that are focused on minimization of the environmental impact of the chemical industry. In this section, some of them are discussed being relevant for the remainder of this thesis. Of course it is impossible to be comprehensive at this point; therefore a reference is made to the recent and very interesting book by Allen (Allen and Shonnard 2002) on environmental chemical process design. Some other tools, like supply chain management and life cycle approach, are discussed in Chapter 3.

Basic principles for green engineering

Green Engineering is (chemical) engineering that is focused on incurring as little environmental impact as possible (Allen and Shonnard 2002; Anastas and Breen 1997). During the design phase, but also during exploration, maintenance, or transport, the following principles are considered (Pereira 1999): 1) higher product selectivity, 2) high conversion, 3) improved energy efficiency, 4) use of benign solvents, 5) raw materials substitution, 6) conversion of hazardous products to less hazardous products prior to shipping, 7) on-site production of hazardous materials, 8) conversion of by-products to products, 9) lower secondary emissions, 10) low aqueous waste.

End-of-pipe technologies

Until recently, environmental solutions to processing facilities occurred mainly in the form of end-of-pipe pollution control strategies. These solutions focus primarily on chemical, biological and physical treatment of waste streams that leave the plant, reducing the toxicity and volume of undesirable pollutants in industrial discharges. Although these pollution control strategies have often resulted in significantly reducing negative environmental consequences of processing facilities, they focused on the symptoms and not the true causes of the environmental problems. Therefore, they lacked cost-effectiveness and sustainability.

Pollution prevention

The design approach of pollution prevention consists in an hierarchy of various steps (Mulholland, Sylvester, and Dyer 2000): 1) minimize generation, 2) minimize introduction, 3) segregate & reuse, 4) recycle, 5) recover energy value in waste, 5) treat for discharge, 6) safe disposal.

This hierarchy holds for preventing pollution during design or in fact any other engineering action. Every action should be focused on minimization of the generation of waste or the introduction of waste. If the presence of a waste stream is unavoidable, then the other steps can be used, from segregation and reuse to, at last, safe disposal. Viewing pollution in this way can generate great awareness and, perhaps even more importantly, transform the question of dealing with waste from a nuisance to a challenge to chemical engineers, thus stimulating design creativity and general professional excellence.

Waste minimization

The approach for waste minimization involves ranking and the generation of alternatives, like technology replacement, source reduction, and on/off-site recycling of waste materials. Other possibilities for improvement of environmental performance through analysis of plant mass balances, improved housekeeping around the existing processes, and finally process redesign, have led some to speculate that a zero-emission plant will one day be the norm. However, such a zero-emission plant will not necessarily minimize the environmental impact, as separation and recycle require energy.

Process intensification

What once started with pinch technology (combining hot and cold streams for optimal energy integration) has now resulted in the widely used and adapted concept of process intensification. In fact, process intensification is one of the core businesses of chemical companies' engineering departments and often forms a part of the Responsible Care program.

The idea behind process intensification is optimal integration of energy, materials, and processing tasks with the goal of minimizing amounts of energy and materials needed and size of equipment required to produce a given quantity of product per unit time. This can be achieved by combining a number of process steps into a smaller number and increasing the rate, conversion, and yield (increasing the 'intensity') of chemical synthesis.

Intensification requires innovation and technological breakthroughs that enable cheaper, cleaner and safer manufacturing of products. Such technological breakthroughs also require less equipment, less space, are simpler to operate, and are more energy efficient. The main improvements and successes of process intensification can be found in the development of new processes (e.g. using better catalysis) and better equipment (e.g. combining distillation with chemical reaction) (Harmsen, Korevaar, and Lemkowitz 2003).

2.4.4 *System levels in the chemical process industry*

The sustainable development of the chemical engineering field is a very broad subject. To focus the discussion and the relevance of problem definitions, it is important to distinguish system levels. The awareness of the existing system levels can give the possibility to clearly define how various levels are interlinked and which kind of information must be exchanged. In this thesis five system levels are defined: 1) social-structure level, 2) market level, 3) chemical routes level, 4) processing level, 5) conceptual level.

System levels are mainly barriers for multi-disciplinary work, e.g. marketing officers ask for a technological innovation, but have no idea what this can be; process designers have experience in technological innovation, but do not know how this can fit in with creating new markets.

Social-structure level; the central question here is: what function is required to provide for a societal need? For example, if the society asks for more comfort, this need can be fulfilled with many materials and constructions.

Market level; of course, there are higher and lower market system levels, such as dealing with global trading, place of multinationals, national governments, etc. However, in an industrial case, the most fundamental choice can be made, within the framework of sustainability, concerning the question of whether or not this kind of chemical should be produced and which chemical compounds are available.

Chemical routes level; it is possible to produce the desired chemical from various chemical building blocks. That is the reason that chemical processes for bulk chemicals mainly produce intermediates, from which end products are synthesized related to the market trends.

Processing level; the real process design is done within the processing level, the focus here is on the question: which chemical process is most suited for the production.

Conceptual level; the lowest system level on which the system of chemical industry operates is on the micro-level, the subsystem of the chemical process. Over the years, due to environmental concern, much have been changed in the framing chemical processes, as shown in Figure 2.7 (Yang and Shi 2000).

Initially many chemical processes consisted only of a reaction and a separation section. Because of the energy crisis in the seventies, chemical processes were extended with heat and power integration systems. Hence, energy consumption decreased resulting in significant cost savings. Although the basis of this change was purely economic, it still can be seen as one of the first changes made within the concept of sustainable development. Other changes of the chemical process were triggered by the increase of environmental regulations. These resulted in the

addition of a waste treatment section to the chemical processes. These days, the demand for more sustainable development requires a more efficient use of raw materials and smaller environmental impacts of the chemical process. (Cano-Ruiz and McRae 1998)

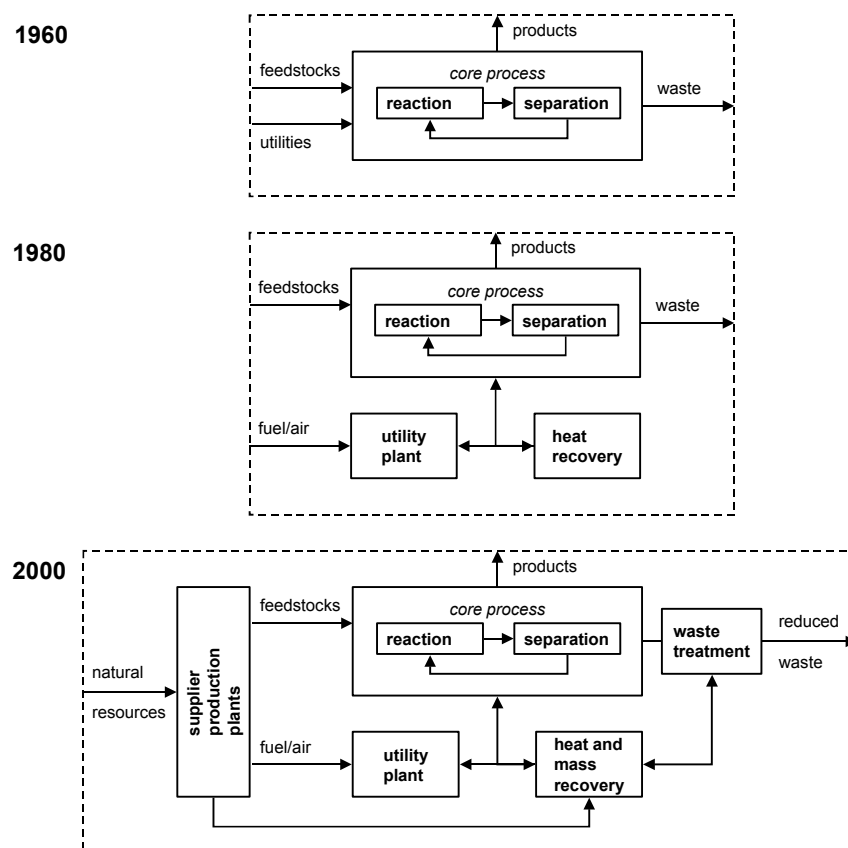


FIGURE 2.7 EVOLUTION IN THE FRAMING OF THE CHEMICAL PROCESS

To complete the evaluation of the influence of sustainability on the chemical industry, some attention has to be given to the interaction between the system levels. As described above, all these subsystems are influenced by sustainability. From a chemical engineering point of view, the interactions and influences of sustainable development are greatest on the chemical process itself, as the chemical process can be seen as the heart of the chemical industry. With this in mind, the chemical process is the place where sustainable development can be introduced most effectively, i.e. will have the most successful outcome. However, it is emphasized here that, although the various subsystems have been described as if they exist autonomously, they actually are organized, operated and directed by human beings. It is decisions made and actions carried out by human beings that in the end will

define the actual result and the ultimate success - or failure - of sustainable development.

Generally speaking a project life cycle comprises *research and development*, *conceptual process design*, *engineering design*, *construction*, *operation*, *maintenance*, and *decommissioning*. The number of options available for reducing environmental impact decreases drastically and the costs associated in implementing an option increase dramatically, as the process life cycle progresses from one stage to the next. (Pereira 1999). This is the main reason why sustainable development of the chemical industry is most effectively and certain most efficiently achieved by focusing on the earliest stages of the project life cycle.

It is apparent that waste management and pollution prevention by means of end-of-pipe technologies will not be the solution to environmental impact minimization. End-of-pipe technologies are applied at the operational stage of the process life cycle. At this stage, some opportunities for environmental impact minimization are left, but these are fulfilled at high cost. Thus, it can also be concluded that most opportunities at the lowest cost can be found in the beginning of the process life cycle, at the stage of research and development and/or conceptual design.

Another important aspect that was identified by describing the influence of sustainability on the chemical industry is that sustainability makes decision-making more complex. Designers of chemical processes not only have to make technical decisions, but also have to identify the influence of any decision made on the other decisions that still have to be made. This identification of possible long-term effect is necessary to ensure that no decision made will cause extra long-term problems with sustainability.

2.4.5 Principles and challenges

Above the main topics of the sustainability debate are described, from this debate principles and challenges are derived. These principles and challenges are the authors interpretation of the relevant criteria for the sustainable development of the chemical industry. From the discussion on sustainable development, *society-focused* and *ecology-focused* criteria are derived.

Ecology focused principles for sustainable chemical engineering

- **Closing the Cycles.** The most important guideline concerns achieving closed systems. The chemical engineer is responsible for the functioning of a certain technology, but also for the malfunctioning and the side effects. A system has to be designed in such a way that all effects are within a reasonable manageability. For example, it is forbidden to do experimental work with toxic chemicals on a large scale in the open air. Three arguments emphasize the working within closed systems: i) closed system make a clear distinction between the human world and the ecological world, the latter being open; ii) closed systems can have an optimized material balance; and iii) closed systems have an unambiguous interchange with other systems.
- **Improved Efficiency.** The chemical industry has a large responsibility in ensuring the continued availability of feedstocks. Modern society cannot avoid the use of non-renewable resources, but their rate of consumption can

be done greatly reduced. Efficient management of every material flow is one of the main tasks of chemical engineering. This holds true even if so-called renewable resources are used. Decoupling of energy consumption and the use of fossil resources is one of the main challenges facing chemical engineering; another is the replacement of precious metals, like the platinum series elements, which are extremely scarce, for by common metals, such as iron, for use in catalyst systems, which are of vital importance to society (e.g. catalytic converters in automobiles).

With these principles the ecological part of sustainable development of the chemical industry can be covered.

Society focused principles for sustainable chemical engineering

The social part of sustainable development is much more difficult for the chemical engineer to envision than the ecological part. Three principles can, however, be helpful:

- **Definition of System Levels.** For every design task it is helpful to distinguish the system level, this places the contribution to sustainable development in the right perspective. It is impossible to solve all problems at once, but with a clear understanding of the system level one is working with, the solution can be interchangeable with other solutions.
- **Systematic Decision Making.** During the design of chemical process plants, many decisions are taken. If this decision-making is done in a systematic way, it is possible to consider many external factors. In the remainder part of this thesis it will become clear how this systematic decision making can be carried out, making use of novel structures and a new design methodology.
- **Involve the People.** Societal issues can only be resolved by societal debate. From my point of view it is impossible and even unwelcome if engineers or scientists attempt to fully manage the discussion of sustainable development. All people are involved in sustainable development and should therefore be invited in various stages of technology development. As the saying goes, sustainable development is too important to be left to experts. The only way to incorporate societal demands during the design of chemical processes is to ask a public forum to react on the conceptual design.

Towards a design methodology for sustainable chemical processes

The principles mentioned here provide the basic framework for the remaining part of this thesis. In the next Chapters, the current status of conceptual process design is reviewed, and present design methodologies are discussed. This gives the opportunity to clearly establish the general demands for a design methodology to stimulate sustainable development in chemical design. It also establishes a general framework for creating a novel design methodology that is able to incorporate sustainability demands during the conceptual process design of chemical plants.

2.5 Concluding remarks

In this Chapter an overview is given of the sustainability debate, from this the following conclusions can be drawn:

- Sustainable engineering differs from green engineering in the sense that it: i) considers both societal, environment, and economic issues at the same time, ii) focuses on issues on a large system level, a large temporal scale, and a large spatial scale, iii) asks for a change in the relation between technology and society.
- The distinction between a *scientific approach* and *worldviews* is very important in the discussion about sustainable development. During the chemical engineering design, it is quite possible to incorporate scientific insights on the sustainable development debate, like the reduction of emission impacts, the use of renewable feedstocks, or the application of alternative energy sources etc. Worldviews might influence the final design result, but mainly this is not directly visible. It is important that the designers are aware of the role that the normative aspects play in their decision-making.
- Sustainable development covers various spatial and temporal scales and various system levels. The incorporation of sustainability issues asks for a clear understanding and distinction of the scale and level of the working field. In this way, it is possible to reduce the broad scope of sustainable development towards a narrowed and more defined engineering scope, without losing the view on the bigger picture.
- The chemical industry is of essential importance to the sustainable development of modern society, but also environmental problems originate from the chemical industry. The chemical industry has a lot of knowledge to solve such environmental problems. Speaking about sustainable chemical engineering has to do with awareness of the dependence of society on chemical engineering and its influence on the environment, of maximizing benefit and minimizing risk; both over long time and spatial scales.
- Existing environmental-focused technologies, like green engineering, pollution prevention, waste minimization, or process intensification etc. do contribute to sustainable development of the chemical industry, but for the traditional chemical engineer it is hard to incorporate or locate these tools in the current practice. Therefore it is necessary to have a general design framework in which these tools are located and their interrelations become clear.
- It is quite possible to derive society and ecology focused engineering principles from the societal sustainable development debate. These principles have the following main characteristics: i) closing the cycles, ii) improving the energetical and material efficiency, iii) defining the system levels, iv) improving the decision-making, v) involving society.

Chapter 3

PRESENT CONCEPTUAL PROCESS DESIGN; PRINCIPLES AND PRACTICES ¹

Summary *In this Chapter, the field of conceptual process design is investigated. Firstly, the relevance of conceptual process design research is identified. Then conceptual design is placed in a societal context. After a brief discussion of generic design principles, the currently standard approaches of conceptual process design are discussed. This description of conceptual process design can be used to put all developments made in the remainder of the thesis into general conceptual process design perspective.*

¹ This Chapter has been written together with Michiel Meeuse (Meeuse 2002), except for section 3.4.3

3.1 Introduction

The objective of chemical processes is to convert a specific feed stream into specified products. The design of the process begins with the desire to produce profitable products that satisfy societal needs (Seider, Seader, and Lewin 1999). The products include petrochemicals, industrial gases, foods, pharmaceuticals, polymers and many other (bio-) chemical products, etc. A large number of steps are taken between the original idea and plant operation, of which conceptual process design is a specific step. Douglas (Douglas 1988) defined conceptual process design as:

(...) to find the best process flowsheet (i.e., to select the process units and the interconnections among these units) and estimate the optimum design conditions.

In the more recent textbooks on process design, Biegler (Biegler, Grossmann, and Westerberg 1997) and Seider (Seider, Seader, and Lewin 1999) give similar definitions. The importance of conceptual process design becomes clear when one realizes that, although a relatively small fraction of the total budget is spent during the conceptual design, the majority of investment costs is assigned in this phase. Figure 3.1 illustrates this schematically.

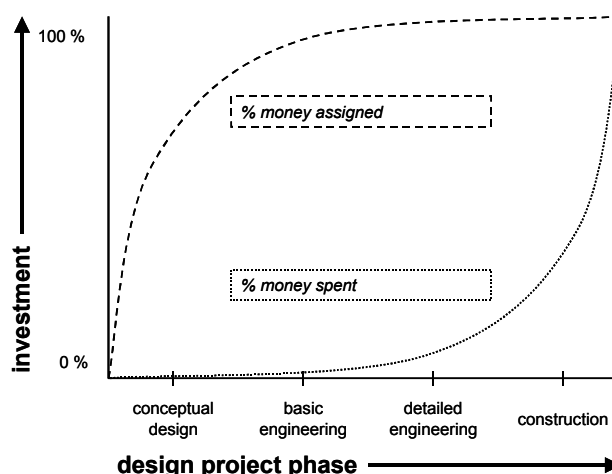


FIGURE 3.1 FINANCIAL CHARACTERISTICS OF CPD

Sirola (Sirola 1997) estimates that decisions made in the conceptual design phase, which accounts for about two or three percent of the project costs, fix approximately eighty percent of the combined capital and operational costs of the final plant. So the success of a chemical plant is for a large part determined by the conceptual design.

Conceptual process design is a highly complex task. Therefore systematic methods for conceptual process design are required. The following characteristics of conceptual design contribute to this complexity: i) a large number of alternatives is

possible, ii) a large variety of requirements should be satisfied, iii) large differences in temporal and spatial scales are involved, iv) these characteristics will now be discussed in some more detail.

TABLE 3.1 EXAMPLE OF EXTERNAL AND ADJUSTABLE FACTORS

Economic	Physical	Operational	Functional	Plant	Site	World
Optimization base Plant optimization Solvent availability Reactor flexibility Sensitivity for fouling Availability Strategic behavior by designers	Material selection Plant layout Reactor choice	Operation/Automation Steady operation Operability	Battery Limits Process technology Process outputs Process inputs Heat integration Waste water treatment Solvent choice Unit to handle emission		Storage facilities Site selection Utilities Quality of raw material	Environment and safety Emission permits
Site selection Raw material and product price Integration with local facilities	Location, lay-out Local weather	Storage possibilities on site Restrictions induced by local plants				
Integration options with local companies Competitors Political stability	Climate	Fugitive emissions Company safety records				

Number of alternatives

Douglas (Douglas 1988) estimates that for a typical design the number of alternatives that might accomplish the same goal can be over 1 billion. Out of these alternatives one wants to select the one that best suits the objectives, e.g. the design with the lowest financial costs that satisfies all other constraints. The main difficulty with this large number of alternatives is that the path from design decisions to the demands to be satisfied is complex and highly non-linear. This requires systematic methods to reduce the number of alternatives early in the design process.

Quality factors

In process design, the designer has to cope with a large variety of requirements. Some of these are explicitly state in the Basis of Design, others not. Herder defined all requirements as quality factors. Based on group discussions with industrial experts, Herder (Herder 1999) identified a large list of quality factors that are relevant for chemical processes. These quality factors are arranged in two dimensions. On one dimension there are the following four classes: i) *functional*; what functions shall the system provide?; ii) *operational*; how shall the system be operated?; iii) *physical*; what are the physical conditions the system shall endure?; iv) *economic*; what are the costs and budget limitations?

The other dimension concerns the system levels: *plant level*, *site level* and *world level*. Table 3.1 shows a representative list of external factors, classified according to these two dimensions, from a case study presented by Herder (Herder 1999).

All those factors are regarded nowadays as relevant, but it stays very hard to consider them during the decision-making in the conceptual phase of the chemical processes, especially since the different criteria play a role at different phases in the design. The problem is that the route from a design decision to the quality factor is quite complex, comprising many causal steps and being highly non-linear in its behavior. So a challenge for conceptual process design is to know when which quality factors should be considered and how the design decisions made have an influence on these quality factors.

Multiple scales

The performance of chemical processes is determined by phenomena operating at various temporal and spatial scales. On the one hand nano-scale phenomena are dominant at for instance catalyst surfaces with typical spatial scales of 10^{-9} m and typical temporal scale of 10^{-3} s. On the other hand phenomena on global scale influence the operational policies of chemical processes with typical spatial scales of 10^6 m and typical temporal scales of 10^6 s. Figure 3.2 shows the various scales schematic.

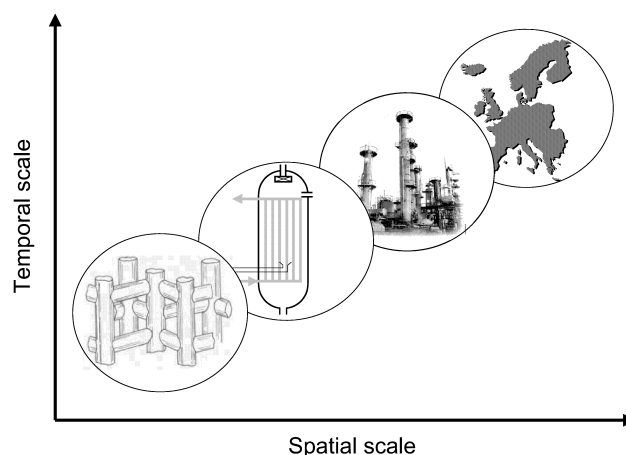


FIGURE 3.2 RELEVANT SCALES FOR CHEMICAL PROCESSES

This Chapter is organized as follows. First some generic design principles will be discussed. These are principles found in other engineering disciplines, but also applicable in chemical process design. Then the context of conceptual process design is sketched. This context contains two dimensions: the supply chain and the process life span. In section 3.4, the conceptual process design practices, as found in the literature, are presented. The Chapter ends with some final remarks.

3.2 Generic design principles

Design is an activity that is carried out in a wide variety of application fields. Railway-tracks, a new engine for a Formula 1 car, a new chair and a CD player are all products that are designed (by engineers). The design of such products is often a multi-disciplinary activity. Despite this wide variety in design, there are several common factors.

Several authors describe the essential element of design as reasoning from *function* to *form* (Gero 1990; Kroes 2000; Roozenburg and Eekels 1995). The design starts with the need for a product that fulfills a specific function. The designer should then determine the product that (optimally) satisfies the required tasks. The form of the product consists of a description of both geometric properties and the physico-chemical properties. In chemical process design the function is generally described as *to convert a feed into products with specified properties*. (Douglas 1988)

A model that describes the various activities carried out in the process of reasoning from function to form is the so-called *basis cycle of design* (Roozenburg and Eekels 1995). This model is found in various alternative design fields, including industrial design engineering (Roozenburg and Eekels 1995), chemical process design (Siirola 1996) and mechanical engineering design (Cross 1984). Figure 3.3 shows this cycle.

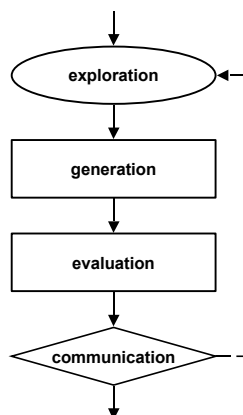


FIGURE 3.3 BASIS CYCLE OF DESIGN

The process starts with formulation of the design problem. In this stage the basis of design is defined. This includes specification of the external factors that needs to be considered, selection of the design space and of the building blocks to be used and identification of the required domain knowledge. Then, in the synthesis phase, alternatives are generated. The (physical) behavior of the alternatives is determined in the analysis phase. In the evaluation phase the performance of the system is compared with the required performance, as specified in the problem formulation phase. So this relates to the societal appreciation of the alternatives. If the performance is not acceptable, one should either reformulate the problem, or generate other alternatives in the synthesis phase. When the behavior is acceptable, one can proceed with the design to the next level of detail.

3.3 Context of conceptual process design

Every chemical process is designed for a given infrastructure within a certain environment; this implies that many interactions exist between the performance of the chemical plant and the world around. The context of the conceptual process design can be sketched in two dimensions (Grievink 2002); the supply chain and the process life span. This is illustrated in Figure 3.4; the context presented in this picture is an *engineering* context, which differs from the *actors'* context presented in Chapter 1.

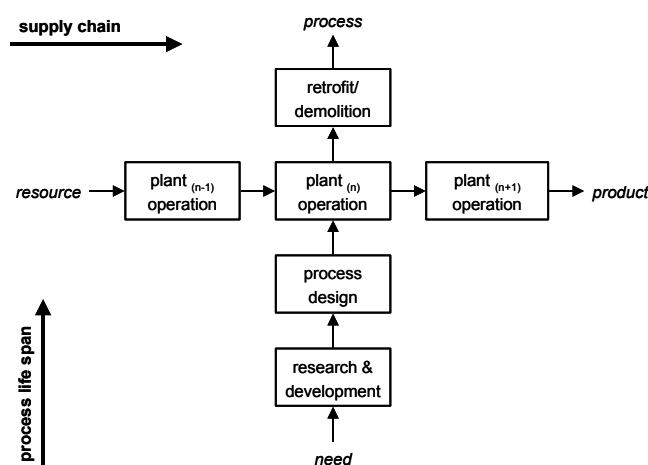


FIGURE 3.4 *ENGINEERING CONTEXT OF THE CONCEPTUAL PROCESS DESIGN*

3.3.1 *Supply chain*

Traditionally chemical processes were studied separately from their environment. Because of the growing urge for industrial symbiosis (Konz and van den Thillart 2002) and growing complexity of industrial product life cycles (Kleineidam 2000) this is no longer sufficient. This is the incentive for the emerging field of supply chain management (Applequist, Pekny, and Reklaitis 2000; Hall 2000; Zhou, Cheng, and Hua 2000). The supply chain is defined, as the whole of processes that surrounds the process and that is required to bring the product to the customer. The supply chain is somewhat related to the product life cycle, which describes the life of a product from cradle to grave. The difference is that the viewpoint in the supply chain is the process whereas the viewpoint in the product life cycle is the product. The supply chain describes all factors influencing the operation of the process. The supply chain starts with the exploration of resource materials and ends with the final product (Backx, Bosgra, and Marquardt 1998), the transportation and inventory steps in between are also taken into account. The chain does not only contain material flows, but also information flows, which determine the purchasing, planning and marketing. This kind of schemes (as presented in Figure 3.5), can be helpful in locating the process in its larger context by considering the input and output of the process as outcomes of the supply chain modeling (Backx, Bosgra, and Marquardt 1998).

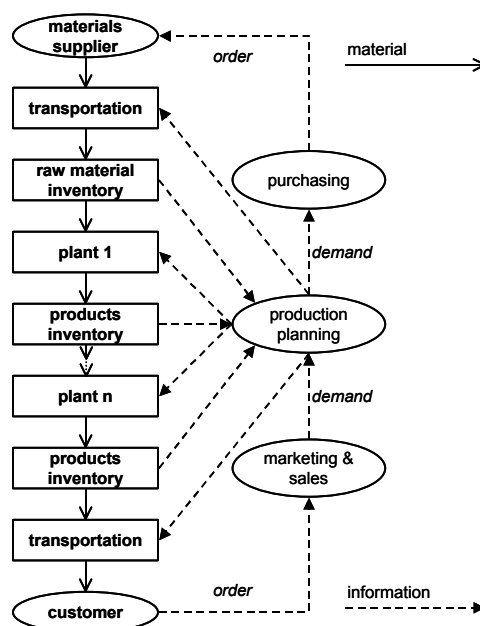


FIGURE 3.5 SCHEMATIC REPRESENTATION OF A SUPPLY CHAIN

The whole supply chain can be modeled (García-Flores, Wang, and Goltz 2000) and optimization tools can be used in supply chain management (Gupta, Maranas, and McDonald 2000). Supply chain considerations will influence some external factors in the Basis of Design. Typical examples are turndown ratios and flexibility requirements with respect to product grades and associated qualities.

3.3.2 Process life span

The conceptual process design is only a part of the process life span of chemical plants, as already indicated in Figure 3.4. Here, a general description of the procedure is discussed to come to a chemical process taken from Siirola (Siirola 1995), see Figure 3.6.

According to Siirola, the building of a chemical plant is an organized multistage goal-directed process. This process leads from the identification of the customers' needs to a plant operation producing a material that fulfils the needs. The construction of a chemical plant is carried out in various ways, depending on the organization of the company or the nature of the chemical process, for example the development of a new facility requires more steps than the improvement of an existing plant.

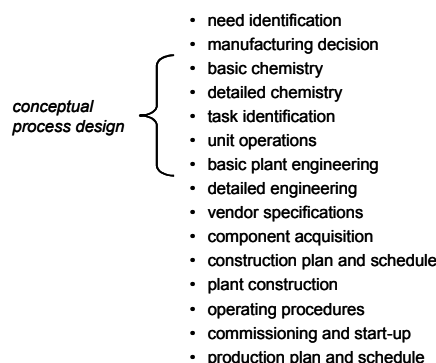


FIGURE 3.6 GENERAL INNOVATION CYCLE

Figure 3.6 shows that the conceptual process design covers the stages basic chemistry to basic plant engineering. In the stage of basic chemistry fundamental reaction chemistry is selected. In the detailed chemistry stage chemical details of catalysis, solvents and reaction conditions are defined. The task identification identifies physical operations to prepare raw materials for reaction and isolate reaction products for sale. In the unit operations stage, chemical and physical operations that are defined previously are associated with actual pieces of equipment and basic plant engineering means the definition of supporting utilities and other facilities infrastructure. This sequence however is strongly focused on petro-chemicals. For processes with micro-structured products the microstructure should be considered explicitly early in the process.

The innovation process is not a linear process, in which each stage is visited once. On the contrary, the process is highly iterative and stages may be revisited several times until an acceptable solution is reached. This implies that each visit to a stage can be conducted at different levels of detail. Especially from the viewpoint of sustainable development, life span issues of the chemical plant are important during the development of chemical processes (Ishii 1997).

3.4 Conceptual process design practices

Traditionally conceptual process design was a kind of evolutionary activity. New plants were designed mainly based on existing plants. In the early seventies some progress was made towards a systematic approach for conceptual process design (Rudd, Powers, and Sirola 1973). This was mainly inspired by the increasing demands both from an economic point of view and from an environmental and energy consumption point of view. But only in the last two decades of the 20th century the major advances in conceptual process design were made. The approaches can be classified into two groups: hierarchical decomposition and superstructure optimization (Daichendt and Grossmann 1997; Douglas and Stephanopoulos 1995). Hierarchical decomposition and superstructure optimization are sometimes presented as two competing approaches. They should however, be considered as complementary rather than competing (Douglas and Stephanopoulos

1995). In the earlier design stages the emphasis will be more on hierarchical decomposition, while optimization methods will be more important in the later design stages. In these stages the number of alternatives is reduced and usually models will be available. Therefore optimization methods will be more useful then in the earlier phases.

3.4.1 Hierarchical decomposition

The basic idea of hierarchical decomposition is that the design problem is too complex a problem to be solved at once. Therefore it is decomposed into several sub-problems with increasing amount of detail. Two different types of hierarchical decomposition are often encountered into the literature. The most often referred to approach is the one originally presented by Douglas (Douglas 1985; Douglas 1988). This approach starts with considering only the input-output structure of the process. In the subsequent design levels, more details are added, finally ending with the complete flowsheet. The design decisions are mainly made using heuristics and short-cut models. The evaluation is done based on economics only. Table 3.2 shows the levels according to Douglas and Stephanopoulos (Douglas and Stephanopoulos 1995).

In all levels the decisions are made based on the total annualized costs. The method was originally developed for gas/liquid processes only (Douglas 1985; Douglas 1988)). Extensions to solid processes (Rajagopal, Ng, and Douglas 1992), polymer processes (Malone and McKenna 1990; McKenna and Malone 1990) and multi-step reaction plants (Douglas 1990) have been presented afterwards.

TABLE 3.2 DESIGN LEVELS OF DOUGLAS HIERARCHICAL DECOMPOSITION.

Hierarchical level	Design information
Level 0	Input information
Level 1	Number of plants
Level 2	Input/output structure
Level 3	Recycle structure
Level 4	Separation structure
Level 5	Heat exchanger network

The second direction into hierarchical decomposition is a task-driven method (Siirola 1995; Siirola 1996). In this method the properties of the product and the feedstocks are compared. The raw materials are considered to be the initial state. The desired product is the goal state. When property differences exist between the initial state and goal state, tasks are required that eliminate these differences. According to Siirola (Siirola 1995) a natural hierarchy among property differences (and hence tasks) exists: 1) molecular identity, 2) amount, 3) composition, 4) phase, 5) temperature, 6) pressure, 7) form.

This hierarchy arises because changing the properties lower in the hierarchy will generally not influence the properties higher in the hierarchy. Table 3.3 (Siirola 1996) shows the hierarchy in property differences and some resolution methods. Once all required tasks have been identified, equipment should be designed to

realize these tasks. In this step significant savings can be achieved when multiple tasks are integrated in one piece of equipment. The last item of the hierarchy, form, however seems not to fit in. Meeuse (Meeuse, Grievink, Verheijen, et al. 1999) showed that for products with in internal microstructure one should start with considering this structure, rather then end with it.

TABLE 3.3 PROPERTY HIERARCHY AND RESOLUTION METHODS

Property Difference	Resolution Method
Molecular Identity	Reaction Mixing
Amount	Splitting, Purchase
Composition	Mixing, Separation
Phase	Enthalpy Change
Temperature, Pressure	Enthalpy Change
Form	Various

The Delft Conceptual Design Matrix (Grievink 2002) is a combination of the task driven method, Douglas approach and the general design paradigm. This matrix is shown schematic in Figure 3.7. In this novel level framework one of the levels contains the task description. This also enables the designer to think into the more fundamental tasks then in terms of traditional unit operations. Meeuse (Meeuse, Grievink, Verheijen, et al. 1999) and Jadhav (Jadhav, vander Stappen, Boom, et al. 2002) have demonstrated the effectiveness of such an approach for structured products.

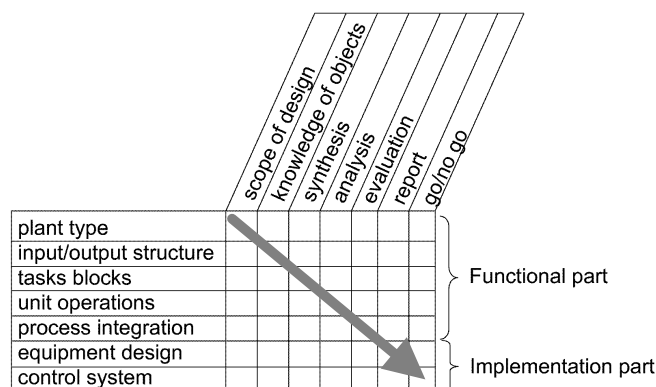


FIGURE 3.7 DELFT CONCEPTUAL DESIGN MATRIX

3.4.2 Optimization-based conceptual design

The process design problem can also be formulated (and solved) as an optimization problem. A typical characteristic of such an optimization problem is that it consists of both continuous design variables, like sizes, temperatures, pressures and flow

rates, and discrete design variables, indicating the structure of the process. These discrete design variables are associated with a so-called superstructure, which has embedded a large set of feasible process operations and interconnections that are candidates for an optimal process design. Figure 3.8 gives an example of such a superstructure. This structure contains a plug flow reactor, a CSTR and all combinations of these two reactors, as well as two different separation sequences. The number of trays and feed tray location are additional design variables. The numerical optimization techniques that can be employed to find the optimum design embedded in the superstructure can be either gradient based, mixed integer non linear programming techniques (MINLP) (Floudas 1995; Grossmann 1997) or genetic algorithms (Emmerich, Grötzner, Groß, et al. 2000). Most applications are for subsystems rather than for complete flow sheets. Floudas (Floudas 1995) presents an overview of several applications: heat exchanger networks, separation systems, reactor networks and reactor-separator-recycle systems. Papalexandri and Pistikopoulos (Papalexandri and Pistikopoulos 1996) present an alternative superstructure based on mass and heat transfer modules rather than on equipment. This approach is closely related to the task driven approach, allowing for the generation of novel type of processes. One of the difficulties in this approach is however to formulate an objective function since there is no direct relation with equipment sizes and hence with the capital costs.

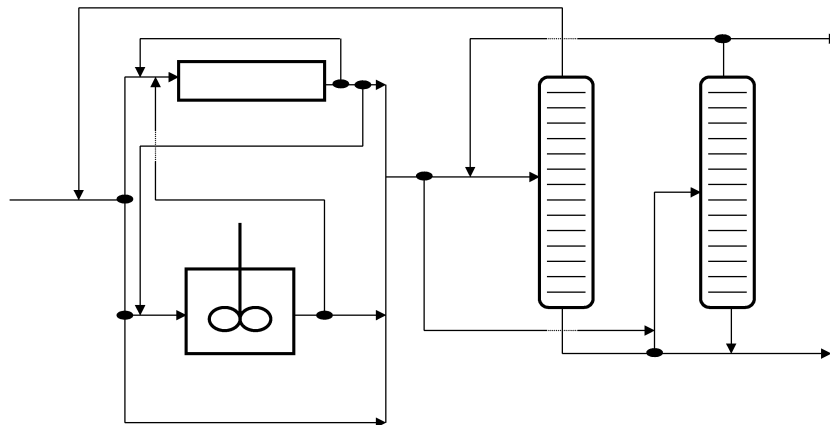


FIGURE 3.8 PROCESS SUPERSTRUCTURE

The main benefit of the optimization-based approaches is that it can really find the optimum solution embedded within the problem statement. However the time required for this is substantial. Especially the formulation of the problem and the efforts required to get the converged solution from arbitrary initial conditions can be significant.

3.4.3 *Multi-objective optimization*

In the former section, it is explained how the economic optimization of flowsheet superstructures can be performed. Especially for environmental design it is important to refer to methods that enable multi-objective optimization, because traditional economic analysis methods can not address environmental issues very well (Jackson and Clift 1998).

A promising theory for that purpose is the construction of a set of solutions using the LCA-approach, which are optimal in the Pareto sense. Originally Pareto is referred to as an economic theory in which it is impossible to improve one objective on the account of the deterioration of at least one other objective.

Many examples exist in literature, in which clean technologies are explored and existing processes are improved in the environmental sense (Azapagic and Clift 1999; Burgess and Brennan 2001). (Alexander, Barton, Petrie, et al. 2000; Vignes 2001) Mainly the authors present their approach as the incorporation or the application of life cycle assessment (LCA) to process design. Although LCA is introduced as a product assessment tool, its framework is useful for the definition of a multi-objective optimization problem in the context of chemical process design (Azapagic and Clift 1999).

3.5 **Concluding remarks**

In this Chapter, the field of conceptual process design is investigated, one of the earliest phases of the design of chemical plants. The conceptual process design problem aims to find a flowsheet that converts a specified feedstock into a specified product and that fulfils the requirements of the assignment. In practice, an assignment is given to design a chemical plant for the production of a certain product or a set of products, within a given environment and with required specifications.

The focus of is to incorporate the quality factors controllability² and sustainability³ in conceptual process design. In the current design practices presented in this Chapter, these quality factors are not considered explicitly. Therefore, design methodologies need to be improved such that these issues can be incorporated. It is important that the design methodology helps to make decisions explicitly. The methodology has to improve the generation of alternatives and locate the analysis tools. During the generation of alternatives, heuristic-based tools are used, because a decision has to be made with lack of quantitative information. In the analysis and evaluation phase, it is necessary to define new tools that can quantify the controllability or the sustainability.

² The thesis by Michiel Meeuse (Meeuse 2002)

³ This thesis

Chapter 4

NEW SUSTAINABLE PROCESS DESIGN METHODOLOGY

Summary *This Chapter starts with an overview of the status quo of design methodologies, with respect to engineering in general and the chemical engineering discipline in particular. Based on this overview, demands to a new design methodology for the sustainable conceptual design of chemical processes and products are derived. From own experience and based on literature sources a design methodology is developed and presented in this Chapter. The methodology consists in three parts: 1) decision-making sequence, 2) design framework, and 3) design tools. The decision-making sequence is the repeating part of the design methodology, consisting of a problem definition stage, a generation of alternatives stage, an analysis of alternatives stage and a design evaluation stage. The design framework is based on current chemical engineering practice and presents the relevant levels of detail. The design tools fill the design framework in relation to the decision-making sequence. It is presented that existing green engineering tools fit in the methodology. Besides that some stages of the methodology are filled in with specific design tools for sustainable chemical processes, developed during this research. In the next Chapters these tools are described more specifically.*

4.1 Introduction to design methodologies concept

Designing a chemical process is a complex activity, because a mostly ill defined and abstract process need, should result in a construction plan for an industrial plant, with satisfying results. Performing this conversion requires a structure (design methodology) that facilitates the generation and analysis of alternatives. Many complicating factors can be distinguished, see also Chapter 3, like *large-scale varieties, unpredictable responses, strongly interacting phenomena, contradicting criteria, large number of various technologies* etc.

The design activity can be characterized as a decision process, involving many decision-makers and levels of detail (Cano-Ruiz and McRae 1998). In Chapter 2 and 3, it was discussed that for improving the sustainable development of chemical industries, it is necessary to carry out changes in the practice of chemical process design. It was argued that the best opportunities for achieving more sustainable processes lie in the stages before the conceptual process design is finished.

This Chapter clarifies the role that the insights of design methodology can play in the development of new methods and tools for the chemical engineering discipline. First definitions of *engineering design*, and *design methodology* are given. The basic concept for the framework of the remainder part of this thesis is presented, by the introduction of the *general design procedure* and the *decision diagram*. Then the various steps and their relation to newly developed tools are introduced, these tools are discussed in the Chapters 5 to 8.

4.1.1 Definition of (engineering) design

The concepts *design* and *engineering* are mainly used interchangeably, but the concept *design* can be used for many kinds of decision-making (e.g. policy development, innovation trajectories, integration of components). That is the reason that definitions of *design* and *engineering design* are given here, from which the latter is used in this thesis. The focus of this work is on the development of new tools and methods for chemical conceptual *design*, within the chemical *engineering* discipline.

Definition of design

In this thesis, a design is defined as: *finding a satisfying solution to the given design problem within given boundary conditions*. Such a definition implies the importance of an accurate design problem definition. That is the reason that within this research, the formulation of a design problem gets a lot of attention. From that design problem it should become clear what the designer and the problem owner see as a satisfying solution and what they consider to be the boundary conditions. If these two are clear, the design consequence is more unambiguous and more feasible.

Three kinds of boundary conditions or constraints can be distinguished, technological, physical, and societal constraints:

- *Technological constraints*; in a long term, the answer depends on expected innovation; in a short term the level of knowledge management is important. The level of acceptability also determines the technological feasibility. At

forehand the problem owner should describe to what extent the designer is free to play with ecological, economical, and social demands. In practice, feasibility is strongly determined by licenses, business innovation, or societal pressure.

- *Physical constraints*; every design is limited by physical and chemical laws, like thermodynamics or kinetics. Although mainly, the profitability of the design or the available knowledge are the limiting factors, every engineering activity is strongly dependent on the knowledge level of science.
- *Societal constraints*; Especially from the perspective of sustainable development, a design should be pointed at fulfilling the societal needs now and in the future. Innovation and development of societal structures can be maintained in a long term (sustained). This is true for physical resources, but also for societal trends.

Definition of engineering design

The Accreditation Board for Engineering and Technology (see webpage <http://www.abet.org>) gives a nice definition for engineering design, which is useful in this thesis:

Engineering design is the procedure of devising a system, component, or process to meet desired needs. It is a decision-making procedure, in which the basic science and mathematics and engineering sciences are applied to convert resources optimally to meet a stated objective.

This thesis is focused both on the development of a novel design methodology for chemical processes, while the validity of the developed design methodology is tested to the design of chemical processes and products. Therefore, the definition of engineering design is the same for both processes and products.

4.1.2 The concept of design methodologies

The first methods that claim the possibility to describe the complex path of technical artifact design appeared in the 1950s. The science of studying the art of designing is called *design methodology*; its main focus is on the study of principles, practices and procedures of design. Contributions to the understanding of design methodologies, can be found in the following areas (Cross 1984): i) the study of how designers work and think, ii) the establishment of appropriate structures for the design process, iii) the development and application of new design methods, techniques, and procedures, or iv) reflection on the nature and extent of design knowledge and its application.

At first, the thinking about artifact design was mainly focused on systematization. Later, roughly from the late 1970s a more fundamental and philosophical approach emerged, which tries to find common concepts between the different areas of design and on the reflection on the context of engineering disciplines.

In the field of chemical engineering, the designers are not used to the more abstract approach of design methodologies; the existing methods or tools are either focused on experience-based decision hierarchies (hierarchical decomposition) or on optimization-based analysis tools (superstructure optimization), see also Chapter 3. That is the reason that the remainder of this Chapter can be seen as a plea for the

use of more abstract design methodologies, in order to gain the possibility for the integration of sustainable development during design.

Definition of design methodology

Now, a definition of design methodology should be derived. According to Roozenburg and Eekels, the following definition can be given:

Design methodology is the science that studies the procedures that are followed in product design, and it provides knowledge about the design process (Roozenburg and Eekels 1995).

This definition emphasizes the scientific nature of design methodology. This thesis uses the expression ‘design methodology’ more specifically as a model that describes the design process, defined as:

a structure for making design decisions and for locating design tools in a consistent way.

According to Roozenburg and Eekels (Roozenburg and Eekels 1995), a design methodology should contain the following three parts: i) models of the structure of design and development procedures, ii) the total of rules and methods for part of the design process, and iii) a glossary of the terminology used to describe the method. A distinction should be made between *descriptive* and *prescriptive* design methodologies. A descriptive methodology describes the sequence of activities that typically occur in designing, mainly based on experience. The general design procedure, defined later in this Chapter, has a descriptive nature. Prescriptive models force the designer to work in a certain order and encourage the designer to adopt improved ways of working. The decision diagram, see later in this Chapter, is an example of a prescriptive design methodology

Definition of design tool

A design tool is defined as any procedure, technique, aid, or method for designing, representing an activity that the designer might use and combine into an overall design process (Cross 1984). In general the designer is free to choose a design tool to solve a certain problem within the context of a given design methodology. In this Chapter new design tools are introduced and the location of existing green engineering design tools is determined.

4.1.3 Opportunities and threats for design methodologies

The purpose for a design methodology is both to execute individual elements of the innovation cycle efficiently, and to link individual cycles so that solutions are coherent. As a result, companies and institutions have developed many methodologies. These methodologies appear to be little more than applied common sense, but Wheelwright and Clark state:

While common sense is an all-too-rare commodity, there is more to structured methods than a straightforward application of what everybody already knows. The difficulty is in finding a method and logic that works where people, information, objectives, and capabilities interact in a complex system. (Wheelwright and Clark 1992)

Working with structural design methodologies, certainly has some drawbacks and benefits; those are summarized below.

Benefits of a structured design methodology

Many examples of structured methodologies can be found in literature, the benefits of applying these methodologies are twofold:

- *Improved quality of the design*; the methodologies help the design team with structuring the complex problem and provide tools and methods to solve the sub-problems. In this way the sequence of design steps gives the possibility to decompose the problem and the presentation of standard design tools can generate a common language.
- *Improved efficiency of the design process*; the rationalization of the design process can lead to reduced cycle time or improved knowledge management.

Possible drawbacks of design methodologies

Heavily structuring a creative process like the design of new technologies, obviously can cause some drawbacks, which are points of attention when applying these methodologies:

- *Restriction of the creative mind*; The main purpose of a design methodology is facilitating the design procedure, so the use of it should not limit the creativity of the individual designer.
- *Endangering adaptability*; Methodologies can create a feeling of complacency, which do not only influence the quality of the design in the short term, but also has an influence on the flexibility and adaptation of the organization in the long term. Constant evaluation and refinement of the methodology is therefore of crucial importance.

4.2 Chemical process and product design strategies

In order to develop a structured methodology, firstly a description is given of existing methodologies to identify the distinct activities in the design process of the chemical engineering field. In this section, prescriptive design methodologies from literature are described, focused on the process synthesis phase of the chemical process and product design. This section can be seen as an extension to Chapter 3; the difference is that in Chapter 3 the current process engineering practice was discussed, while here various strategies for process and product design are considered related both to chemical engineering and other engineering practices.

4.2.1 Synthesis of chemical process flowsheets

Through history, three fundamental approaches for the synthesis of chemical process flowsheet have been developed (Cano-Ruiz and McRae 1998; Siirola 1995): *systematic generation*, *evolutionary modification*, and *superstructure optimization*.

- *Systematic generation*; in this approach, a flowsheet is generated from scratch, by building the flowsheet from smaller, more basic components. The components are put together in such a way that raw materials can be transformed into the right products. Systematic generation cannot guarantee

structural optimality, therefore analysis tools like simulation and modeling are needed to ensure optimization of the rough ideas.

- *Evolutionary modification*; this approach seems to be the approach most traditionally used by conceptual engineers. It starts with an existing flowsheet for the same or a similar product and then makes structural or operational changes as necessary to adopt the design to meet the objectives or the specific case at hand. The quality of solutions generated by evolutionary modification depends critically on the starting flowsheet as well as on the methods used to modify it.
- *Superstructure optimization*; this approach can also be seen as the mathematical programming approach to process synthesis as it is an optimization over structure. A reducible superstructure is optimized to find the best combination of process units that achieve the design task. It offers the promise of simultaneous optimization of structural as well as other design parameters. However, it requires the starting superstructure from somewhere (which for some problems may be implicit in the formulation), as well as very extensive computational capability.

Superstructure optimization or multi-objective optimization can be very promising, especially with nowadays computer development. Yet, it cannot be said that the process designed with this method is sustainable, as this is not only dependent on the designer, but also on the objective functions defined, computer tools used and programming. Evolutionary modification cannot be compared equally with systematic generation and superstructure optimization as this approach is merely used to adjust minor modifications on existing plants. Although the method at this moment cannot generate entirely new sustainable designs, as it is based on existing unsustainable practice, but it can be successively used to adapt processes to sustainable criteria.

In this thesis, the goal is to cover the whole path from need identification to flowsheet generation. This can only be done by systematic generation, since evolutionary modification and superstructure optimization are useful for parts of the design cycle. In other words, in this thesis evolutionary modification and superstructure optimization are seen as design tools or simplifications of the systematic generation of alternatives.

In practice, a design objective should be derived by systematic generation and after that the designer can decide to work from an existing plant (evolutionary approach), or define object functions (optimization approach). From this it also becomes clear that the life cycle approaches as presented in some chemical engineering literature are very useful in analyzing and improving process structures. However, for the systematic generation of entirely new processes it is necessary to develop a methodology that spans the process development from need to plant.

4.2.2 *Four textbooks on conceptual process design*

In the following part, four textbooks are compared that are used extensively in the field of chemical engineering education. It is not the aim of this section to give a comprehensive evaluation of those books, but the purpose is to see whether existing texts on conceptual process design can be used to incorporate external factors in

general or sustainability in particular. Therefore all books are compared on descriptions of *economical*, *environmental*, and *social* issues. For every issue, three stages are considered: the *definition of design problems*, the *generation of design alternatives*, and the *evaluation of design results*.

J.M. Douglas, *Conceptual Design of Chemical Processes*

One of the most well-known teaching books is *Conceptual Design of Chemical Processes* by Douglas (Douglas 1988). In the first Chapter Douglas stresses the creative aspects of the design process and compares the process with painting: first a rough sketch is made, then modifications are introduced and, finally colors are added. This comparison results in his approach towards designing, in which the design problem is reduced to a hierarchy of decisions.

The engineering method, described by Douglas indicates that first developing very simple solutions and then adding successive layers of detail should solve design problems. The method starts with determining the most significant details of the design to discover the most expensive part of a process and the significant economic trade-offs (this approach is also called *decomposition*). Next, first guesses are made of the design and a number of process alternatives are generated that might lead to improvements. In this way, a *reasonable-looking rough process design* is generated, before much detail will be added. Then, more rigorous and costing procedures for the most expensive equipment items are used and the accuracy of the approximate material and energy balance calculations are improved. Detail can be added in terms of the small, inexpensive equipment items that are necessary for the process operations but do not have a major impact on the total plant cost.

A systematic approach to this way of process design is reducing the design problem to a hierarchy of decisions, see also Chapter 3: 1) batch versus continuous operation, 2) input-output structure of the flowsheet, 3) recycle structure of the flowsheet, 4) general structure of the separation system, 5) vapor recovery system, 6) liquid recovery system, 7) heat-exchanger network and utility systems.

This approach to process synthesis has two advantages. Firstly, it allows the calculation of equipment sizes and the estimation of costs while proceeding through the levels in the hierarchy. Then if the potential profit becomes negative at some level, process alternatives can be looked for or the design project can be terminated, without having to obtain a complete solution to the problem. Secondly, if decisions about the structure of the flow sheet at various levels are made and these decisions are changed, process alternatives will be generated. Therefore, with a systematic design procedure for identifying alternatives, it is less likely to overlook some important choices.

TABLE 4.1 EVALUATION OF DOUGLAS' METHODOLOGY.

<i>Stages Issues</i>	Definition of Design Problems	Generation of Design Alternatives	Evaluation of Design Results
Economical	+	+	+
Environmental	-	-	-
Social	-	-	-

The evaluation of the Douglas' methodology is presented in Table 4.1. In the design problem definition (Douglas calls this step *Input Information*) mainly technical and economical information is discussed, such as thermodynamic data, the production rate and its purity. In this stage, Douglas only briefly mentions constraints as a result of the explosion limits of the mixtures used.

Later in his book, Douglas very briefly discusses non-economic aspects of the design problem among which safety, health and environment constraints. Those constraints do not influence the generation of alternatives. Douglas only describes technological solutions to the design problem and uses corresponding heuristics, which are implicitly based on economic considerations. The analysis is focused on economic performance and Douglas stresses that: *...it is essential to consider the processing costs necessary to meet any environmental requirement*. These costs are caused by end-of-pipe treatment and illustrate the economic perspective of this methodology.

R. Smith, *Chemical Process Design*

Smith's *Chemical Process Design* (Smith 1995) immediately starts with the hierarchy of chemical process design and does not include a general introduction to the design process. Smith's approach to process synthesis can be compared with the one introduced by Douglas. The book includes Chapters on safety and health issues, waste minimization and effluent treatment, and ends with a brief Chapter on overall strategy.

The design methodology of Smith can be seen as a spherical model, see Figure 4.1. A typical statement in this book is: *the purpose of chemical processes is not to make chemicals, the purpose is to make money. However, the profit must be made as part of a sustainable industrial activity, which retains the capacity of ecosystems to support industrial activity and life. (...) Following the hierarchy, all to often safety, health and environmental considerations are left to the final stages of the design*. Here, Smith points out a crucial gap in process design, but unfortunately does not offer much guidance in defining nor in evaluating these problems.

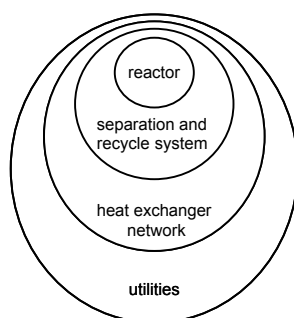


FIGURE 4.1 THE SPHERICAL MODEL OF PROCESS DESIGN

Figure 4.1 shows the hierarchy of the Smith's design model, which can be used as an approach for process design: 1) choice of reactor type, 2) choice of separator type, 3) synthesis of reaction-separation systems, 4) determination of distillation sequence, 5) choice of heat exchanger network and utilities targets, 5) making economic tradeoffs, 7) effluent treatment, 8) process changes for improved heat integration, 9) heat exchanger network design.

Now the evaluation of Smith's methodology can be done, see Table 4.2. It must be stated that the methodology has a very poor design problem definition, which is based on implicit assumptions, such as maximization of profit, and obviously on the assumption that the designer can manage without guidance. During the generation stage, Smith does provide extensive information on economic trade-offs, waste minimization and effluent treatment, and safety and health considerations. In spite of the guidance in the generation of alternatives, Smith does not provide information on non-economic analysis and evaluation.

TABLE 4.2 EVALUATION OF SMITH'S METHODOLOGY

<i>Stages</i> <i>Issues</i>	Definition Design Problems	Generation of Design Alternatives	Evaluation of Design Results
Economical	-	+	+
Environmental	-	+	-
Social	-	-	-

L.T. Biegler, *Systematic Methods of Chemical Process Design*

The textbook by Biegler et al. *Systematic Methods of Chemical Process Design* (Biegler, Grossmann, and Westerberg 1997) starts with an introduction, in which a typical scenario for the design process is sketched. Accordingly, Biegler describes the steps in process synthesis as shown in Figure 4.2. Biegler's definition of process

synthesis includes the entire process from an abstract description, defined as the problem definition received from management to a refined definition, resulting in the conceptual process design.

The evaluation of this textbook is summarized in Table 4.3. In this book the design process is elaborated more explicitly than in those mentioned above. Biegler also employs Douglas' approach, but it is expanded with a large number of numerical optimization methods. Besides that more guidance is given to the designer on converting ill-posed problems to well-posed ones. The process designer is advised to: 1) establish goals, 2) propose tests one can carry out to assess if one is meeting one's goals, 3) identify the starting points, 4) identify the space of design alternatives.

The book also discusses criteria on economy, environment, safety, flexibility and controllability. These criteria are considered as part of the evaluation stage. A typical example: *Environmental concerns involve satisfying the very large number of regulations the government imposes on the operation of a process*. This statement illustrates that non-economic concerns are seen as constraints instead of objectives, which does not result in a multi-objective optimum. The methodology provides many numerical optimization techniques to search among alternatives, mainly on economic grounds. Furthermore, the book provides guidance in designing flexible processes. Although non-economic criteria are discussed, no corresponding analysis methods are mentioned in order to assess and select the alternatives.

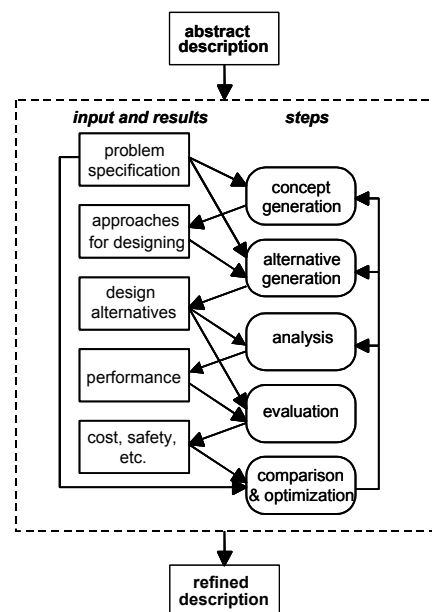


FIGURE 4.2 BIEGLER'S MODEL FOR PROCESS SYNTHESIS

TABLE 4.3 EVALUATION OF BIEGLER'S METHODOLOGY

<i>Stages</i> <i>Issues</i>	Definition of Design Problems	Generation of Design Alternatives	Evaluation of Design Results
Economical	+	+	+
Environmental	+	-	-
Social	-	-	-

W.D. Seider, *Process Design Principles, Synthesis, Analysis, and Evaluation*

Finally, the book by Seider et al. entitled '*Process Design Principles, Synthesis, Analysis and Evaluation*' (Seider, Seader, and Lewin 1999) is considered. Seider starts with an extensive hierarchical model of the design process, this model is the framework of the book and for each detailing stage design tools are given. The method provides heuristics based on safety and waste and energy minimization. The hierarchical structure can be summarized as follows: 1) reaction operation, 2) distribution of chemicals, 3) separation operation, 4) heat removal and addition, 5) pressure-change operations.

Though Seider addresses environmental and safety issues in his introduction, they still remain rather vague: Environmental objectives are normally not well defined because economic objective functions normally involve profitability measures, whereas the value of reduced pollution is not easily quantified by economic measures. Unfortunately, this statement is not followed by suggestions for improvement and is still from an economic perspective.

TABLE 4.4 EVALUATION OF SEIDER'S METHODOLOGY

<i>Stages</i> <i>Issues</i>	Definition of Design Problems	Generation of Design Alternatives	Evaluation of Design Results
Economical	+	+	+
Environmental	+	+	-
Social	+	-	-

In Table 4.4, the evaluation is summarized. The book adopts the hierarchical strategy and adds a large number of heuristics. Some of those include safety, health, and environment considerations, which is a significant improvement compared to previous discussed methods. An extensive appendix shows examples of

environmental problem statements and corresponding technological solutions. Just like the books discussed above, economic analysis methods are discussed. Seider also discusses thermodynamic analysis, which is rather new and a nice contribution in the field. Evaluation methods for environmental and social issues are not available.

Concluding remarks

Four textbooks are compared on their integration of economical, environmental, and social issues during three stages of design: design problem definition, generation of alternatives, and evaluation of design. The following conclusions can be drawn.

Design Problem Definition; although problem analyses are scarce and typically based on economic issues, a trend is noticed towards a growing awareness of non-economic issues (Smith 1995) (Seider, Seader, and Lewin 1999). Economic issues are quantified and non-economic issues are qualitatively stated, which implies that the economic issues can have a larger impact on the final design decisions. A trade-off framework for both quantitative and qualitative criteria is not available.

Generation of Alternatives; the teaching books discussed are dominated by theories on process synthesis ranging from hierarchical methods to numerical optimisation techniques. All those techniques are mainly based on the choice of unit operations, rather than on the choice of functions. A trend is noticed towards the incorporation of guidelines that should help the designer to deal with non-economic issues, but these are still scarce (Seider, Seader, and Lewin 1999).

Evaluation; current teaching books focus on economic analysis and alternatives are evaluated accordingly. Evaluation criteria are not developed by the designer, but are in some way delivered by the problem owner. In this way, a strong interaction between the design problem definition and the evaluation of the result is very difficult to obtain.

Overall it can be concluded that present design methodologies are mainly written from a technological-economical perspective. As a result, sustainability metrics, guidelines, and analysis methods are needed to support the evaluation of non-economic issues more as they do now.

4.2.3 Chemical product design

It is striking that less information is available on the teaching or training for structured chemical *product* design. While in the former section four textbooks (out of many more) are chosen for conceptual process design, only one textbook can be found focused specifically on chemical product design. One of the hypotheses of this research is, that a methodology developed for chemical processes also holds for chemical products. Therefore, after the discussion on conceptual process design methods, the book by Cussler and Moggridge on *Chemical Product Design* (Cussler and Moggridge 2001) is discussed.

The method of Cussler and Moggridge consists in a four-step procedure: need identification, idea generation, idea selection, and manufacture information. This procedure is relatively similar to the procedures used by mechanical engineering

methods like those by Cross (Cross 1984), as discussed already in Chapter 3 and in more detail later in this Chapter.

- *Need Identification*; chemical product design starts by identifying customer needs. Four steps are distinguished that must be treated by the design team in this phase: 1) interviewing customers, 2) interpreting their expressed needs, 3) translating these needs into product specifications, 4) revising product specifications. In the third step, translation of needs into product specifications, chemistry and engineering becomes important. Here the qualitative needs that are usually assembled and edited by marketers have to be translated to product specifications. The following strategy is presented for this translation step: i) write complete chemical reactions for all chemical steps involved, ii) make mass and energy balances important in product use, iii) estimate all important rates that occur during product use.
- *Ideas Generation*; this part is the most creative part, also called the generation of alternatives. There are two steps in this phase: 1) ideas from human sources can be collected through techniques like brainstorming; ideas from chemical sources can come from techniques like *natural product screening*, *random molecular assembly* and *combinatorial chemistry*, 2) for the screening of ideas, criteria are needed to define which aspects are considered most important. Strategies can help to choose which are the most important factors to evaluate the product ideas on. Examples of such strategies are the definition of *scientific maturity*, *engineering ease*, *lowest cost*, or *environmental impact*. Weighting factors can be used for final decision-making.

After this phase usually another management decision must be made about the continuing of the project. Experience shows that management tends to be too supportive at this stage. It is thus important at this stage that the project team is objective, and presents both the advantages and the risks concerned with a concept.

- *Selection of Ideas*; two kinds of criteria can be used when selecting an idea: chemical or engineering criteria, and intuition-based criteria. To make a selection with chemical criteria, experiments have to be performed. It is important to find out which consumer attributes are related to which physical properties. Technical criteria and non-technical can be used: i) Selection using thermodynamics (what is physically possible), based on *ingredient substitutions* or *ingredient improvements*, ii) selection using kinetics (how fast – how expensive), based on *chemical kinetics* or *heat and mass transfer coefficients*, iii) selection using intuition-based criteria (what is feasible in an industrial or academic context), based on *innovation*, or *integration* of knowledge. A concept selection matrix can be used here: generate some important criteria on which to judge the ideas; weight the criteria according to their perceived significance; score each idea for each criterion. Summing the products of weighting factors and scores over all criteria gives an overall score for an idea. A reference product or benchmark can be used for comparison, which will receive an average score for each criterion.

- *Manufacturing Information*; the following issues are addressed concerning this last phase of product design: i) intellectual property, ii) supplying missing information, iii) final specification, iv) micro structured products, v) device manufacture.

4.2.4 *Comparing process and product design methodologies*

If the chemical product design method by Cussler (Cussler and Moggridge 2001) is compared to the methods for chemical *process* design, discussed above, two main conclusions can be drawn. Firstly, the incorporation of consumer demands throughout the design of a chemical product is rather usual. This makes the methodology rather flexible to external factors, because the designer is forced to make rigid need identification and a translation of those needs into engineering functions. In the methodologies for conceptual process design, those steps are not mentioned that explicit, so a new methodology for chemical processes and products should contain these steps. Secondly, the use of creativity and intuition during the design is an integral part of the chemical product design, as it is for the design of technological artifacts in general. The chemical process designer should learn from this and could be forced to the use of creativity and intuition-based methods for the generation of conceptual process design.

4.3 **Design approaches in various disciplines**

After discussing the strategies for chemical process and product design, the scope is now enlarged to a discussion of some general visions on design. Those visions are not really developed into a concrete design methodology, but they form more or less the philosophical background of the design methodology that is developed at the end of this Chapter. Here, design is described as a *strict problem definition*, a *satisfying process*, a *concurrent approach*, and a *decision-making procedure*.

4.3.1 *Design as problem definition procedure*

The publications by Yoshikawa describe a very general approach to design in the form of a general design theory. To start with a quote: *design theories are no more able to change real design activities than linguistic theories are able to change our language life*. The General Design Theory described by Yoshikawa has a strong relation with the discussions on the development of computer-aided design tools at that time (1970s-1980s). That makes the construction of the theory in some way outdated, because it wants to describe design procedures as strict algorithms that can be handled by computers. This section is based on an article by Tomiyama and Yoshikawa (Tomiyama and Yoshikawa 1985) and a critical review article by Reich (Reich 1995).

The authors give the following reasons for the development of a General Design Theory (Reich 1995; Tomiyama and Yoshikawa 1985): i) clarify the human ability to design in a scientific way, ii) produce practical knowledge about the design methodology, iii) frame design knowledge in a certain formality, suitable for implementation, iv) most design theories only deal with ‘how to design’

(phenomenological), v) the GDT wants to answer ‘what is design’ (epistemological).

Short overview of the *General Design Theory*

It would be beyond the scope of this thesis to give an extensive discussion on the contents of the General Design Theory, thus only the main points are summarized here. The basis of the GDT is a division of reality into three *worlds* (see also Figure 4.3): a) the real world, b) the conceptual world, and c) the logical world.

Design theories are then defined to deal with mapping from the *conceptual* world (the world in the designer’s mind) to the *real* world (where all concrete entities exist) via the *logical* world (the world of science, symbols, philosophy etc.).

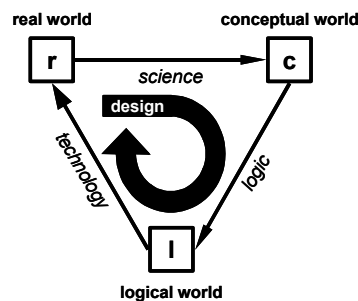


FIGURE 4.3 DESIGN MODEL BY YOSHIKAWA

The General Design Theory defines many axioms, theorems and definitions. In this short overview the definitions are not repeated entirely, because in most cases the meaning of the used terms is clear, and the interested reader is referred to the literature sources. Some of the axioms and theorems are mentioned, only if they are valuable for the final design specification.

Axiom of recognition; any entity can be *recognized* or *described* by its attributes and/or other abstract concepts.

Axiom of correspondence; the entity set in the real world and its representation in the conceptual world have *one-to-one* correspondence.

Axiom of operation; the set of abstract concepts is a *topology* of the set of entity concepts.

The aim of the three axioms is to make clear that it is possible to describe an idea in the conceptual world by logical terms, so that it can become entities in the real world. In this stadium nothing is said about the effort, knowledge and time it would take to create such entities. Therefore it is necessary to distinguish between *ideal* knowledge and *real* knowledge.

Ideal knowledge is the one that knows all entities and can describe each of them by abstracts concepts without ambiguity. It follows from this definition that in the ideal case, a problem definition immediately leads to a design solutions. This is the ideal case, because the designer has all information and knows all possible combinations.

Real knowledge is the set of feasible entity concepts, which are made compact by coverings selected from the physical law topology. Speaking about reality, brings us at the hypothesis about real knowledge. The real knowledge can not be defined in the sense of the ideal knowledge, but a hypothesis can be formulated about the contents of the real knowledge. While discussing the item of the real knowledge, it is necessary to introduce a metamodel. Such a metamodel covers the lack of information that is the peculiarity of a real design.

In summary, the General Design Theory discusses two kinds of knowledge or reasoning based on the definition of ideal knowledge and the hypothesis of real knowledge. This leads to an Ideal and a Real General Design Theory:

Ideal General Design Theory

- Has the ability to separate between two entities
- Needs knowledge to have two perfect properties
- Guarantees the termination of design on basis of the two properties

Real General Design Theory

- Is an adaptation of the concept of ideal knowledge to the real world
- The topological nature of knowledge (as in GDT-ideal) remains intact
- Entities are described by a finite number of attributes (as in GDT-ideal)
- In reality this finiteness can be too large, therefore metamodels are introduced
- Requires the ability to continually model the designed artifact

Concluding remarks on the *General Design Theory*

The power of the concept of a General Design Theory lays in the precise definition of the relation between experience and reasoning. The logical world is a medium to create things for the real world, but the creativity is coming from the conceptual world. From this design can be defined as a creative and logic process that brings us from a problem to solutions, while lacking information. The design process is located between the design problem specification and the design solution. The design specification is based both on the experience of the designer and the language that is used. The experience of the designer is going from the real world into the conceptual world and the reasoning of the designer brings that to a design problem in the logical world.

If the design problem is specified, technology can help the designer to generate solutions for the problem by using technology, and entities for the real world are created. The main idea is that, the more precise the design problem is defined, the easier it is to generate a solution. It is also true that the more a design methodology approximates the ideal case; it costs more time and gains insight and detail. The more the design process can be described by the real-case design theory it loses detail and becomes more trivial. Every design methodology can be seen as somewhere between a fully logical framework and consolidated experience.

4.3.2 *Design as satisfying activity*

During the conceptual process design of chemical plants, mainly optimization tools are mentioned, as is shown in Chapter 3. However, it might be discussed if those tools really can be seen as design tools, in the sense that they contribute to the generation of new ideas. A useful contribution to this discussion is given by publications of Simon (Simon 1996). Simon opposes that during design, optimization does not occur and engineers can never use optimization, but only can find satisfactory solutions. In this section, this thesis participates in this discussion and takes from this discussion the hypothesis that a design methodology cannot be focused on finding the optimal solution, but only on finding a *satisfying* solution.

Introduction to the concept of *satisfying design*

Simon bases his book (Simon 1996) mainly on experiences and thoughts from the field of economics. From that viewpoint he writes about Operational Research (OR), which can be seen as *science*, and Artificial Intelligence (AI), which can be seen as *design*. Operational Research is defined by Simon as

algorithms for handling difficult multivariate decision problems, sometimes involving uncertainty. (...) To permit computers to find optimal solutions with reasonable expenditures of effort when there are hundreds or thousands of variables, the powerful algorithms associated with OR impose a strong mathematical structure on the decision problem. (...) Of course the decision that is optimal for the simplified approximation will rarely be optimal in the real world, but experience shows that it will often be satisfactory (underlining: GK).

The underlined sentence shows that Simon concludes from experience that optimization is never leading to an optimal solution, but he gives no fundamental reason for that. What if a method is found that gives optimal solutions in the real world; does such a method provide optimal solutions or are they only satisfactory? Simon is convinced of the impossibility of the existence of such a method. He states that all kinds of methods that are not using strong limitations on the original problem cannot be optimized and thus only give satisfying results.

He summarizes this statement in the next quote about Artificial Intelligence: The alternative methods provided by AI, most often in the form of heuristic search (selective search using rules of thumb), find decisions that are 'good enough', that satisfy. The AI models, like OR models, also only approximate the real world, but usually with much more accuracy and detail than the OR models can admit. (...) The price paid for working with the more realistic but less regular models is that AI methods generally find only satisfactory solutions, not optima.

Some critical remarks on the use of optimization

Above, the concept of *satisfying design* is introduced. One of the arguments made by Simon is that the models used for optimization are always imperfect. Therefore design cannot be carried out by optimization. In this section, the assumptions underlying optimization as design methodology are discussed into more detail,

because it does not follow very clear from Simon how he defines optimization and its relation to designing.

Optimization can obviously only be carried out when mathematical models are available; models used for design consist of equality constraints, inequality constraints and a domain of validity (as already described in Chapter 3). With the definition of design and optimization, as given in Chapter 3, it becomes clear that optimization can be an important part in chemical process design. Chemical engineers are aware of the limits of optimization models and use their results imbedded in the larger picture. This implies that optimization of a superstructure does not deliver the final design of a chemical plant, but that the optimization of superstructures is a very helpful tool in generating an overview of all possibilities and thus a strong basis for decision-making.

Design as *satisfying* process

The definition of design as a satisfying process seems to be very useful, because it focuses the development of a design methodology on the description of general frameworks and tools, rather than the definition of exact procedures that will lead to unpractical or unmanageable approaches. Besides that, the book by Simon also clarifies the difference between a scientific approach, which is really focused on finding the most accurate description of the solution to a given problem, and the design approach, which should be satisfied with rough descriptions and rough ideas. It is already stated above that design at best can be seen as decision-making with lack of detail.

4.3.3 *Design as concurrent approach*

The most important theme in this research is the translation of non-technological factors to technological constraints and criteria. In most designs, only the economical performance of the process or product is taken into account. This leads to a large emphasis on efficiency, both chemical and physical. However, if the question has to be answered how to take long-term effects into account, other kinds of efficiency should be considered. For this, the concept of concurrent engineering is very important, because it is a feasible approach, to work with different disciplines on one subject.

In many product development trajectories, the concept of concurrent engineering is introduced successfully. Concurrent Engineering provides a cooperative teamwork between multiple disciplinary functions to consider all interacting issues in designing products, processes, and systems (Huang 1996). The concept of concurrent engineering is also gaining progress in the field of chemical engineering (Han, Kim, Lee, et al. 2000; Herder and Weijnen 2000).

In Figure 4.4 (Hubka 1980), the engineering process is placed between various management processes and auxiliary processes, which are available in an industrial context. This gives a clear overview of the place of the design methodology that will be developed in this thesis, as stated in Chapter 1.

Concurrent engineering is a management tool for product development and its objectives include improving quality, reducing costs, compressing cycle times, increasing flexibility, raising productivity and efficiency, and improving the social

image. These objectives, as Huang (Huang 1996) states, are achieved through cooperative teamwork between multidisciplinary functions to consider all interacting issues in designing products, processes and systems from conception, through production, to retirement, simultaneously.

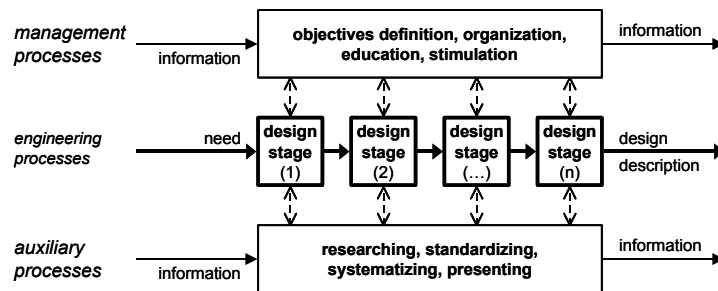


FIGURE 4.4 CONTEXT OF ENGINEERING DESIGN

Design for X

In the field of concurrent engineering, the so-called Design for X method is developed. The X in this expression stands for 'x + bility', in other words this methodology is applicable to all kinds of external factors, like total quality, total life cycle costs, environment etc. (Huang 1996). DfX can be described as:

a tool in which a long series of relationships have been formulated, together with their dispositional effects, measured in relation to the universal virtues. In this way the designer is given dispositional insight into the technical areas in which he does not naturally belong (McAloon 2000).

Besides this, DfX provides specific tools that can be used during the design. The idea is that designers cannot be expected to be subject experts on every factor that arises during the design process, so these tools can help designers in areas they are not familiar with.

This concept is useful, because it distinguishes the framework of the design from the purpose of the design. In this thesis, the following learning points are taken from the DfX-method, i) at every moment during the design project, the designer should be able to rationalize the decision-making and to communicate clearly to external parties, ii) a design project starts with the determination of the design procedure and the evaluation tools that will be used. In this way, the design methodology is flexible to the purpose of the design, iii) design procedure and design methods are distinguished; the design procedure defines the detailing steps on which decisions have to be made to reach the final goal, the design methods are tools that help the designer to make the decisions in a structured way.

Design for Environment

Design for Environment (DfE) is a member of the DfX family and is almost as broad itself. DfE has been emerging during the last decade and many similar methodologies exist with a large variety of names: Environmentally Conscious

Design, Ecodesign, Green Design, Clean Design, Life Cycle Design, etc. Although these terms can differ in detail, the main goal can be considered the same (McAloone 2000).

Fiksel (1996) describes DfE as follows:

DfE is a systematic consideration of design performance with respect to environmental, health, and safety objectives over the full product life cycle. (...) DfE seeks to discover product innovations that will result in reduced pollution and waste at any or all stages of life cycle, while satisfying other cost and performance objectives.

Furthermore, Fiksel describes the following key elements of DfE, which are required for an effective implementation: 1) *Metrics*; driven by fundamental customer needs or corporate goals, to support environmental performance measurement, 2) *Design Practices*; based on in-depth understanding of relevant technologies and supported by engineering guidelines, 3) *Analysis Methods*, to assess proposed designs with respect to the above metrics and to analyse cost and quality trade-offs.

In a true DfE approach, requirements do not address only product performance but also other downstream issues such as environmental quality, service, etc. are addressed. The requirements are translated in objectives using measurable and verifiable performance metrics. After requirements have been defined, the actual design is made by employing guidelines. Fiksel distinguishes two types: i) *prescriptive guidelines* are strict statements about what designers should or should not do, and are sometimes called ‘design rules’, ii) *suggestive guidelines* are based on previous experiences, but do not pretend to be strict rules.

A large variety of guidelines exist and most of them are still in development. They can be expressed as verbal rules of thumb, multidimensional look-up tables, diagrams, etc. Fiksel describes the following benefits of using these guidelines: i) they encourage consistency among different development teams in areas where consistency is desirable, e.g. standard material-labelling schemes, ii) they promote continuity through the accumulation of knowledge over successive design cycles, and allow that knowledge to be preserved and passed down, iii) they lead to a more systematic design process that is less dependent upon the idiosyncrasies or particular biases of individual designers, iv) they expand the scope of issues considered during design, allowing the team to anticipate downstream pitfalls or constraints that they may have ignored.

Once initial designs have been formulated, the verification begins. The earlier this stage begins, the sooner the design team will recognize design shortcomings and will be able to take steps to overcome them. In an integrated approach, DfE must be balanced against other cost and quality factors, which requires a well-structured decision framework. Finally, after sufficient cycle loops the design is released to the next stage of product development.

4.3.4 *Design as decision-making sequence*

Many visions can be given on the description of a valuable design methodology. In this section, the focus is on the literature that treats design methodologies as a

sequence of decisions. First, some authors are introduced and then some concluding remarks are made.

Cross

Cross (Cross 1984) describes design as *the sequence of distinct activities that occur during designing*. Cross states that a design model should be *heuristic*: using *previous experience, general guidelines and rules of thumb* that lead in the right direction. And more important than that: be explicit in every decision that is taken. The design sequence of Cross has already been discussed in Chapter 3, therefore only the accompanying figure is presented here.

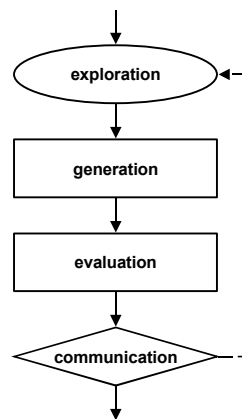


FIGURE 4.5 CROSS' DESIGN SEQUENCE

French

French has developed a detailed model of a *product design procedure*, which can be seen in Figure 4.6. This model begins with an initial statement of a need, and the first design activity is analysis of the problem, which comprises according to French: i) a proper statement of the design problem, ii) limitations placed upon the solution (e.g. codes of practice, statutory requirements etc.), iii) the criterion of excellence to be worked to.

Alternatives are generated in the form of *schemes* during the conceptual design phase. This stage is the most creative part of the process and has a profound influence on the final outcome. The alternatives are elaborated in greater detail during *Embodiment of Schemes* and, if there is more than one, a final choice is made between them. These steps are repeated when the alternatives do not meet the criteria. Finally the best option is completed in the detailing phase, after which it should be ready for implementation.

The final stage of the process is the communication of the design to other disciplines in the development process, such as marketing. French' model also describes the design process and explicitly focuses on the design of technical artifacts that can be both products and processes. In the diagram, the circles

represent stages reached, or outputs, and the rectangles represent activities, or work in progress.

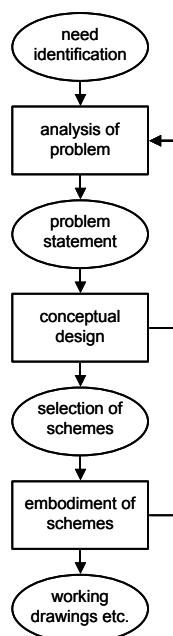


FIGURE 4.6 FRENCH' DESIGN SEQUENCE

Sinnott

The sixth volume of Coulson and Richardson's handbook on Chemical Engineering deals with chemical engineering design (Sinnott 1993). In this handbook, a sequence for conceptual process design is presented as given in Figure 4.7. Such a sequence is different from the design methodologies, discussed in section 4.2.2 (Four textbooks on conceptual process design), because it is meant as a *descriptive* design methodology.

The design sequence consists of several main stages, which have to be completed before accomplishing the final design. These steps are, reduced to three, the *Design Specification and Collection of Data*, the *Generation of Designs*, and the *Selection, Evaluation, and Optimization*.

Design Specification and Collection of Data; in this phase, the designer should obtain, as complete and as unambiguous as possible, a statement of the requirements. The real requirements have to be elucidated through discussion, as it is important to distinguish between the real needs and the wants. The designer should also assemble all the relevant facts and data, this will include information on possible processes, equipment performance and physical property data. How this stage is performed is dependent on the background of the designer. Many design organizations will prepare a basic data manual, containing all the process know-

how on which the design is to be based. Most organizations will have design manuals covering preferred methods and data for the more frequently used, routine, design procedures. The constraints, particularly the external constraints, should be identified early in the design process.

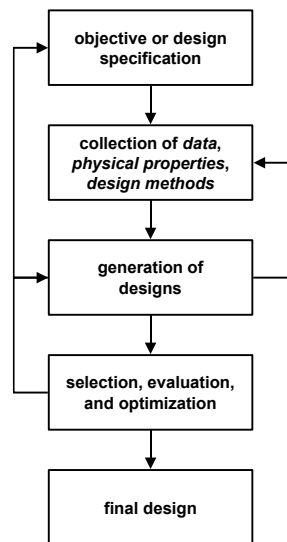


FIGURE 4.7 SINNOTT'S DESIGN SEQUENCE

Generation of Designs; only a very small fraction of the information needed to define the design problem is available from the problem statement. To supply the missing information, assumptions have to be made about what types of process units should be used, how those process units will be interconnected, and what temperatures, pressures and process flow rates will be required. This is the synthesis activity for which methods like hierarchical decomposition or superstructure optimization can be used, see also Chapter 3.

Selection, Evaluation, and Optimization; after completing all possible solutions, they have to be analyzed to make sure they correspond to the previously defined boundaries and requirements. After this, the best candidate has to be selected. This can be done by a process of progressive evaluation and selection, which narrows down the range of candidates to find the best design for the purpose. The selection process can be considered to go through the following stages: i) possible designs (credible), i.e. within the external constraints, ii) plausible designs (feasible), i.e. within the internal constraints, iii) probable designs, i.e. likely candidates, iv) optimal designs, i.e. judged the best solution to the problem, based on criteria. Note that the above-described steps are part of an iterative process.

Cano-Ruiz

Cano-Ruiz (Cano-Ruiz and McRae 1998) gives a similar model for the design methodology, the difference is that the problem-framing is now concurrent to all

the remainder design steps, see Figure 4.8. In this way, it becomes clear that the interaction between problem statement and final result is very important. The problem statement delivers system boundaries, uncertainty constraints, and even stopping rules that define the performance of the decision-making process during the design.

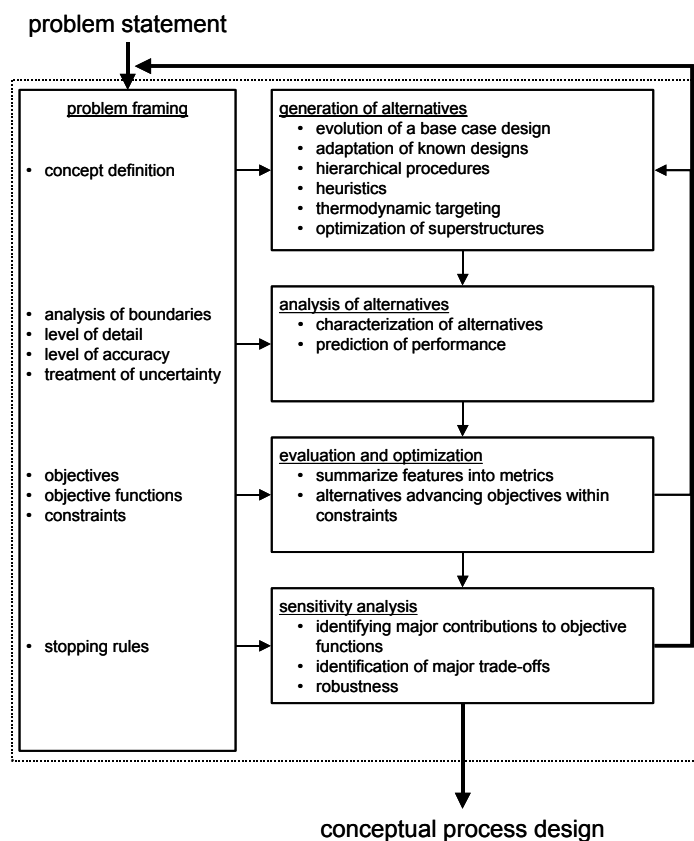


FIGURE 4.8 CANO-RUIZ' DESIGN SEQUENCE

Sirola

Sirola (Sirola 1996) provides a detailed model for the design procedure of chemical processes, see Figure 4.9; the author considers the analysis as a distinct phase. Furthermore, the generation of alternatives is called *synthesis* and shows an internal analysis loop. In fact, alternatives are not generated blindly but are guided by synthesis methods and guidelines so that they are conceived with anticipation to the desired performance.

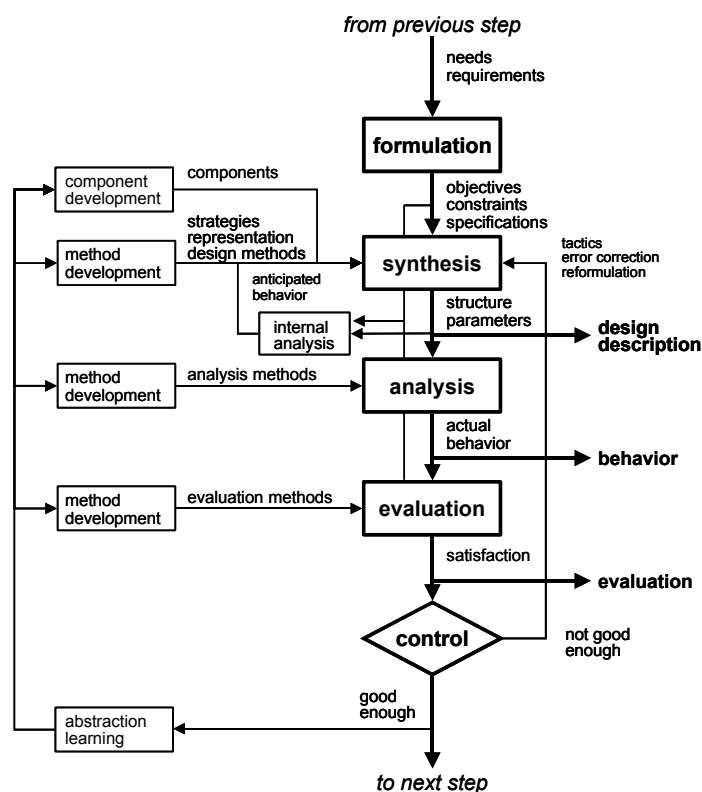


FIGURE 4.9 SIROLA'S DESIGN SEQUENCE

Concluding remarks on design sequences

In this section, various design sequences are discussed; three concluding remarks can be made. Firstly, general design methodologies mainly focus on prescriptive decision-making like the methodology of Cross and in a more extended form by French; although these design methodologies pretend to describe the entire design process. Secondly, the methodology by Sinnott is meant to help designers to find a structured way through the decisions that have to be made and the knowledge that have to be generated during the design. Thirdly, the more extended methodologies of Sirola and Cano-Ruiz give a place to the common practice design methods of the chemical engineering field along a decision-making structure like those presented by French and Cross. In this way the structure of those methodologies tend to be rather complex, but it is still rather difficult to present in a simple and logical way the iterations that have to take place.

In conclusion, it is stated that the presented design methodologies only are describing the design process, without making explicit how to deal with the complexity that will be met by the designer. A reason for that behavior could be the wish of the authors to present a prescriptive methodology based on experience. In

that way the methodologies are focused on how the practice should be, rather than how the practice really is.

The presented design sequences are summarized in one figure (Figure 4.10); later in this Chapter, this simple model will be extended to the decision-making sequence as the heart of the newly developed design methodology.

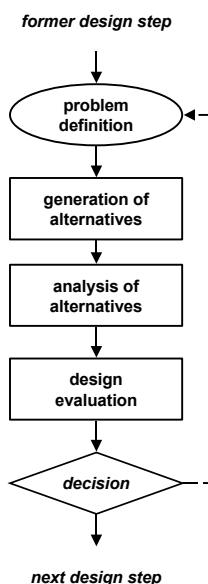


FIGURE 4.10 DECISION-MAKING SEQUENCE AS USED IN THIS THESIS

4.4 Demands to the design methodology development

One of the hypotheses of this thesis is that if structured ways are introduced to make constraints and criteria explicit during the design, *integrative solutions* can be reached and *innovation paths* can be traced. In that way, sustainable development of the chemical industry can be obtained. This changes the design methodologies and procedures and some specific demands are distinguished for a design methodology. In this section, the distinction is made between demands from a *sustainability perspective*, an *engineering perspective*, and a *methodological perspective*.

4.4.1 Sustainability perspective

The following demands can be given from a sustainability perspective:

- Mainly, incorporation of sustainability during design has to do with the problem definition from a sustainability perspective and the evaluation afterwards that ensures that the design really contributes to sustainable development. This implies that a well-defined link between the problem definition phase and the evaluation phase must be present, to ensure that the

design deals consistently with external factors and trade off. This link defines the structure of the methodology and asks for the development of design methods for structured problem definition, structured decision-making, and evaluation methods.

- Innovation towards a sustainability direction asks for new and inventive ideas. Thus, tools have to be improved or developed, that structures the generation of alternatives. In this way the integrative or synthesis part of the design can be focused more constructively towards sustainability considerations by using hints, guidelines, creativity, intuition etc. New design methods have to be developed that effectively deal with the issues of the sustainability debate and translate vague and broad societal considerations into concretely defined chemical engineering criteria

It is emphasized here that these points are not mentioned so explicitly in discussions about sustainable design at this moment. Many discussions about sustainability are focused on the question how a certain problem (e.g. minimization of waste, heat integration) can be solved. However, not only the content (*how to solve*), but also the structure (*in which order*) have to be considered if the above-mentioned two demands have to be met.

4.4.2 *Engineering perspective*

In general, designing is the main umbrella for all specific engineering disciplines, this is sketched schematically in Figure 4.11. Every engineering discipline has its own way of designing; so many approaches and procedures exist. The larger part of all those design approaches seems to be the same, so all this knowledge is integrated to a general design methodology. From literature and experience, the following guidelines for the development of such a new design methodology for sustainability are suggested:

- Use a progressive design procedure; the framework of the procedure is equal for all kinds of design, the filling-in of the steps depends on the nature of the design. The design procedure conceptualizes and structures the approach of the design problem and locates appropriate design methods. This is important, because in this way the design methodology can function as a common language between various disciplines.
- Every step of the design procedure is a clearly defined decision-making step. Designers are trained in structured decision-making with lack of information, this skill is very useful and helps to work efficiently
- The methodology and the methods should increase the insight of the designer into the whole product and process innovation cycle and also increase the openness towards other design disciplines.

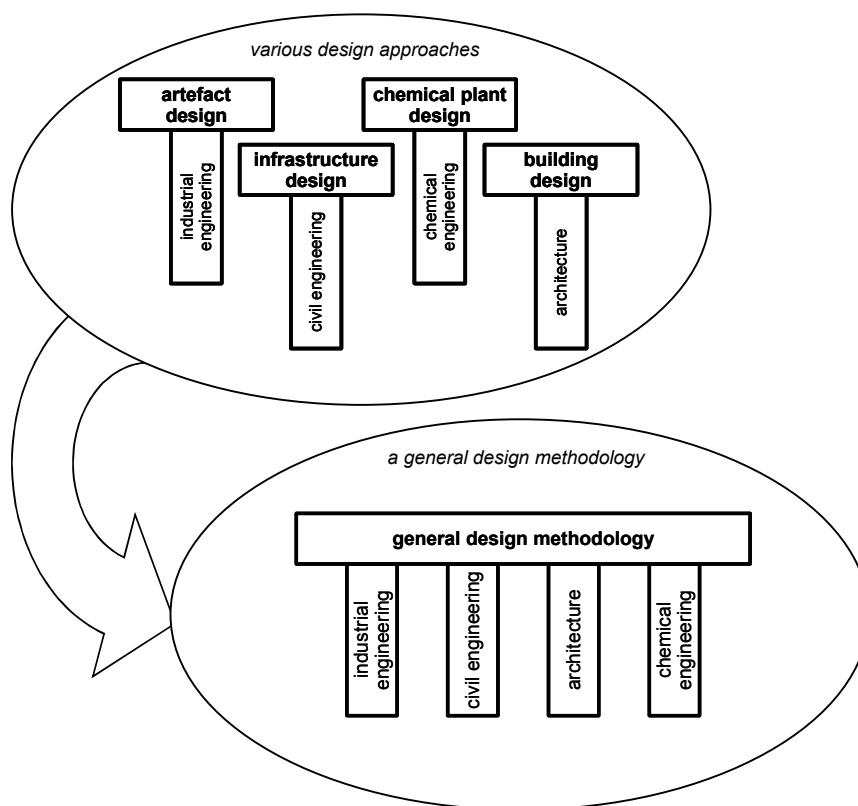


FIGURE 4.11 TOWARDS A GENERAL DESIGN METHODOLOGY

4.4.3 Methodological perspective

From a methodological perspective, the following demands can be set to the methodology:

- For sustainable development of the chemical industry, it is essential that the process designer can explore a free space in the beginning of the design. This design freedom ensures innovation and creativity; freedom can be obtained by aiming at least information for the first stage of design.
- Develop a framework by which designers can determine which method leads to the most sustainable outcome of their design problems; the design framework should be flexible to the application towards different design cases (Macmillan, Steele, Austin, et al. 2001). A methodology should be generic in order to be used for a wide range of applications, but specific to be practical at a working level. Developing a general methodology that can be made specific by the use of design tools can solve the problem this contradiction possesses. It should be clear what the scope and purpose of the tool is, and how results should be treated, and valued.

- The design methodology and the design methods are developed concurrently in this research and in the same way their application should be done concurrently in the design practice. In this way the integration of design methodology and design methods is ensured. It is really important that design methods reflect the constraints and criteria as should have been defined in the objective definition phase.

4.5 The new design methodology

The new design methodology is now presented; it consists of three main parts: 1) *Decision-making sequence*; this is a prescriptive model, which forces structured decision-making, 2) *Design framework*; this is the general framework consisting in various iterating decision-making steps that describes the levels of detail; the framework is dependent on the engineering context, like in this thesis the two frameworks for process and product design 3) *Design tools*; these tools help the designer in being creative and in taking rigid decisions.

Process design tools form a part of the overall process design methodology. The design methodology presents a framework for the steps in the development of a conceptual design, whereas a design tool performs a certain part of the conceptual design. The new design methodology comprises all the employed tools, their interaction and their integration.

4.5.1 *Decision-making sequence*

During the design many decisions are taken. Based on literature (as presented in the first part of this Chapter) a *prescriptive* model can be proposed: the decision-making sequence, see also Figure 4.10 and Figure 4.12. This model is prescriptive, which implies that the designer is forced to do the decision-making along the stages of the sequence. This decision-making sequence consists of five stages, each containing three detailed elements: 1) problem definition, 2) generation of alternatives, 3) analysis of alternatives, 4) design evaluation, and 5) decision.

Decisions are taken continuously in every step and every stage of the design trajectory. Thus, it can be argued that the behavior of the decision-making sequence is behaving like a *fractal*; every larger design decision consists of smaller partial decisions. Every time a decision step is magnified, various partial decision steps appear, as schematically shown in Figure 4.13. In this thesis, however, this behavior is not considered explicitly, but it emphasizes the importance of decision-making during design and it makes clear that the more the design methodology is expanded, the less generic the methodology becomes. The extent to which the methodology is specified depends strongly on the design team.

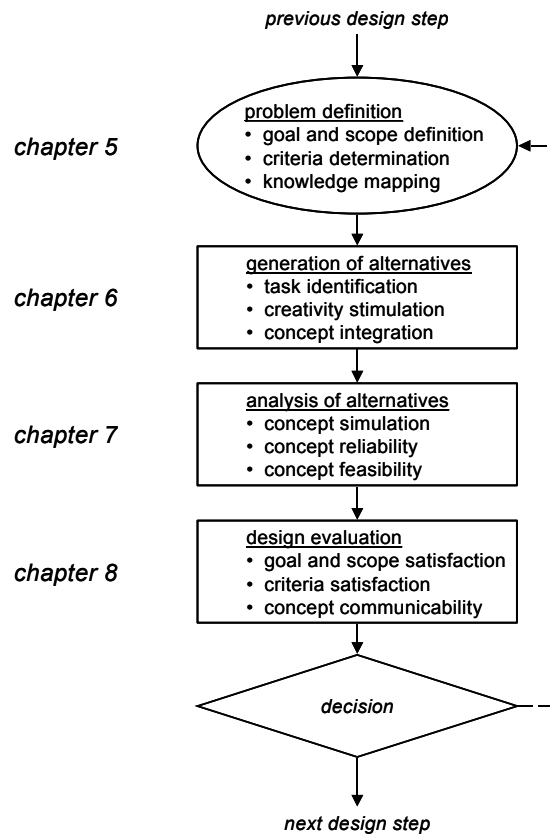


FIGURE 4.12 EXTENDED DECISION-MAKING SEQUENCE

During this decision-making various tools and methods can be very useful and the designer is free to choose which method is used during the decision-making. Below the five stages of the decision-making sequence are discussed; those steps are also used as setup for the following Chapters on design tools.

Problem definition (see also Chapter 5)

The system boundaries are defined at the start of the project. From the perspective of sustainability the designer is responsible for the effects and controllability of every flow (both mass and energy) entering or leaving the system to be designed. Additionally, the designer should obtain as complete and as unambiguous as possible a statement of the requirements. The problem is defined in the following terms, which are the three elements of this decision-making stage:

- *Goal and scope definition*; The goal and its constraints have to be defined as part of the problem definition. The best way to do this is, is by setting hypotheses or clear objectives. The direction of the design is set by needs, and limited by the final conditions, which a design has to meet.

- *Criteria determination*; The criteria specify the final requirements of the product. The criteria are used at the end of the cycle to evaluate whether the synthesized answer is the real answer to the problem. Criteria have to be set clearly in the beginning of the design project and should decide in which way the criteria are evaluated at the end of the design.
- *Knowledge mapping*; Investigation of available knowledge, gives the designer insight in possible solutions within the given time-span. The designer should also assemble all the relevant facts and data, this will include information on possible processes, equipment performance and physical property data. From the perspective of sustainability, it is important to be knowledgeable of (newly developing disciplines) such as Green Chemistry, Industrial Ecology, Pollution Prevention, Life Cycle Assessment, etc.

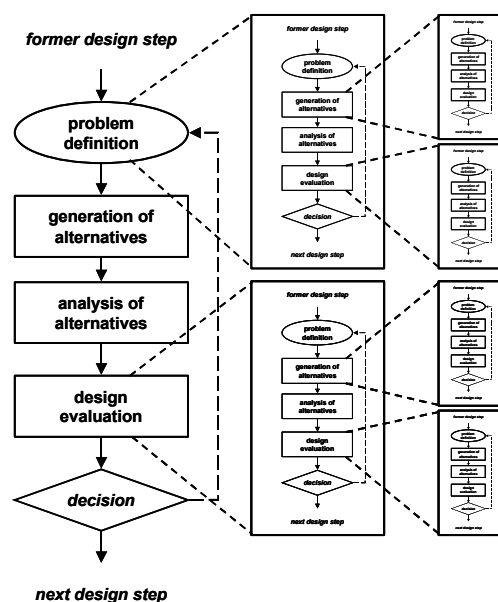


FIGURE 4.13 BEHAVIOR OF THE DECISION-MAKING SEQUENCE

Generation of alternatives (see also Chapter 6)

Only a very small fraction of the information needed to define the design problem is available from the problem statement. To supply the missing information, assumptions have to be made about the kind of solutions. This part is the most creative part of the design in which decisions are made by experience and intuition. Existing chemical engineering methods mainly focus on this or the next stage with specific interest for unit design and flowsheet design; denoted as the synthesis activity (Douglas 1988). The generation of ideas depends on the following elements:

- *Task identification*; in the preceding decision stage, the design problem is defined; mainly this is done as a question for which an answer has to be found. Such a question is not necessarily formulated as an engineering assessment. Thus in the generation of alternatives stage, it is for most important that the designer in some way reduces or decomposes the abstract problem to one or more design tasks. Design tasks are defined here as: unambiguous design problems that fit in consistent decision-making. Later it is needed that those tasks are evaluated and it is checked that the reduction to functions did not lose the value of the original design problem.
- *Creativity stimulation*; being creative gives the designer the possibility to come up with non-trivial or even innovative solutions. So in every decision-making sequence, it is important that it becomes clear how the creativity can be improved. This can be done by various tools, like associative methods, creative confrontation methods, or analytic systematic methods (Roozenburg and Eekels 1995). In this way solutions and ideas are generated to the various tasks that are identified.
- *Concept integration*; the problem was decomposed into various tasks, then ideas for solutions were created and now, at the end of the synthesis activity, the solutions should be integrated to one concept or some concepts. A concept is defined here as an integral solution or answer to the given design question.

From generation of alternatives to analysis of alternatives

In the analysis of alternatives stage an idea from the generation of alternatives stage is rejected or accepted. In practice, the iteration between the generation and analysis step is highly frequent and mainly done implicitly in one stage, but it is crucial to distinguish between those stages to ensure transparent explicit decision-making. The feedback from the analysis stage to the generation stage is a decision as well. It is important to emphasize that a separation between the analysis and generation stage makes the design more structured and forces the designer to make more deliberated decisions.

Analysis of alternatives (see also Chapter 7)

After completing all possible solutions, they have to be analyzed to make sure they are feasible within the goal and scope of the design trajectory. In other words, this decision stage has to ensure that the alternatives are no nonsense. Therefore, the following elements are considered:

- *Concept simulation*; if the design is performed well, it generates rather new concepts. This is nice, but it also places the designer for the difficulty of how to assess the properties of something that does not exist. Therefore it is necessary that in some way the concept is represented by common knowledge, in such a way that the idea is communicative to colleague designers. For example, in the early steps of the design this can be done by a rough sketch, while in the later steps the design is represented by a detailed prototype.

- *Concept reliability*; in every stage of the decision-making sequence assumptions are made, it is very important that as far as possible those assumptions are made explicit and their relation is clear to the designer or within the design team. It can be very helpful to use a logbook for this or even to draw a tree of all made assumptions and their derivatives.
- *Concept feasibility*; from the scope and goal setting of the problem, it should be clear for which (engineering) field or which time span the design is performed. This limits the feasibility of possible solutions; for example if a process or product has to be realized within a few years, only concepts based on existing and proven knowledge can be taken into account. Besides that the feasibility of the concept is also dependent on physical and chemical laws, which also should follow from the simulation step.

Difference between analysis of alternatives and design evaluation

The analysis of alternatives stage is meant as a check to which extent the proposed solution fits within the given design problem. In the design evaluation stage, more value-laden criteria are used to decide whether the solution is satisfying towards the stakeholders. This implies that the analysis step is seen as a more scientific assessment done by the designer (e.g. there is no loss of mass or the solution is technologically feasible within the current state-of-art, etc.), while the evaluation step is more normative, done by societal groups (e.g. it is expected that people like this design, or sustainable development can be guaranteed, etc.).

Design evaluation (see also Chapter 8)

After the analysis phase it still is possible that various alternatives exist, which are all possible and challenging solutions to the given problem. The expected properties of the alternatives, following from the analysis have to be compared with the criteria from the problem definition stage. The difference between the criteria and expected properties gives the design a value. On the basis of this value the decision is made which of the alternatives is passed to the next design step. From the design evaluation stage it becomes clear if a design really meets the needs of the design problem. Also in the case that only one solution passes the analysis stage, it should be ensured that all criteria and requirements of the problem definition are passed. This is done by three elements:

- *Goal and scope satisfaction*; during the decision-making many assumptions are made and mainly the original problem is reduced to some extent, therefore in the final stage it should be ensured that the original design problem is solved and that the given solution is not beyond the scope of the given system boundaries. This and the next element actualize the statement that a strong link should exist between the problem definition and the design evaluation stages.
- *Criteria satisfaction*; the criteria determined in the problem definition stage have to be met by the design concept. This implies that a trade-off should be made between the various external factors that play a role in the complex decision-making during chemical product and process design.

- *Concept communicability*; the final concept has to be transferred to the next level of detail, this means that all assumptions, criteria, and definitions should be reported in such a way that the decision-making is transparent. Doing this in a structured way makes it an integral part of the evaluation stage, because it forces the designer(s) to be consistent and structured.

Decision

Based on all the steps above a final decision can be drawn, it is still possible to go back to the problem phase and walk again through the decision-making sequence. After the decision is taken, the final result goes further to the next level of detail in the design framework. Then it is not possible anymore to make an iteration step.

4.5.2 *The design framework*

The decision-making sequence provides a structural model to the problem definition, problem solving, and solution evaluation. However, this model does not make explicit how to deal with levels of detail during the design. Although a design could be performed with the decision-making sequence only, it is more reliable to deliver a framework for the iterations path that have to be followed by the designer. Here a proposal is given of the various design steps that are passed by during the chemical process design up to the detailed engineering phase. This is called the *design framework* and can be seen as a *descriptive* methodology based on the practice of the chemical engineering field. The design framework lines up the various design steps from need to construction. Within those steps, the stages of the decision-making sequence are repeated; the detail level of the decision-making depends on the step size between two design steps. The design framework can be changed depending on the design practice that exists within an institute or company.

In Figure 4.14 and Table 4.5 the design framework is presented. In Chapter 9, this model will be used for chemical *product* design. The remark is made here that the steps are ranked in a graduated level of design detail. Studies like concurrent engineering investigate the possibilities to perform various levels simultaneously, this is not taken into account here, but with the use of knowledge on this topic, it would be possible to use this method along with other models. This makes the design framework flexible to both a hierarchical and a concurrent approach.

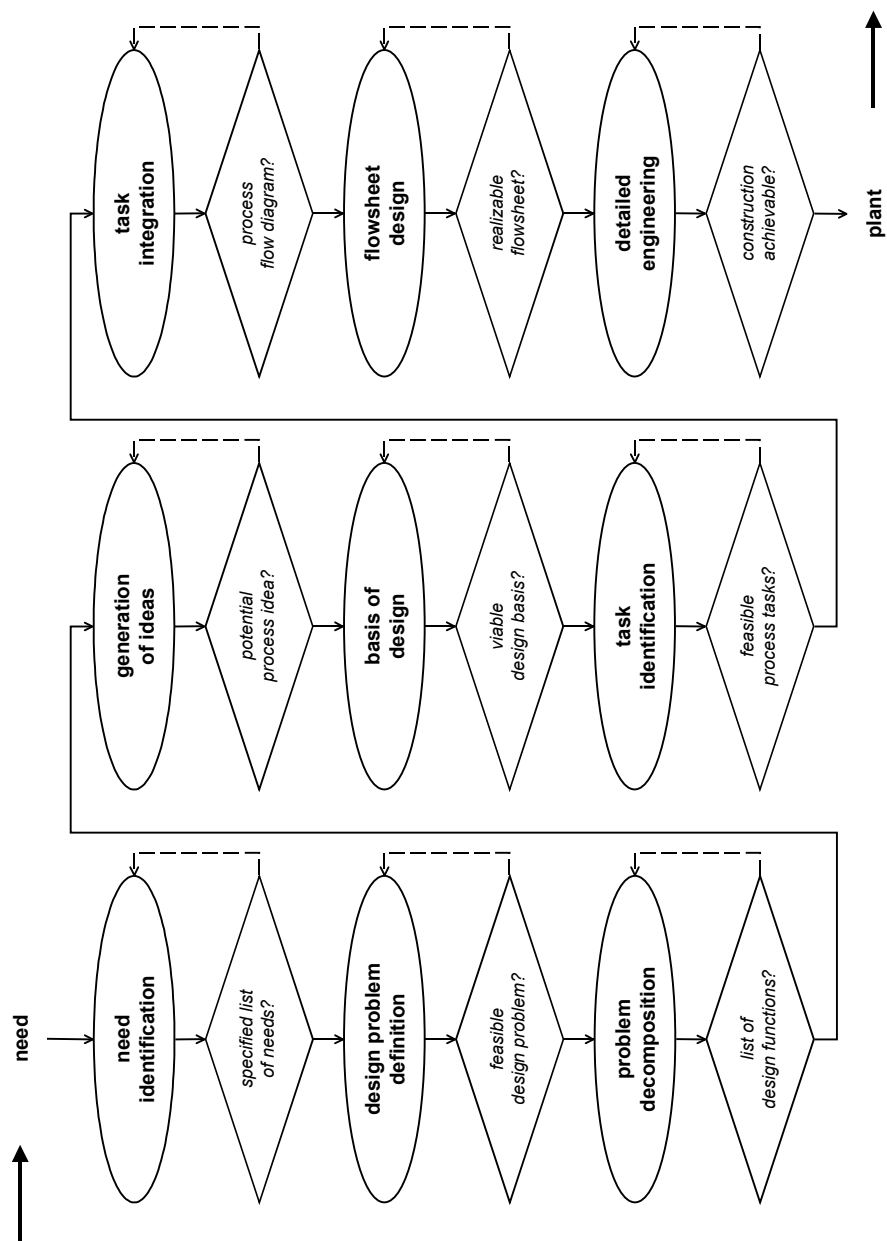


FIGURE 4.14 GENERAL DESIGN FRAMEWORK FOR CHEMICAL PROCESSES

TABLE 4.5 GLOSSARY OF THE DESIGN FRAMEWORK

need identification	The whole design project starts with a question for the fulfillment of a need, its character can be societal, economical, environmental, and technological. <i>specified list of needs?</i>
design problem definition	From the need a design problem is derived that can be solved within given constraints. Together with the design problem, the system boundaries and the evaluation criteria are defined. <i>feasible design problem?</i>
problem decomposition	Mainly, the identified needs and the derived design problem are abstract and can be solved in many ways. Thus, the designer decomposes the design problem in various design functions. <i>list of design functions?</i>
generation of ideas	Possible solutions are generated based on the existing knowledge, experience, and creativity. These are rough ideas of basic chemistry, plant innovation, market strategy or whatever. <i>potential process idea?</i>
basis of design	While the final result is a chemical plant, the designer or the design team have to come up with a design basis that, within the given goal and battery limits, ensures that a solution is feasible. <i>viable design basis?</i>
task identification	Within the basis of design, tasks are identified that represent the original design problem and that give the possibility to be innovative. <i>feasible process tasks?</i>
task integration	The various process tasks are integrated into an optimal flow diagram along with correct mass and energy balances, based on simulation results. <i>process flow diagram?</i>
flowsheet design	In the flowsheet generation, a conceptual process flow diagram is created that the critical specifications of the process. Evaluation on economics, safety, health, environment, and sustainability is performed. <i>realizable flowsheet?</i>
detailed engineering	The process unit operations are designed in order to manufacture on large scale. The plan for construction is developed, in such a way that the decision for final construction can be made. <i>construction achievable?</i>

The design framework is constructed by combination of the authors practical experiences with conceptual process design and literature sources, like the general innovation cycle by Siirola (Siirola 1995), see also Chapter 3. Besides that the design framework follows a same structure as the decision-making sequence, while going from the first to the final level more and more detailed information is gained, see Figure 4.15 (compare this also with Figure 4.13). The structure ends with a

decision stage, which is the final management decision to conclude that the design can be realized as operational plant.

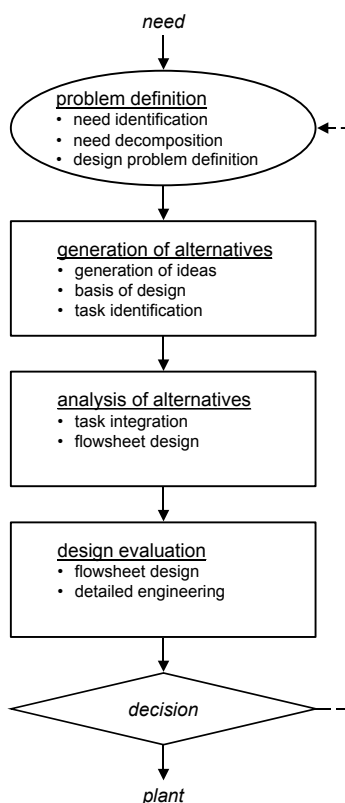


FIGURE 4.15 THE DESIGN FRAMEWORK AS A DECISION-MAKING SEQUENCE

4.5.3 The design tools

The design framework, presented in the former section, can now be filled with design tools. In Table 4.6, this is done for existing tools related to environmental and sustainable engineering. After that, in Table 4.7, the tools developed in the rest of this thesis are presented.

The design framework and existing green-engineering tools

Table 4.6 is based on some main references from the chemical engineering field, from the last five years. It is not pretended to give a profound overview of the chemical engineering field, but it only illustrates how the various tools fit in the proposed general design framework. Besides that it shows clearly where gaps have to be filled in the sustainable chemical engineering field.

The following groups of tools or approaches are distinguished:

- CD: *(environmental) criteria definition* (Herder and Weijnen 1998; Kheawhom and Hirao 2002; Lemkowitz, Korevaar, Harmsen, et al. 2001; Sharatt 1999)
- CP: *cleaner or greener production* (Boyle 1999; Brennecke 2000; Dunn and Bush 2001; Khan, Natrajan, and Revathi 2001; Pauli 1997; Pereira 1999)
- ECM: *environmentally conscious manufacturing / design* (Allen and Shonnard 2002; Brennecke 2000; Cano-Ruiz 2002; Cano-Ruiz and McRae 1998; Gungor and Gupta 1999; McAloone 2000)
- GC: *green chemistry* (Anastas and Breen 1997; Curzons, Constable, Mortimer, et al. 2001; Lankey and Anastas 2002; Mulholland, Sylvester, and Dyer 2000; Sheldon 1994)
- LCA: *life cycle approach* (Alexander, Barton, Petrie, et al. 2000; Azapagic and Clift 1999; Burgess and Brennan 2001; Ishii 1997; Lankey and Anastas 2002; Mellor, Wright, Clift, et al. 2002)
- NI: *need identification for sustainability* (Jansen 2003; Lemkowitz, Harmsen, and Nugteren 1999; Lemkowitz, Korevaar, Harmsen, et al. 2001; Robèrt, Schmidt-Bleek, Aloisi de Larderel, et al. 2002)
- PI: *process intensification* (Harmsen, Korevaar, and Lemkowitz 2003; Stankiewicz 2003)
- PP: *pollution prevention* (Anastas and Breen 1997; Berger 1999; Cano-Ruiz and McRae 1998; Mulholland and Dyer 1999; Oldenburg 1997)
- SCM: *supply chain management* (Backx, Bosgra, and Marquardt 1998; Baumann, Boons, and Bragd 2002; Hall 2000)
- WM: *waste minimization / closing the cycles* (Dantus and High 1999; Mellor, Wright, Clift, et al. 2002; Mulholland, Sylvester, and Dyer 2000; Sheldon 1997; Young, Scharp, and Cabezas 2000)

Table 4.6 shows that the green engineering design tools can be located in the design methodology. It also clarifies that the methodology is a guideline for the development of new design tools, because the empty spaces give clear definition of the tools that have to be developed for the design of sustainable chemical processes. From Table 4.6 it becomes clear that at least for the following design steps design tools have to be developed: i) problem decomposition tools regarding to sustainable development, ii) structured problem definition tools for the more detailed process design steps, iii) evaluation tools for the more detailed process design steps.

The design framework and new design tools presented in this thesis

Here the design tools and their location in the design framework is introduced. The following Chapters discuss the tools in more detail, these Chapters are organized along the four steps of the decision-making sequence, see also Table 4.7. All tools are developed or evaluated in the specified location or locations, e.g. the Chemical route selection tool (CRS) is used for the determination of chemical routes during the basis of design phase. This does not mean that the tools are exclusive for only that location; for sure it would be possible to use them on more locations in the design methodology. However, this is not validated during this thesis, but can be done in follow-up research or case studies.

TABLE 4.6 EXISTING DESIGN TOOLS FROM THE GREEN-ENGINEERING FIELD

<i>Design framework</i>	<i>Decision Diagram</i>			
	Problem	Synthesis	Analysis	Evaluation
Need identification	CD NI		CD NI	CD
Design problem definition	CD		CD	CD
Problem decomposition				
Generation of ideas	GC SCM	GC SCM	GC SCM	
Basis of design	GC SCM	GC SCM	GC SCM	
Task identification	GC	GC	LCA	
Process integration		CP LCA PI	CP LCA PI	LCA
Flowsheet design		LCA PI PP WM	LCA PI PP WM	LCA
Detailed engineering		ECM PP	ECM PP	

TABLE 4.7 LOCATION OF THE DESIGN TOOLS DEVELOPED IN THIS THESIS

<i>Design framework</i>	<i>Decision Diagram</i>			
	Problem	Synthesis	Analysis	Evaluation
Need identification				
Design problem definition	DSR			ESC ¹⁾
Problem decomposition				
Generation of Ideas				SRT
Basis of design	SBDCC	CRS		
Task identification				
Process integration		GPS	EA	
Flowsheet design				
Detailed engineering				
<i>Description tools</i>	Chapter 5	Chapter 6	Chapter 7	Chapter 8

¹⁾ Described in Chapter 9

Decision sequence ranking tool (DSR)

The decision sequence ranking tool helps the designer to make decisions based on intuition and network analysis. The designer or the design team gives a value to every relation between a pair of decisions. Then the average is calculated and a hierarchy is derived, which gives insight into which alternative most influences the others and therefore should be decided first. This tool is applied to some industrial cases and it appeared to be very fruitful in facilitating decisions making in a complex situation involving many external factors. The tool gives a decision path for the design and in that way it defines the design problem definition.

Evaluation of sustainable consumables tool (ESC)

The problem definition for a sustainable product design can be evaluated by using a matrix in which values can be given to the possible contributions that can be made to various areas. This tool is developed by application in an industrial case and helps to make a problem definition in such a way that it incorporates all of the most important sustainability topics.

Sustainability ranking tool (SRT)

Often many ideas are available after a brainstorm session, from which the most sustainable one should be chosen. This SRT gives a value to a broad collection of ideas and gives insight in which idea contributes the most to sustainable development. The tool is developed in an industrial case for a chemical process design.

System boundaries definition and closed cycles tool (SBDCC)

The way, in which system boundaries are defined, often makes the difference between a sustainable design and a conventional design. Essential in sustainable development of chemical processes and products is the concept that the design team is responsible for every flow that is entering and leaving the system boundaries. Therefore this tool is very useful in stating a sustainable design problem.

Chemical route selection tool (CRS)

A chemical route selection tool is developed, based on insight from the exergy concept, which helps achieving efficient use of energy and mass. The exergy concept mainly is used as an analysis tool for chemical processes, but here it is also useful for comparing chemical routes without any process information. The CRS tool is useful in defining the basis of design.

Guidelines for process synthesis tool (GPS)

Based on the exergy analysis of various processes, guidelines can be derived that help the designer to integrate the different process tasks into one process concept. In this way experience and theory are condensed to a simple list of rules of thumb that can be handled during decision-making. It also avoids the tendency to generate many details that only block the progression of the design project.

Exergy analysis tool (EA)

After the concepts are integrated to a process, an exergy analysis can give insight in the level of heat integration. The level of exergy loss is a measure for the energy efficiency of the process operation, which can be used as a measure for the sustainability of the process.

4.6 Concluding remarks

In this Chapter, a comprehensive methodology for the design of chemical processes and products is introduced. The methodology is based on existing chemical engineering practice, insight from other engineering disciplines, and industrial experience. The methodology presented here consists in three parts: 1) a general procedure, 2) structured decision-making, 3) methods for design. The structured decision-making model is the heart of the design methodology, consisting of a problem definition phase, a generation of alternatives phase, an analysis of alternatives phase and an evaluation phase.

It is concluded that a design methodology for sustainable chemical engineering has the following characteristics:

- A structured design methodology improves the quality of the design and the efficiency of the design process by creativity stimulation and the stimulation of incorporating external factors.
- The present textbooks on chemical process design are mainly written from a technological-economical perspective. As a result, sustainability metrics, guidelines, and analysis methods are needed to support the evaluation of non-economic issues more as they do now.
- Comparison of the chemical *process* design with a chemical *product* design strategy shows two main differences: i) the incorporation of consumer demands throughout the design of a chemical product is rather usual; this makes the methodology rather flexible to external factors; ii) the use of creativity and intuition during the design is an integral part of the chemical product design, as it is for the design of technological artifacts in general. The chemical process designer can learn from this by the use of creativity and intuition-based methods for the generation of conceptual process design.
- Four important characteristics of a design methodology are discussed, which are the basis of the design methodology presented in this thesis: i) design as a problem definition procedure, ii) design as a satisfying activity, iii) design as a concurrent approach, iv) design as a decision-making sequence.

Chapter 5

SUSTAINABLE PROCESS DESIGN METHODOLOGY, PART I: *PROBLEM DEFINITION STAGE*

Summary *The design problem definition stage consists in three elements: 1) the goal and scope definition, 2) the criteria determination, 3) the knowledge mapping. These three elements are elaborated in this Chapter, together with an important tool that is evaluated during this research: the identification of stakeholders. Then two tools, developed during this research, are described extensively and illustrated with case studies: the decision sequence ranking tool and the system boundaries and closed cycles tool.*

5.1 Problem definition (see also Chapter 4)

In the first phase of the design, the problem has to be defined precisely. Mainly designers are confronted with a question like ‘produce a certain amount of a product per year’. Such an assignment is given within an industrial context, which implies many boundary conditions, like utility facilities, infrastructure, feedstock availability, and existing unit operations. Within all those boundary conditions, a design has to be made, which is an (sub)-optimum regarding given constraints.

In this problem definition phase, the direction of searching for the sustainable solution can be decided. The coherence between physical and normative aspects of sustainability is crucial in this stage and the involved external parties must be concerned, the so-called stakeholders. The goal and the scope of the design study are thoroughly analyzed, so that at the end a more exact project goal can be formulated. If the project concerns the design of a new artifact and no concept exists at this stage, it is necessary to first identify a reference design.

In Chapter 4, it was discussed already that the problem definition stage consists in three elements: 1) *Goal and scope definition*, 2) *Criteria determination*, and 3) *Knowledge mapping*. In Chapter 4 an introduction was given to these elements, here they are discussed in more detail and after that some design tools are introduced and evaluated.

5.1.1 Goal and scope definition

In this phase the main goal of the design project and the general outline and scope of the project are set. The following subjects should be covered: the *main drivers*, the *level of innovation*, and the *market*.

The *main drivers* for the design are identified, i.e. what are the motivations to do this project? Does knowledge and experience exist on which the design can rely? How does the project idea fit with the company’s business strategies? What is the urgency and the importance of the outcome.

The *level of innovation* of the design must be determined; whether it concerns a product or process improvement, product or process redesign, function innovation or system innovation. This will determine the degree of freedom the designers have. What is the *market* the new product should be launched in, who will be the target group? Possible partners can be identified. Can the company do the project on its own, or should other lines of business be included?

In the scope, the aim of the design is determined and the final requirements are listed. In this case, the design starts with need identification and ends with a conceptual process design; the detailed engineering step is beyond the scope of this thesis (see also Chapter 4). The design steps towards the Conceptual Process Design (CPD) form the earliest part of the process development. Starting from existing knowledge (like chemistry, operation data, catalyst behavior, etc.) and the investigated needs, a new or modified flowsheet is generated, which is the basis of the later engineering steps.

Identification of stakeholders

A specific task in the goal and scope definition stage is the identification of stakeholders. Designers should question whether every need is taken into account at the start of the design project. A *need* is defined as an actual need, or a certain issue that have impact on a stakeholder. Summarizing the needs of the design gives an overview of the functions that the design has to fulfill. In a company context mainly other departments of the company will carry out this step. However, it is rather necessary that all required information on needs and stakeholders is available to the design team.

In the early, exploratory stage of the design process it is important that a basic analysis is performed that helps to signal problems and identifies possible critical issues and gaps in the available knowledge. Besides this, experience has shown that a collectively reached sustainable solution has more legitimacy and is more efficient (Jansen 2003; Robèrt, Schmidt-Bleek, Aloisi de Larderel, et al. 2002). Thus, before a sustainability project is started, a social map should be derived, for which stakeholder identification is a concrete approach.

Firstly, a definition of a stakeholder should be found. A 'stake' can be defined as *an interest, a right (legal or moral) and / or an ownership. From this a (environmental) stakeholder can be defined as individuals or groups with a legal, economic, moral and/or self-perceived opportunity to claim ownership, rights or interests in a firm and its past, present or future activities- or in parts thereof (Madsen and Ulhøi 2001).*

Madsen and Ulhøi (Madsen and Ulhøi 2001) introduce a model to analyse and identify the most significant stakeholder groups and their influence on corporate behaviour. Different categories of stakeholders can be identified, e.g. employees, shareholders, customers, suppliers, regulators, NGOs etc. They can be classified into *primary* and *secondary* stakeholders.

Primary stakeholders are stakeholders without whose direct participation the design or the result of the design can not survive. Such stakeholders include owners, investors, employees, suppliers, customers and competitors, as well as the natural system (e.g. physical resources and carrying capacity).

Secondary stakeholders can be defined as those who in the past, present, or future influence or might be influenced by the design operations. Examples of secondary stakeholders are local communities, local government, social activist groups and business support groups.

Some of the stakeholders can be more easily identified than others. Consumers, who can be considered as the ultimate stakeholder, and internal stakeholders are relatively easily identified and contacted. External business stakeholders can be suppliers, partners, buyers, distributors, etc. External stakeholders that represent the society or the environment are more difficult to recognize. Environment can be split up in local environment, for instance people who live around a factory, and global environment. The latter can be represented by environmental organizations. The last group, stakeholders representing the society, are the most difficult to recognize and consult. These stakeholders can be concerned about issues like health and safety, noise, or very complex issues like equity and problems of developing

countries. Representatives can be the (local) government, international organizations (United Nations) or non-governmental organizations (NGOs).

The depth of the stakeholder analysis depends on the estimated impact a project will have on a stakeholder. Tools exist that help to identify key stakeholders, who should always be consulted. Some important steps to be taken in a stakeholder analysis are the following, adapted from Turner (Turner 1995): 1) identify stakeholders (who are they and what are their stakes), 2) investigate stakeholders (gather information), 3) identify mission (estimate their support/opposition), 4) SWOT stakeholders (what are their strengths and weaknesses), 5) predict behavior (what will they do), 6) make action plans (formulate plans and procedures/ maintain contact with key stakeholders)

Important is that a plan is made that shows which stakeholders should be contacted in each phase of the project. Although it is desirable, it is usually not feasible to contact all stakeholders at the problem analysis phase of the project. It is, however, important to think of their possible objections, and prepare to talk with them in a later stage. An attempt should be made however to contact/consult stakeholders as early as possible in the project. Key stakeholders should always be consulted.

5.1.2 *Criteria determination*

As said before, constraints are the final boundaries that a design has to meet. The direction of any development is given by the needs as discussed in Chapter 2, but sustainable development in particular is limited. The environment, society and economy deliver the constraints of a sustainable production of chemicals, so that the optimum of the final design is somewhere within the triangle. Constraints are defined as the final conditions that a design has to meet, like the return on investment, maximum emission targets, safety of operations, or the acceptability by the stakeholders. The idea of sustainable development is to integrate the aims of all those constraints into one 'best practice' for innovations.

The determination of the design criteria is a specific task for the designer or design team. Here a framework is delivered to come to a coherent set of criteria: 1) conduct a debate on sustainable development, 2) compose a list of general criteria, 3) derive a list of specific criteria.

Debate on sustainable development. While sustainable development still is a moving and changing societal debate, the design team has to carry out a debate on its own definition of sustainable development related to the design topic. For this debate, the text of Chapter 2 and related literature can be used as background. The basic criteria (see Chapter 2) are the framework for a discussion on the sustainable development of the chemical industry: i) ecology-focused principles for sustainable chemical engineering, ii) society focused principles for sustainable chemical engineering.

Compose a list of general criteria. From the debate on sustainable development, a list of general criteria can be composed, for this the checklist of criteria can be used as discussed in this Chapter.

Derive a list of specific criteria. The list of general criteria can be made specific related to the design subject. For this it is necessary to distinguish three kinds of criteria and to determine which kind of criteria is best to represent the meaning of

the design team. The reason for the definition of the three kinds of criteria is the enormous amount of criteria that are available in the field of sustainability and environmental benignity. A designer has to decide which criteria are useful in the particular design, and to make a rationalized consideration. It can then be helpful to formulate criteria in all three categories, in such a way that the relevant issues of the sustainability debate are covered.

Make a framework for criteria evaluation. The sustainability debate considers both hard engineering constraints (like the minimization of emissions) and soft societal criteria (like the inter- and intragenerational inequity). A coherent set of sustainability criteria should cover both areas and also provide a framework for final evaluation. This framework has to be set at this early stage of the design, before the alternatives are generated.

The derivation of sustainability criteria

In the framework presented above, the designers are urged to derive specific and general criteria. In this thesis, three kinds of criteria are distinguished: *knock-out*, *normative*, and *reference* criteria.

Knock-out criteria; formulated as a statement, with the possible answer yes/no; the result is go/no go. For example: *this process runs only on solar thermal energy*. The aim of those criteria is to be able to distinguish very fast between a large number of alternatives, without going into much detail. A knock-out criterion functions as a very rough filter.

Normative criteria; formulated as a question, with a spectrum of answers (e.g. weak/medium/strong, or yes/no/don't know); the result is a weighed trade-off. For example: *this product popularizes environmental thinking and functions as trendsetting*. The aim of those criteria is to qualify in some way the normative aspects of sustainable development in such a way that the results can be weighed and a trade-off can be made.

Reference criteria; formulated as an equation, with relative number as an answer; the result is a measure of improvement or worsening achieved by the alternatives. For example: *the total amount of raw materials used per unit product (kg/kg)*. The aim of those criteria is to quantify the technological or economical progression related to a bench case.

5.1.3 Knowledge mapping

In the problem definition, also an overview should be given of the required knowledge domains. From the perspective of sustainability, it is important to know about fields like:

- green chemistry (Anastas and Breen 1997; Curzons, Constable, Mortimer, et al. 2001; Sheldon 1994)
- industrial ecology (Allenby 1999; Ehrenfeld 1997; Erkman 1997; Graedel and Allenby 1995; Lemkowitz, Pasman, and Harmsen 1999; Mellor, Wright, Clift, et al. 2002; O'Rourke, Connelly, and Koshland 1996)
- life cycle approach (Andersson, Høgaas Eide, Lundqvist, et al. 1998; Azapagic and Clift 1999; Burgess and Brennan 2001; Ishii 1997; Pereira 1999)

- waste minimization or reduction (Dunn and Bush 2001; Young and Cabezas 1999; Young, Scharp, and Cabezas 2000)
- pollution prevention (Berger 1999; Cano-Ruiz and McRae 1998; Dunn and Bush 2001; Gungor and Gupta 1999; Hostrup, Harper, and Gani 1999; Mulholland and Dyer 1999)
- cleaner or greener production (Dunn and Bush 2001; Khan, Natrajan, and Revathi 2001; Pauli 1997)
- environmentally conscious design or manufacturing (Allen and Shonnard 2002; Brennecke 2000; Cano-Ruiz and McRae 1998; McAloon 2000)
- process integration and intensification (Han, Kim, Lee, et al. 2000; Harmsen, Korevaar, and Lemkowitz 2003; Kravanja and Grossmann 1990; Schembecker and Tlatlik 2003; Sirola 1995; Smith 2000)

This kind of knowledge can be obtained by i) literature studies and ii) by a careful composition of the design team. The choice of the final design solution strongly depends on many external factors that can not be influenced by the design team based on engineering expertise only (Herder 1999). Factors like the available data, the available research and development facilities, the applicable licenses, the possibility to use new and other design tools, the involvement of stakeholders, the estimation of market competence, etc. It is strongly recommended that on the first meetings, when the problem definition is discussed, all these factors are made explicit together with their expected influence on the final design. The DSR tool is very useful for this.

5.2 Decision sequence ranking tool

Chemical process design involves a sequence of decisions that have to be made to successfully accomplish the design task. Decision making in the chemical process design task mainly is done based on experience and knowledge, mainly without the use of a tool that facilitates decision-making. At least no tool that facilitates decision-making in chemical process engineering can be found in literature or books on chemical process design.

However, the influence of sustainable development on the chemical industry increases the complexity of all subsystems that could be defined for the chemical industry. This section describes the *decision sequence ranking* tool (DSR) that enhances the structured decision-making during chemical process design, as is illustrated in an industrial case study. The DSR is based on an influence analysis tool, originally developed for scenario planning, but in this research converted to be used for ranking of the influencing factors.

5.2.1 Decision-making in chemical process design

Based on the input of the design task, the design team has to make decisions on, for example, which chemical route to use, which catalyst type would fit best or the process route. Besides that many external and quality factors influence the design, while the designer can not influence those factors. Every decision made will influence other decisions that still have to be made and the possibility to successfully fulfill the design task. An additional difficulty in the decision making in chemical process design is that the conceptual design of a chemical process

involves a wide variety of people within the firm, like the business management, the project manager, the research scientist, the process design engineer, or the safety specialist. All these people influence the design, and all must come to agreement in order to realize the design.

All designers function within a different world of knowledge and experience on the same project. Each of them has unique responsibilities and interests. The overall design task requires that all of the individuals involved join together to plan, decide, critique and integrate their knowledge and experience (Bucciarelli 1994). The decision-making process within the design task is not something that has to be done individually, but is a group activity. Hence, it is possible that difficulties arise on the agreement of a decision, because of conflicting interests or different professional experience and backgrounds.

After the considerations made above and in Chapter 3, it becomes clear that decision-making in a conceptual process design task is complicated for two reasons: i) complexity in decision-making, because each decision influences other decisions *vice versa*, ii) decision-making is performed in a design team of which the members have different knowledge backgrounds and experiences.

5.2.2 *Influence analysis tool in scenario building method*

So, it would help to facilitate decision-making. Therefore, a tool is needed that analyzes the influence a decision has on the other decisions or that ranks the order of decisions. In that way the complexity of the decisions can be untangled. A tool that tackles the decision-making by integrating the different background of knowledge and experience of the members of the design team would at least avoid conflicts because of incompatible interests.

However, no methods or tools are known in chemical engineering that could do this, but in the field of strategic planning management a tool exists that performs an analysis of the external areas of influence that affect a company and assesses the interrelationship between these areas of influence. A team, featuring a diverse mix of specialists, uses this tool in a method to define future scenarios, on which a strategic company planning can be based. A clear and practical description of the influence analysis tool and how it is used in scenario planning is given in the book on *Scenario Techniques* by Von Reibnitz (von Reibnitz 1988). This book is used for the explanation of how the tool works, presented in this paragraph, and is the basis for the remainder of the influence analysis part of this project.

The influence analysis tool is used in brainstorm sessions performed by a multidisciplinary team to set up scenarios that will help in strategic planning. The quality of the resulting scenarios will be influenced by the composition of the team. Therefore, a team should be composed of a wide diversity of specialists who have knowledge, experience and expertise in the subject as well in some other areas of influence.

5.2.3 *Background on network analysis*

The main idea behind this tool is the disentanglement of a complex network. In Figure 5.1 such a network is sketched schematically, it represents 8 different

decisions (A ... H). These decisions are influencing each other and in that way they are influenced by each other.

Some relations between decisions are stronger than other relations, this is sketched with thick and thin lines. The question is now how within a complex network, as depicted in Figure 5.1, the best order can be given for solving the problem. The point of departure is that first a decision should be made on the point in the network that has the most relations with the others, because this point is influencing the others and therefore very *active* in the network. The last decision is made for the point that is not influencing the other points, and thus is *passive* in the network. The tool described below, is focused on how a decision-maker can decide which item has the most influence on the others. Completing a matrix does this, for every item the question is answered: if one item is fixed, does that limit the decision freedom of the others? The answer is given with three numbers: 0 for *no* (no line in Figure 5.1), 1 for *in some way* (thin line in Figure 5.1), and 2 for *yes* (thick line in Figure 5.1).

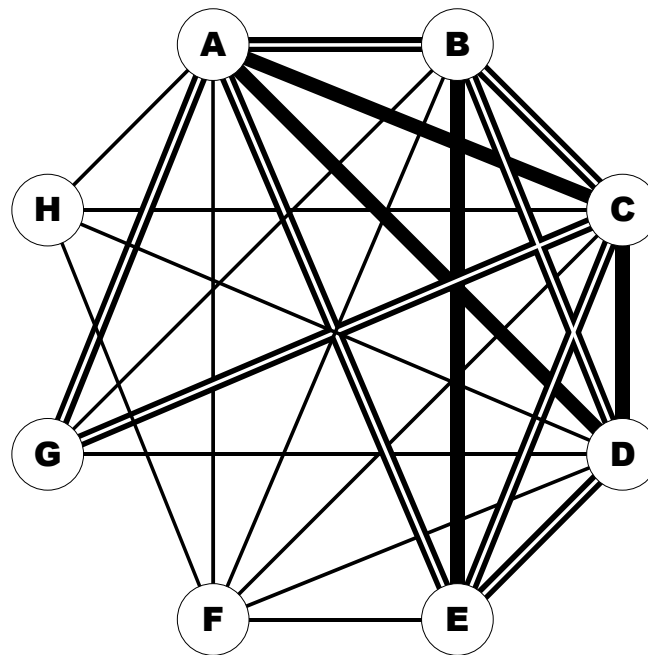


FIGURE 5.1 COMPLEX NETWORK

Identifying and assessing the areas of influence

The influence analysis tool starts by identifying the external areas of influence affecting a company. Typical areas of influence are sales market, competition, legislation, technology, society and economy. Then, for each area of influence, the influencing factors are determined by assessing the interrelationships between the areas of influence. In this way, the extent to which each area, characterized by its

most important influencing factors, influences all the other areas is meant. To find this, every area is compared with every other. This so-called network analysis, normally produced with the aid of a network matrix, results in an active total which expresses for each area the extent to which it influences all the other areas, and a passive total which indicates how much each area is influenced by others.

Network matrix

A network or interrelationship matrix (Table 5.1) determines the influence that each decision has on the others. The network matrix is evaluated from left to right, to find the extent to which each system element affects all the other systems elements. The degrees of influence are weighted as follows:

0 = no influence

1 = weak/indirect influence

2 = strong/direct influence

TABLE 5.1 NETWORK MATRIX FOR FIGURE 5.1

	A	B	C	D	E	F	G	H	act.
A		2	2	2	2	1	2	1	12
B	1		1	1	0	0	0	0	3
C	0	2		2	2	1	2	1	10
D	0	2	2		2	1	1	0	8
E	1	2	1	1		0	0	0	5
F	0	1	0	0	1		0	1	3
G	1	1	1	0	0	0		0	3
H	0	0	1	1	0	1	0		3
pass.	3	10	8	7	7	4	5	3	5,9

Adding the total for each element across the row gives the so-called *active total*, which is the total extent to which one element affects all the other system elements. Adding the columns gives the so-called *passive total* for each system element, which is the extent to which each element is influenced by all the other elements. The sum of the active or passive total, divided by the number of system elements gives the grid, used for defining the fields in the system grid, as will be explained in the next section. When determining the degree of influence it is also important to establish the type of influence that element A has on element B, etc. and to note the justification for the degree of influence on a separate sheet so that the system analysis can later be verified.

The influence assessment is performed by asking the following question for each combination of areas of influence: *If a decision is made in X, does this have a zero or very weak, a weak or indirect, a strong or direct influence on the decision-making for Y?* In other words, the assessment is done from an active point of view and the matrix is completed in a horizontal way from left to right and from up to down.

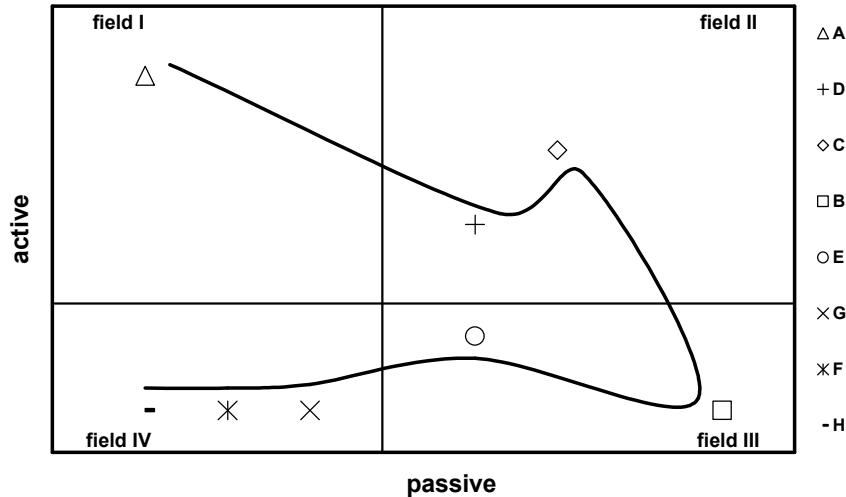


FIGURE 5.2 SYSTEM GRID AND SYSTEM HIERARCHY FOR FIGURE 5.1

System grid

The network matrix can be transferred to a so-called system grid, which for Table 5.1 is presented in Figure 5.2. Such a system grid, exists in four fields, which are produced by taking the mean of the active or passivity total. The fields represent four degrees of activity:

Field I Active field, which contains the active system elements. A relatively high activity and relatively low passivity characterize the elements located in this field. In other words, these elements have a relatively strong influence on all the others in the system and are relatively little influenced by them.

Field II Ambivalent field, which contains the ambivalent system elements. A relatively high activity and passivity characterize the elements located in this field. Hence, elements in this field influence the system as strongly as they are influenced by the system.

Field III Passive field, which contains the passive system elements. A relatively low activity and a relatively low passivity characterize the elements located in this field. These elements are very strongly influenced by all system elements and have relatively little influence on the system.

Field IV Buffering field, which contains the so-called buffering system elements. A relatively low activity and passivity characterize the elements located in this field. Therefore, elements in this field have relatively little influence on the system and are relatively little influenced by it.

System hierarchy

To define the hierarchical order of the elements in the system the fields of the system grid have to be analyzed according to the importance of each field. So

examining the fields from I to IV, each field from left to right, and top to bottom, gives the defined hierarchy. This hierarchy can be used to obtain the maximum synergy effect in a system. Elements in the active area have to be used in such way that these in turn will influence the elements in the other areas. When no elements in the active area exist, the elements of the ambivalent area have to be used, and so on. It is of no use trying to influence the system by directly influencing the elements in the passive or buffering area, as they have little effect on the other elements.

The hierarchy derived from the network analysis is in this example case: A,D,C,B,E,G,F,H. This implies that using this order in decision-making, gives a structured entanglement of the network. In Figure 5.3, the decision-making is illustrated by presenting the network from Figure 5.1 and the stepwise removing of the influence areas.

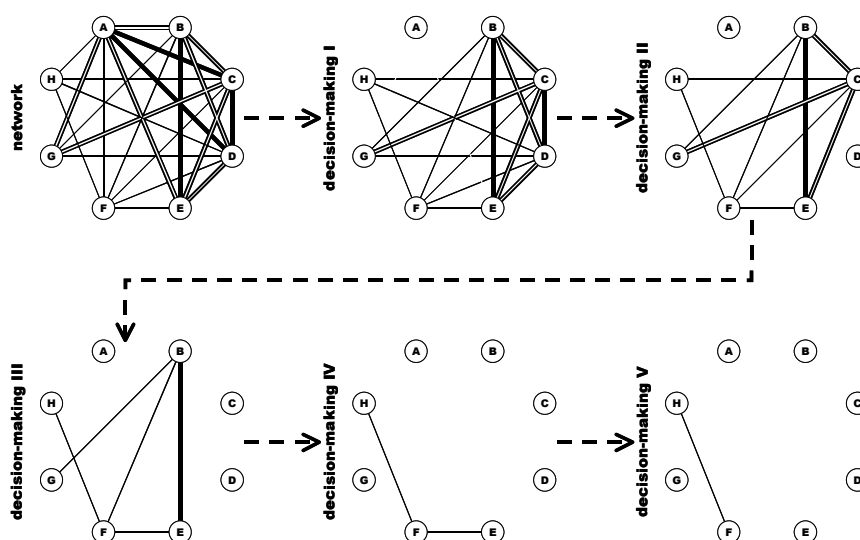


FIGURE 5.3 ILLUSTRATION OF THE DECISION SEQUENCE RANKING TOOL

5.2.4 Decision management in chemical process design

The decision sequence ranking tool described and defined how the influence analysis works. Now some ideas can be generated on how to use the tool in decision making in the chemical process design. It is assumed that a chemical process has to be designed to operate over 20 years and that it is desired to design a robust as possible chemical process. The following possible uses of the tool are discussed: i) identifying stakeholders influence, ii) identifying influence of sustainable technological input, and iii) identifying hierarchy of design decisions.

Identifying stakeholders influence

To perform the influence analysis a team is needed that has knowledge and experience in the behavior and future development of the defined areas of influence.

Objective: To identify which stakeholders have the most influence on the chemical process to be designed, regarding sustainable development and the idea of a robust as possible process.

Input: The areas of influence of the chemical company as well as the chemical plant (mostly stakeholders), such as government, society, buyers, non-profit organizations, economy and technology. Together with this areas of influence, the accompanying influence factors are investigated, focused on sustainable development.

Approach: The team should perform an influence analysis of the areas of influence. The most active areas should be used to determine a future idea of their development and changes according to sustainable development. The identification of areas of influence and influencing factors, the influence analysis and the future ideas should be performed in brainstorm sessions.

Output: Future ideas that will offer a framework for the design team to determine sustainability criteria and constraints, which will facilitate decision making. When future ideas will be used, they can function as a future goal. Decisions have to be made so the resulting design will fit to the future goal.

Identifying influence of sustainable technological input

To perform the influence analysis a team is needed that has knowledge and experience in the areas of technological input: chemists, process engineers, SHE specialists, equipment designers.

Objective: To identify which sustainable technology will have the most influence on the chemical process to be designed.

Input: The areas of influence which determine the technological input of the design task, like chemistry, reaction engineering, separation engineering, process design, equipment design and SHE specialist. Along with this influence areas, the accompanying influence factors have to be given, focused on sustainability input of the design task. For example for chemistry: chemical routes, use of renewable raw materials and the conversion of by-products to products.

Approach: The team could either perform an influence analysis of the areas of influence or an influence analysis of the influencing factors. The identification of areas of influence and influencing factors and the influence analysis should be performed in brainstorm sessions.

Output: The hierarchy of the areas of influence will determine which discipline will have the most effect on the outcome of the design. For instance, if equipment design is higher in the hierarchy than process design, the results of the sustainable development of equipment design should be used by process design. It should not be attempted to influence equipment design with issues of sustainable development in process design, as this will have little effect.

The hierarchy of the analysis of the influencing factors should be used to determine which sustainable input should have priority, as sustainable inputs higher in the hierarchy will influence sustainable inputs lower in the hierarchy.

Identifying hierarchy of design decisions

To perform the influence analysis the complete design team is needed.

Objective: To identify a hierarchy of design decisions which has to be followed in decision making in the design task.

Input: The areas of influence on which decisions has to be made, like chemical routes, catalyst type, process routes and process conditions. Also the accompanying influence factors (the decisions) are mentioned, for example for process conditions: temperature, pressure and pH. For catalyst type: homogeneous / heterogeneous, catalyst itself.

Approach: The team could either perform an influence analysis of the areas of influence or an influence analysis of the influencing factors. The identification of areas of influence and influencing factors and the influence analysis should be performed in brainstorm sessions.

Output: The hierarchy of the areas of influence as well as the hierarchy of the influencing factors will determine in which order decisions has to be made. For instance, when process conditions are higher in the hierarchy than equipment size, process conditions have to be chosen first.

It is noted that all the above options have some advantages and disadvantages in the practical use and the implementation of sustainable development in chemical process design. The last option is most useful for the design team, however it is difficult to implement sustainable development issues directly. When using this method, also sustainability constraints have to be defined to ensure decisions made will still fit within the idea of sustainable process design.

5.3 DSR case study: Industrial design project

The use and application of the decision sequence ranking tool is described above. Here, an industrial case is presented where the DSR is applied to illustrate the possibilities of its use. The opportunity to test the method was offered by a multidisciplinary design team from Shell Research and Technology Center in Amsterdam, the Netherlands. The team members allowed the observation of their meetings and brainstorm sessions and were very willing to give interviews.

This Chapter describes the performed case and starts with the case set-up and background information of the Shell project (further denoted as *industrial project*, some relevant information is presented in **Appendix A**). Then, based on meetings and interviews the influence analysis tool is used to define a hierarchy in decision issues. The section concludes with a discussion of the results and some concluding remarks.

5.3.1 Industrial design practice

During decision-making in chemical process design, the impact on the outcome decreases as the process advances. The most important decisions are made in the early stages of the innovation process. In order to develop structured

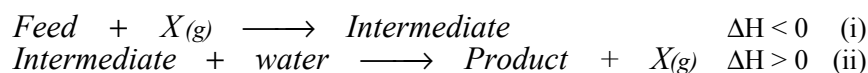
methodologies, one has to look first at the behavior of designers to identify their distinct activities in the design process. Then, opportunities can be found to apply structured methods, which should always be tailor made for the type of product/process and organizational structure. The presented industrial project is considered to be a good example of industrial design practice. The process is not described in detail due to its confidentiality.

Background of the industrial project

The industrial project deals with the development of a new production technology for an existing base chemical. The main incentives of this project are the poor selectivity and high-energy requirements of the existing production process. Furthermore, the new chemical route that is being developed is interesting, because it is possible to co-produce a promising new base chemical.

The project proved to be a nice example of concurrent engineering: the conceptual flowsheet was already being developed while the detailed chemistry was still fully in development. The design team, a sub-team in the project, therefore consisted of several engineers and chemists in order to streamline the communication between the disciplines. This organisational structure made sure that the engineers were provided with important data on the chemical reactions and catalysts. Furthermore, the chemists obtained insight in downstream issues, such as separation steps and recycle structures.

The basic chemistry consists of two principle reactions:



An intermediate is formed through a strongly exothermic reaction of the feed with a gaseous component X. This intermediate is hydrolyzed in the subsequent reaction to the product and the component X. Reaction ii is slightly endothermic. It is the intention that both reactions are heterogeneously catalyzed. Component X is not used during the overall reaction and can therefore be recycled.

In order to perform the case study, several meetings of the design team are monitored. These meetings are divided in three types in order to illustrate the synthesis approach: i) the *reactor selection*, ii) the *flowsheet generation*, and iii) *progress meetings*.

Reactor selection meetings; although the design team called these *reactor selection* meetings, they were actually more a reconnaissance of reactor conditions. The team used a software package in which the designer is systematically led through the selection process. The software tool first requires information on the basic chemistry and then provides the designer on a *question-answer basis* with advice on reaction temperature, pressure, supply strategy of reactants, etc. During these meetings it was noticed several times that the designers anticipated on other issues such as separation and integration of units. However, the strategy was to first develop the reactor and separation system separately and then to investigate integration opportunities. Furthermore, it was noticed that designers considered it useful that the software program reminded them of issues such as explosion limits,

phase equilibria, deposition, etc. The catalyst sub-team could then further investigate these issues.

Flowsheet generation meetings; during these meetings conceptual flowsheets of the separation system were conceived. The designers used a structured approach, in which first an input-output structure was defined, i.e. the reactants, products, trouble components, and recycles. Then the design problem was divided in several cases according to the possible product mixtures from the reactions. Subsequently, alternative flowsheets were generated and discussed. This exercise can be described as a *task identification* design step. Figure 5.4 shows the reaction and separation tasks.

The figure shows that there are three possible product mixtures: 1) product/intermediate/X through an excess of intermediate in reaction ii, 2) product/water/X through an excess of water in reaction ii, 3) all components when the reactants are not fully converted. A mixture of product and X resulting from a stoichiometric feed was considered not realistic. The designers used a synthesis hierarchy similar to that described by Sirola in order to develop the conceptual flowsheet, see also Chapter 6. Several separation techniques were discussed but the use of distillation seemed inevitable. After these sessions, the separation steps could be further investigated. This was not monitored.

Progress Meetings; the objective of these meetings was to decide which alternative to elaborate. Accordingly, simulation results were discussed and potential problems identified, e.g. product specifications, difficult separations, etc. It was interesting to notice that the heat integration was already discussed in this stage. Estimations were provided on the heat requirements with the corresponding temperature levels. Then it was argued that the temperature of reaction A should be maximized in order to efficiently use the heat.

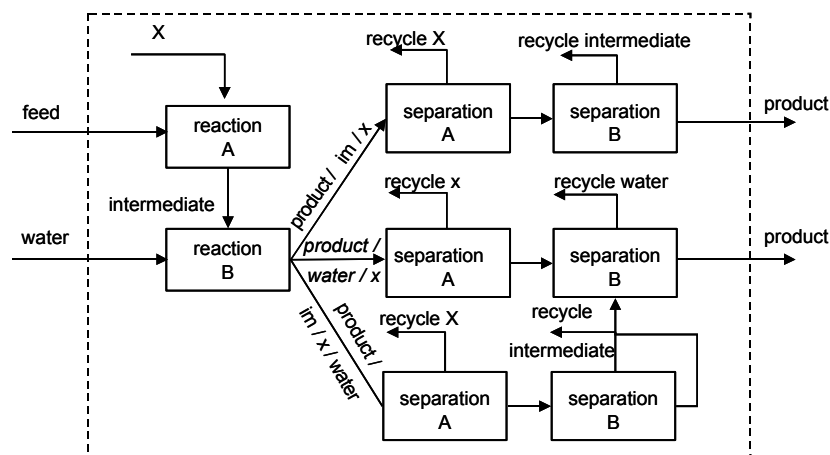


FIGURE 5.4 SCHEMATIC REPRESENTATION OF THE TASK IDENTIFICATION

5.3.2 Case set-up

Before starting the case of the industrial project, the case set-up was defined, by stating an *objective*, *approach* and *expected results*.

The *objective* of the case study is to test if and illustrate how the influence analysis tool of the scenario building method can be used in decision making by a multidisciplinary design team in conceptual chemical process engineering. The case study will be performed within the concept of sustainable development.

Approach; some ideas of how the influence analysis tool can be used in chemical engineering already were presented in a former section. These ideas have been the starting points for this case, resulting in the following two approaches: i) to use the influence analysis tool and the scenario building method in its original way; building a future image in which the designed plant has to operate and try to develop sustainability criteria and design objectives from this future image, ii) to use the influence analysis tool, to identify which discipline is the most effective in implementing sustainable development, or to determine which criteria of sustainability are the most influencing. Both approaches should be performed in brainstorm sessions in which the whole design team participates. Details of the brainstorm sessions will be worked out if it is determined if and how much time is available for these sessions.

The *expected result* of the design case is a well-described and defined influence analysis tool for use in chemical process design.

5.3.3 Design team

About two years ago, in 2000, a multidisciplinary design team has been given the assignment to design a competitive chemical process that manufactures product P and byproduct Q, as well as a competitive process that manufactures product P only. The commercial plant has to be designed for 20 years of operation and sustainability issues have to be taken into account. However, the cost of the design has to be lower than other reported designs. After a recent break of almost half a year, to give the chemical scientists of the design team time to find a feasible catalyst system for reaction (iii), the design process will now be continued.

5.3.4 Opportunities and threats for case study

To perform the case successfully, it is important to define *opportunities* and *threats* in advance. By doing so opportunities can be strengthened and threats minimized by adjusting the case set-up. For the Shell project the following opportunities and threats can be defined.

Opportunity I; a multidisciplinary design team performs the design. This is a great opportunity for the use of brainstorm sessions, because people with different technological or scientific backgrounds will only stimulate each other in ideas and problem solving.

Opportunity II; sustainability issues have to be taken into account in the design. However, implementing sustainable development in design can be very difficult and therefore the team members could be open for testing different ideas to facilitate this implementation.

Threat I; the project already started two years ago, so maybe some preliminary designs have been made. People could base their perception and ideas on these designs what could block them in generating new ideas. This could not be resolved easily, but has to be taken into account when performing brainstorm sessions.

Threat II; due to the deadline given with the design assignment, time pressure will speed up the design process and therefore maybe not all ideas for using the scenario building tool in process engineering can be tested. This threat can not be eliminated already, but agreements have to be made with the design team on what can be done and what not.

5.3.5 *Meetings and interviews*

The case started with the kick-off meeting, in this meeting the current status of the project would be outlined, followed by defining where and how to go from there. The team worked under high time-pressure as the design had to be finished very soon. It was clear that a lot of work had been done already and that the team preferred to continue from this basis. This means that unsolved problems from the past had to be solved in a short time. Therefore solving these problems had priority over implementing sustainability

However, due to its structuring and analyzing character in scenario building, the influence analysis tool could still be used. In this case, not for structuring and analyzing influences of sustainability issues, but for organizing decision issues and problem solving.

Instead of starting with brainstorming, individual interviews were held, as it was too time consuming and difficult to organize a brainstorm session with all the team members. The observation and description of the kick-off meeting and the interviews is given in the following subparagraphs. Note that the observations are personal observations. It is not the intention to offend people or even criticize the design process as it is performed within this company. Observations, whether positive or negative will only be used to identify in what way the influence analysis tool can help or be used in chemical process engineering.

5.3.6 *Kick-off meeting*

Four people of the following disciplines: project leader, chemistry, process flow sheeting and reactor process design, were present at the kick-off meeting. The purpose of the meeting was to define the approach of the project and the current status in about an hour and a half. The goal of the project was to design a process that initially manufactures product P only.

Summary of the meeting

After a short introduction of all the persons present, the project leader gave an overview of the economical constraints, the capacity of the plant (product mass flow) and the deadline for commercial plant start-up. This commercial plant could only be constructed when the design was economically justified.

The next agenda item was the presentation of the input-output structure, which was defined by the person from reactor process design. In the past it was already decided on which site location the commercial plant would be build. Therefore the

input-output structure did not only consist of the process boundary, but also of the site boundary. A remarkable thing of this input-output structure was the fact that sustainability issues were already implemented in the structure. The only stream that was allowed to cross the site boundary was the product stream. To prevent waste and emissions, CO₂ and H₂O had to be fully recycled and other wastes (light / heavy ends) were mixed with fuel used in the utility system.

The person from chemistry gave an overview of the catalyst status. The main problem of the project is to find a feasible catalyst to carry out reaction (iii). A feasible heterogeneous catalyst could not be found and the homogeneous catalyst tested so far showed stability problems at temperatures in excess of 150°C. However, a similar process of another company uses the same homogeneous catalyst without any stability problems reported so far.

During the meeting, the opportunity was offered to present the set-up of the case and the advantages and practical possibilities of the use of the influence analysis tool in the project. Although people were open for using the tool, they were not enthusiastic about participating in brainstorm sessions, as this would be very time consuming.

Defining the domain knowledge required for completing the design concluded the meeting. A list of required domain knowledge consisting of the following disciplines: chemistry, process design, safety engineering, construction materials, reactor engineering and distillation engineering was presented. The list was discussed and completed with the following disciplines: physical chemistry, safety, health, environment, sustainability, and economics.

Observations

During the kick-off meeting it was observed that all team members continuously used their professional experience and knowledge. Therefore, an enormous amount of (useful) information was provided, however it could not be observed that this information was clearly noted in a way that it could be recovered after the meeting. Although the aim of the kick-off meeting was to define the current status and the approach for the remainder of the project, a lot of detailed technical questions were asked. By doing so, sometimes one focused more on details than on the systematic generation of an outline of the current status. Focusing on details however did have the advantage that new ideas were generated and that one already tried to find solutions to problems that could be identified so far.

TABLE 5.2 KEYWORDS FROM SUSTAINABILITY PART OF THE INTERVIEWS.

<i>Discipline</i>	<i>Comments on sustainable development</i>
chemistry	minimum costs efficient use of feed, energy and chemicals waste – how can waste be returned to environment? use of renewable resources for heat, energy, or feed improve the quality of the stakeholders environment usefulness of the produced product ensure employment
project leader	100% recycle of CO ₂ and H ₂ O energy savings and efficiency, lower emission of CO ₂ biological input for the cracking processes production of p based on biological resources
process flow sheeting	decommissioning taken into account during the design of a plant main design objective: no effluents uncertainty about the feedstock in 10 years process integration is important
health & environment	lower capital costs lower energy consumption, this also improves environmental and social issues
safety	strive for inherent safer design
construction materials	prevent material leaking acceptable rate of corrosion critically rating factors of materials in the beginning of the design process more systematic approach of the conceptual design process

5.3.7 Interviews

To obtain a complete and diverse as possible input used by the influence analysis tool, the following disciplines were interviewed: chemistry, project leader, process flow sheeting, health & environment, safety and construction materials. In the interviews, two topics were discussed: how to implement sustainability (10 min.) and what are the main (decision) problems of the design project (20 min.). The point of view in the interviews was the professional experience and knowledge of the interviewer.

Sustainability

Although not directly important for the use of the influence analysis tool in this industrial project, as it was decided to use the tool only to facilitate design problems, the topic was still discussed to find out if and how people see the issue of sustainable development. The outcome of this might be useful to determine if the influence analysis tool can be used to structure issues of sustainable development. The main question was: *What factors/issues are important when designing a plant,*

like the one in this project, that still fits in our world and society over 20 years. In Table 5.2 a short overview of the comments is presented in keywords.

TABLE 5.3 KEYWORDS FROM PROBLEM IDENTIFICATION INTERVIEWS.

<i>Discipline</i>	<i>Problem identification</i>
chemistry	catalyst choice temperature waste unknown toxicity effects of the catalyst feed choice (crude <i>versus</i> pure)
project leader	catalyst choice temperature waste construction materials selection
process flow sheeting	catalyst (stability homogeneous cat, selectivity heterogeneous cat) temperature (conflicting process conditions and energy integration) waste construction materials selection energy integration is important acceptable concentration of acids feed choice (pure <i>versus</i> crude) process conditions
health & environment	catalyst choice (homogeneous cat is corrosive) wastewater energy integration toxicity of some chemicals is unknown runaway of the reactor acceptable concentration of acids
safety	
construction materials	temperature construction materials selection acceptable concentration of acids feed choice (pure <i>versus</i> crude)

Main decision-making problems

The problem identification part of the interview was focused on the identification of the influence areas and the influencing factors, needed for the use of the influence analysis tool. The main question was: *What design issues have to be solved in the design project and what are the main problems?* The interviewee was only allowed to identify problems. No solutions to problems or generation of ideas were allowed, as was observed in the kick-off meeting, because this would only impede the identification of problems. In Table 5.3 a short overview of the comments is

presented in keywords. Unfortunately, the safety engineer was not able to answer this question.

5.3.8 Use of tool

Now all the problems and design issues have been identified, DSR can be used to structure the problems and to order the design issues.

Identification areas of influence

The identification of the area of influence was done based on the outcome of the interviews. At first it was determined how many times an issue was mentioned, based on the problem identification part of the interviews. When an issue was mentioned at least 3 times (> 50% of the interviewees), it was said to be an area of influence. When an issue was mentioned less than 3 times, it was checked whether this issue was mentioned in the sustainability part of the interviews. If the issue was mentioned in the sustainability section, it was defined to be an area of influence, as sustainability issues had to be taken into account.

This approach resulted in the following areas of influence:

Type of catalyst	(mentioned 4 times)
Temperature	(mentioned 4 times)
Waste	(mentioned 4 times)
Construction materials	(mentioned 3 times)
Crude/ pure feed	(mentioned 3 times)
pH	(mentioned 3 times)
Energy	(mentioned 2 times, but a sustainability issue)

TABLE 5.4 SUMMARY OF THE NETWORK ANALYSIS

	Cat	Mat	PI	Feed	CO2	pH	P/T	Specs	Act.
Cat		1	2	0	1	1	2	2	9
Mat	1		1	1	0	2	1	1	7
PI	1	1		0	1	0	2	0	5
Feed	0	1	0		0	1	0	2	4
CO2	1	0	2	0		2	0	0	5
PH	0	2	0	0	1		0	1	4
P/T	2	2	2	0	0	0		1	7
Specs	1	0	1	2	0	1	1		6
Pass.	6	7	8	3	3	7	6	7	5,9

Influence analysis

The influence analysis was performed based on the areas of influence. It was started by defining the influencing factors for every area of influence, based on the information obtained from the interviews. Also the person from reaction process design was consulted to help with the assessment; it was determined that one area

of influence was not taken into account. This was the partial pressure of CO₂ (P_{CO2}). The resulting network matrix can be found in Table 5.4. More background on the assessment can be found in **Appendix A**.

System grid / decision hierarchy

From the influence analysis network matrix (Table 5.4) a system grid can be constructed. For the industrial project, this grid is presented in Figure 5.5. The hierarchy of the areas of influence can be found by analyzing the different fields of the system grid in the following order: active, ambivalent, passive and robust. Each field has to be read from left to right, top to bottom. As shown by the arrow in the system grid.

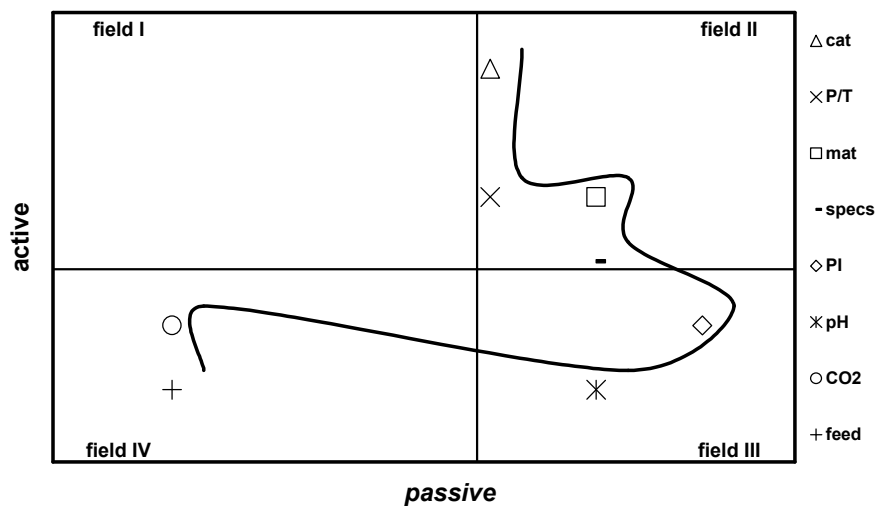


FIGURE 5.5 SYSTEM GRID OF THE INDUSTRIAL PROJECT

For the industrial project, the hierarchy of the areas of influence is as follow:

- I Catalyst choice (homogeneous or heterogeneous)
- II Process conditions (temperature/pressure)
- III Type of construction materials
- IV Product specifications / Waste streams
- V Level of process integration / Energy integration
- VI Level of pH
- VII Choice of CO₂ partial pressure
- VIII Choice of feed type (crude *versus* pure)

This means that the catalyst has the highest influence on the design and will influence the other areas of influence. The feed has little influence on the design, but is also little influenced by the other areas of influence. For the design team this would mean that they have to focus on solving the catalyst problem first, then the issues concerning temperature and construction materials and so on. If all these

problems are solved, they can use the hierarchy as a decision order. Meaning, they can use the decisions concerning the catalyst to influence the other areas of influence as the catalyst is very active in the system. This is more effective than using a decision concerning the feed to influence the other areas of influence, because the feed is very inactive.

5.3.9 *Concluding remarks on the DSR case*

In the decision-making meeting of the industrial project, the hierarchy was presented. Some participants and the chairman of the meeting expected this decision-making to be chaotic and emotional, as important decisions had to be made on many conflicting issues. During the meeting, not only the people of the design team were present, but also people from management, representatives of the plant that delivers the feed stream and people from other disciplines.

In the meeting, the influence analysis hierarchy was presented and explained in less than 10 minutes. This was followed by a presentation of the research performed concerning the catalyst and the results obtained so far. The last outline was given on the process flow sheeting stage to explain the decisions and problems concerning the technical details of the design.

Then the decision-making process was started, in which the order of decisions as presented in the hierarchy was followed. The participants were urged to focus only on one decision at a time; whenever a person tended to discuss another issue too much in detail, the group asked him to focus only on the issue they were discussing. In no longer than 30 minutes all decisions were made and people left the meeting enthusiastic.

This experience shows that this method indeed can structure decision-making. The tool used the experience and knowledge of the members of the design team reflected their intuitions well. The contradiction between a kick-off meeting that was expected to be structured but finally seemed to be a little chaotic and a decision making meeting that was expected to be chaotic and emotional but ended up to be structured is seen as a successful result of the case.

5.4 **System boundary definition and closed cycles tool**

One of the approaches, which ensure that no emissions and wastes are produced during the process, is a closed cycle approach. The strategy behind the *System Boundary Definition and Closing the Cycles* approach is to choose a system in such a way that the process within that system can consist of complete closed cycles. This idea is mainly based on the *precautionary principle*. In this approach, a box is drawn around the process and no flows are allowed to enter this box except the feed and product flow. This is illustrated in Figure 5.6.

The drawing of system boundaries is one of the essentials of the chemical engineering discipline; system boundaries define clearly the design area. Such a design area can be called the *battery limits*, or the *system boundaries*, or the *design basis*.

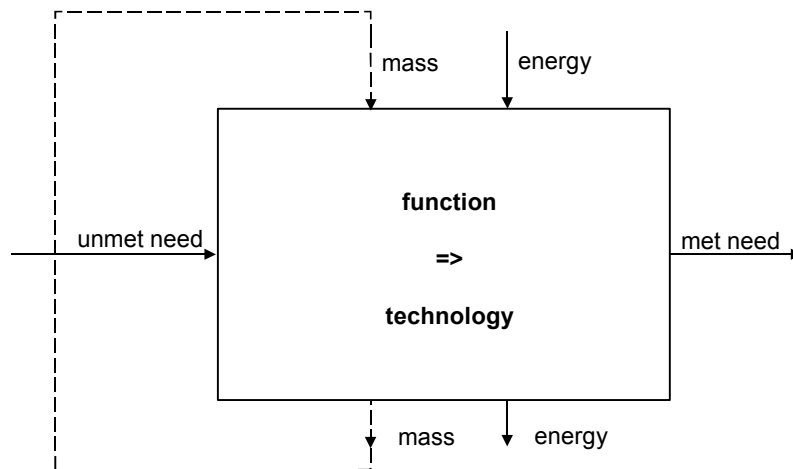


FIGURE 5.6 SYSTEM BOUNDARY DEFINITION

Here it is discussed to draw a system boundary around the system in such a way that the system contains closed loops of materials, especially those of wastes, emissions, and by-products. Before the design starts it should be clear what streams are allowed to enter or leave the process (*primary flows*). All other streams should either be created, or decomposed within the battery limits (*secondary flows*). The main idea is that the design has to meet a need and by doing that all secondary flows belong to the responsibility of the design team. Too often the design is focused on the main route (from feed to product), which results in waste or emissions flows that are simply ignored or should be treated in an expensive way. Here some ideas and results are discussed from the field of *Industrial Ecology*, which can be helpful in creating a closed system. It is not the goal and scope of this discussion to completely cover the field of the Industrial Ecology, but the main items are considered that help the designer for System Boundary Definition and Closing the Cycles.

5.4.1 Introduction to industrial ecology

Industrial Ecology is a rather new discipline, which can be seen as one of the possible approaches to deal with the increasing complexity of industrial systems, while incorporating external factors. The following definition can be found:

Industrial ecology is the means by which humanity can deliberately and rationally approach and maintains a desirable carrying capacity, given continued economic, cultural and technological evolution. The concept requires that an industrial system be viewed not in isolation from its surrounding systems, but in concert with them. It is a systems view in which one seeks to optimize the total materials cycle from virgin material, to finished material, to component to product, to obsolete product, and to ultimate disposal. Factors to be optimized include resources, energy and capital (Graedel and Allenby 1995).

Industrial Ecology tries to change one complex system (Industry-Society) to the likes of another complex system (Ecology) in the hope that the first one will function better. Mainly Industrial Ecology tools are analysis-based, like Life Cycle Assessment and Mass Flow Analysis. Although those tools give much insight, they have the tendency to become very complicated when using them in larger industrial systems. Besides that, the tools do not give direction to the design of more ecological-like industrial complexes.

5.4.2 Design principles of industrial ecology

The basic idea behind industrial ecology, conceptually illustrated by Figure 5.7, is to design industrial systems that imitate nature. In the *ideal case*, industrial systems are created that are materially self-sufficient and closed and are powered by renewable energy sources. Through a life cycle approach with total recycle (as occurs in nature), no non-renewable resources are used and no wastes are created.

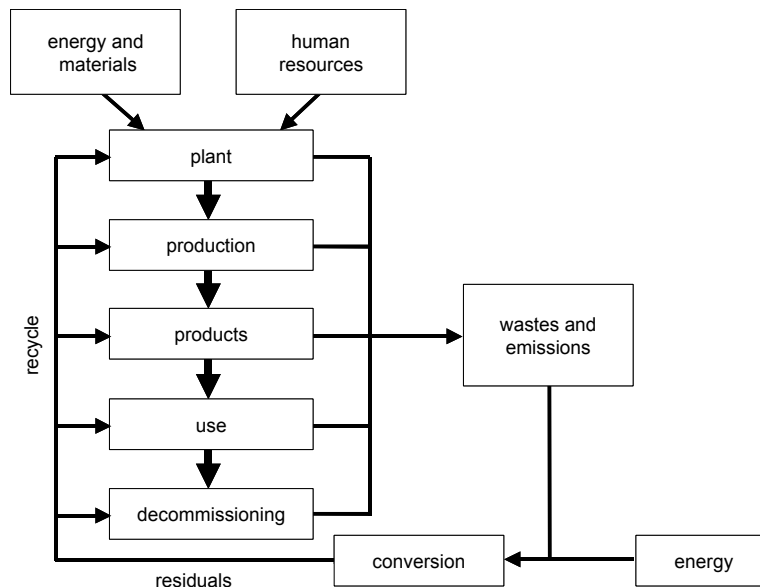


FIGURE 5.7 INDUSTRIAL ECOLOGY APPROACH

From this metaphor, the following design principles can be derived (Allenby 1999; Graedel and Allenby 1995; Lemkowitz, Korevaar, Harmsen, et al. 2001; Lemkowitz, Pasman, and Harmsen 1999):

- Improve the metabolic pathways of industrial processes and materials use, by creating loop-closing industrial ecosystems and dematerializing industrial output. Design products, processes, services, and operations to produce no *wastes*, only *residuals* (wastes have no use and must be disposed of; residuals are wastes that can be reused as a resource).
- Design every process, product, facility, infrastructure, and system to be adaptable to innovation.

- Ensure that all mass entering a process leaves as a saleable product (either primary or as a residual).
- Improve the energy and material efficiency of the system by integration of functions.
- Design, develop, and construct every industrial facility with attention to maintaining or improving local habitats and species diversity; idem to minimize impacts on local/regional resources.

5.5 ***SBDCC case study: methanol from biomass***

A students group within the scope of the course *Sustainable Technology I* (project in fall 2000) performed the case study discussed here. The case study illustrates the use of a closed system approach. The conceptual process design done by the students' case study relates to a process for manufacturing 250.000 ton/year of industrial grade methanol out of a biomass feedstock. The design is made in order of an industrial company. With criteria to determine the sustainability of a process, a selection has been made between several processes.

5.5.1 *Basis of design*

The conceptual process design described in this section relates to a process for manufacturing 250.000 ton/year of industrial grade methanol out of a biomass feedstock. The methanol produced should meet the available steam reforming technology specifications. A reasonable and available dry feedstock has to be selected; in this selection and also in the selection of the process the possibility is considered to divide the process in smaller units on different locations, because of the very large amount of biomass that will be needed to produce the asked quantity of methanol. The variable costs are not of interest, but the relative cost increase of this design compared to the available technology with natural gas as feedstock should be presented.

Methanol has a number of industrial applications, mainly as an intermediate in, for example, the production of formaldehyde. It is also increasingly used in the energy sector. Commercial methanol is produced from natural gas. This natural gas is used for the production of synthesis gas (CO and H_2) by steam reforming. Important commercial processes are the ICI-process, the Lurgi process, and a process developed by Haldor Topsoe (Kirk and Othmer 1998).

5.5.2 *Criteria for selection of process alternatives*

A choice has to be made between the possible process alternatives. First, a short description of the possible process alternatives is given. Next to this overview, a choice is made between the alternatives. The first rough selection between the alternatives is made by common sense, between the remaining alternatives, a choice is made with the help of sustainability criteria. Finally, the chosen alternative will be subjected to a first sustainable evaluation. With the help of this evaluation, certain conditions will arise that have to be satisfied during design.

In Figure 5.8, the closed cycle approach for this design is presented, all things within the box have to be designed and belong to the responsibility of the final

design. This means that the main goal for the process is the production of energy from sunlight. The energy is stored and transported by the material flows of water and carbodioxide to methanol. Eventually an additive flow like a fertilizer can be used.

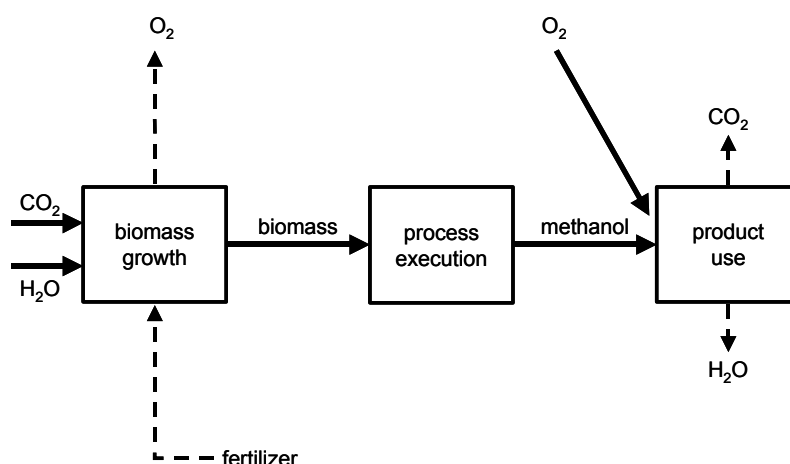


FIGURE 5.8 CLOSED CYCLE APPROACH

5.5.3 Process alternatives

Any kind of biomass is possible for use as feedstock, like wood, grass sources, or municipal organic waste (MOW). The process routes mentioned below are thus the result of a literature survey on methanol production from all kind of biomass. The number of possible biomass feedstocks depends of course on the process alternative. The possibility to carry out the process in different locations is very important for the process choice, because of the very large amount of biomass that is needed for the production of 250.000 tons/year of methanol. Six process routes are distinguished for the synthesis of methanol, three by *thermal process routes* and three by *biochemical process routes*.

- Thermal process routes:
 - Path 1: biomass to methanol (by pyrolysis)
 - Path 2: biomass to syngas (by partial oxidation) to methanol
 - Path 3: biomass to syngas (by steam reforming) to methanol
- Biochemical process routes
 - Path 4: biomass to ethanol (by fermentation) to methanol
 - Path 5: biomass to methanol (by fermentation)
 - Path 6: biomass to methane (by digestion) to syngas (by steam reforming) to methanol

Below, these reaction paths are described in more detail, after that comments are given on the different reaction paths, to make clear which routes are achievable in practice.

Path 1: biomass to methanol (by pyrolysis)

This route, also called dry distillation, was the commercial route for the production of methanol from 1830-1930. In this process, wood is heated to a temperature between 525 and 790 K. The charcoal produced was removed at the bottom of steel retorts, the liquid and gaseous products were removed at the top and were further distilled to useful products. The biomass has to be transported to the methanol factory. As can be seen in literature (Klass 1998) the methanol yield in this process is less than 10 mass% of the feedstock.

Path 2: biomass to syngas (by partial oxidation) to methanol

The Paths 2,3, and 6, all use syngas (mixture of CO and H₂) as intermediate for the production of methanol. All large industrial production sites for methanol are based on the synthesis of methanol from syngas. Therefore, it is here assumed that the production of methanol from syngas is common practice. The difference of the Paths 2,3, and 6 is in the way biomass is converted into syngas.

According to some literature (Klass 1998; Moulijn, Makkee, and van Diepen 2001) many thermal conversion processes can be classified as partial oxidation processes in which the biomass is supplied with less than the stoichiometric amount of oxygen needed for complete combustion. Both air and oxygen have been utilized for such systems. The product distribution of such processes depends on a whole range of parameters like the feedstock, the temperature, the pressure, the oxygen/biomass ratio, and more. For a detailed overview of commercial processes as well as the status of research on this topic, reference is made to Klass (Klass 1998).

Path 3: biomass to syngas (by steam reforming) to methanol

In this process, the oxidation is carried out with steam (Moulijn, Makkee, and van Diepen 2001); steam blended with air or oxygen is also a possible process option. Again, an extended overview of possible processes, together with yields, process conditions and product distribution is given in Klass (Klass 1998). An important feature of Paths 2 and 3 is the necessity to perform all the process steps on one site, because the transportation over long distances will need a complete new transportation network, with high costs.

Path 4: biomass to ethanol (by fermentation) to methanol

The fermentation of biomass towards ethanol is used in the production of alcohols by enzymes present in yeast. About the final step however, no information could be found, but this would be some cracking-like chemical reaction. According to some discussions with experts in the field of microbiology, it is not very likely that microorganisms can be found that can convert ethanol to methanol.

Path 5: biomass to methanol (by fermentation)

Klass (Klass 1998) dedicates some pages to this process route. Due to thermodynamic reasons (Gibbs free energy change of reaction), the fermentation reaction towards ethanol is preferred above the route towards methanol, thus in most microbiological reactions, the methanol is only byproduct. It is possible, however, to consider routes from biomass to methane with consecutive methane oxidation by bacteria. Another possibility is the fermentation of biomass to acetate with consecutive conversion of acetate to methanol. These processes however, are still far from commercial applications.

Path 6: biomass to methane (by digestion) to syngas (by steam reforming) to methanol

The process of converting biomass to methane has been studied since 1786 (Klass 1998). As stated above, it may be possible to convert the methane formed immediately to methanol, but at the moment this step is far from commercial exploitation. Therefore, the methane formed must be processed in a conventional way that is via synthesis gas towards methanol. An important feature of this option is the possibility to locate the different process steps on different locations, because it is rather simple to construct small and low-tech digestion vessels. The methane formed in the digestion step can be transported easily via a natural gas pipeline system, the next steps can take place at one central location afterwards.

5.5.4 Alternatives selection

After the description of the possible reaction paths, now the most feasible and sustainable one has to be selected. First, this is done based on some rough selection regarding literature and assumed feasibility. After that a sustainability criteria system is applied, which selects the most sustainable process route in this case. In this, the reaction blocks for the closed system can be filled rather simply, without applying a large sustainability analysis on processes which are not usable at all.

Selection based on feasibility and literature

Path 1, the pyrolysis of biomass, yields less than 10 % methanol, the rest is hardly usable char. This selectivity is not acceptable and thus this option can be rejected. Path 4 and 5 are rejected after some literature research. If at all possible to produce methanol from ethanol as in path 4, it would be very expensive and from common sense it is too inefficient. For path 5, no microorganisms have as yet been discovered, probably due to the thermodynamic difficulties, as already explained. Path 2 and 3 look very much alike. According to Klass (Klass 1998), the steam reforming of biomass is preferred above partial oxidation with the help of oxygen or air, when the steam reforming can be carried out adiabatically. Advantages of steam reforming include: i) acceptability of a wide range of green biomass feedstocks without pretreatment, ii) lower process energy consumption, iii) direct internal heating of the reactants, iv) efficient energy utilization, v) environmental benefits: steam reforming is reported to avoid the formation of dioxins and to convert any chlorinated compounds that may be present to salts and clean gas. These advantages are the reason that path 3 (steam reforming) is chosen in favor of

path 2 (partial oxidation), although the difference between the two paths is not that large.

Path 6 is also a feasible route. A more detailed sustainability selection has to be made between Path 3 (the steam reforming of biomass to produce syngas and then to methanol) or Path 6 (the digestion of biomass to produce methane, which is next converted to syngas, and then to methanol). In both cases, the synthesis gas is converted to methanol in a conventional way via steam reforming.

Applying of the selection procedure on the process routes

Based on the main sustainability debate and on the discussed criteria checklists, a set of sustainability criteria is formed. The criteria set is mainly based on four criteria discussed by Moser (Moser 1996), which are considered to be the criteria for ecotechnology: 1) Safe for human beings, 2) Safe for the environment, including animals, plants and other species, 3) Resulting in a clear benefit for society and not only in some profit for the factory, 4) Contributing to sustainability; i.e., long-term effects according to an ecocentric view having an economic, ecological and social dimension.

These four basic principles are elaborated to a more extensive set of criteria

- 1.1 Is the exposure to humanly toxic materials inside and outside the plant acceptable?
- 1.2 Is the inherent level of risk acceptable?
- 2.1 Does the use of this technology hold waste emissions within the carrying capacity of the environment?
- 2.2 Does the use of this technology keep the harvest rates of the renewable feed within regeneration rates?
- 2.3 Is the inherent level of environmental risk acceptable?
- 3.1 Does this technology have a positive influence on the well being of the Dutch people?
- 3.2 Are there no ethical or religious restrictions for the use of this technology in the Dutch situation?
- 3.3 Does this technology fit into the Dutch culture?
- 4.1 Does the technology have a positive influence on decreasing the gap in level of wealth, power and knowledge between the rich and the poor world?
- 4.2 Is the contribution of this technology to the overall emission levels acceptable in the Netherlands?
- 4.3 Is the use of this technology competitive over a long period of time, including the external costs?

The Paths 3 and 6 are now evaluated using those criteria (see Table 5.5), only the process steps to make syngas will be taken into account, because the step from syngas to methanol is the same in both cases. The criteria 3.2 and 3.3 are answered positively for both processes. No ethical and religious restrictions are present in the two processes and both processes certainly fit into the Dutch culture.

Due to the very rough level of information at this moment, the criteria 1.1, 2.3 and 3.1 can not be used to distinguish between the processes. It is argued that these criteria have to be considered as main design objectives and in this way the both designs certainly will meet the criteria in the final design stage. The same holds for

criterion 4.1, a criterion not very useful in the case of a methanol plant in the Netherlands.

A choice should be made now on basis of the criteria 1.2, 2.1, 2.2, 4.2 and 4.3. It is also taken into account that the process should have the possibility to be built in different locations, because as already mentioned, a lot of biomass is needed to synthesize such a large amount of methanol and this will cost a lot of transportation effort.

Criterion 1.2: Building various different reforming plants on different locations is not possible, because when the syngas is pressurized for transportation, a large explosion danger exist (this criterion is answered with no). The need for different plants is explained at criterion 2.2. So, on basis of criterion 1.2, the choice must be made for the digestion route.

The 'waste' criteria 2.1 and 4.2: The waste from the digestion step can be used again on the land as fertilizer and the only waste is the carbon dioxide later produced. Because the carbon source of this carbon dioxide comes from a renewable feed, this is no problem at all. In the reforming plant, ash is produced which cannot be re-used very easily. Therefore, on basis of these criteria, the digestion plant is the better one.

Criterion 2.2: To produce 250.000 tons of methanol a year, enormous amounts of biomass are necessary. According to Smith (Smith and Frank 1988), an area of 13 by 13 km is necessary to produce these amounts of methanol out of napier grass or water hyacinth. With the space limitation in the Netherlands one area of this size can not very easily be found for biomass production. It is therefore advantageous to choose a process option where different sources of biomass on different locations can be used. As explained earlier, the digestion route is ideal for this application. Of course, also with the steam reforming plant, it is possible to have sources of biomass on different sites, but in that case syngas has to be transported (see criterion 1.2).

Criterion 4.3: The main difference between the implementation of the steam-reforming and the biological process is the location of the plants and the location of the feedstock. With the digestion route, the process can be carried out near the biomass source. On different locations, different sources of biomass can be used. Especially in The Netherlands it is not easy to find a large area dedicated to one single process; it will be necessary to have different sources of biomass locations as explained above.

Besides this, it will be rather very expensive to transport various kinds of biomass from different biomass sources in Holland to one methanol producing plant. In the case of one reforming plant, this transportation is necessary; in the case of the digestion route, the methane produced can be transported easily via the existing natural gas network under the ground. The biogas or methane can easily be introduced to that network when, of course, some conditions are satisfied.

The digestion process therefore is chosen as the process route. A summary of this selection is presented in Table 5.5, in this table NDP (no distinction possible) means that there is not enough information available to distinguish between the two processes on basis of the criterion, but that it is expected that there is no problem to satisfy the criterion during the design of the process.

TABLE 5.5 SELECTION OF A SUSTAINABLE PROCESS

Criterion	Description	PATH 3	PATH 6
1.1	Acceptable level of toxic materials?	NDP	NDP
1.2	Acceptable inherent level of human risk?	NO	YES
2.1	Emission or wastes within the carrying capacity of the environment?	NO	YES
2.2	Are harvest rates within regeneration rates?	YES	YES
2.3	Acceptable inherent level of environmental risk?	NDP	NDP
3.1	Positive influence on the well-being of the Dutch people?	NDP	NDP
3.2	No ethical or religious restrictions?	YES	YES
3.3	Does the process fit into the Dutch culture?	YES	YES
4.1	Is there a positive influence on the level of inequity?	NDP	NDP
4.2	Acceptable contribution to the overall emission levels?	NO	YES
4.3	Does the process stay price competitive?	NO	YES
		3 x YES	7 x YES

(NDP means no distinction possible)

5.5.5 Basis of design

The assignment for this design is to come up with a process in which methanol is produced from a renewable feed instead of natural gas. Based on the evaluation presented above, here a design is described, in which a conventional part of the methanol plant is combined with a new design for the production of syngas. A short summary is given here of the process concepts chosen; a detailed description of the basis of design is given in this section. The design is elaborated on the level of a basis of design, which means that the main functions are described, like the reaction paths or the needed separation steps. This basic scheme can then be used as basis for the conceptual process design, which is not be carried out for this design.

The process consists basically of several steps:

Growth of the biomass

Pretreatment of the biomass

Digestion of the biomass to methane

Purification of biogas (methane)

Pipeline transportation (the methane is added to the Dutch gas grid)

Conversion of methane to methanol

Purification of methanol

Use of the methanol

} Design Part I

} Design Part II

The first four steps take place at different locations in the Netherlands with different feedstocks. In the remainder part of this section, the focus will be on possible feedstocks; while one feedstock (*verge grass*) will be worked out. Then the pretreatment, digestion, and purification are described as Design Part I. The next steps, denoted as Design Part II, are not elaborated, because this can be a

conventional methanol process. The transportation between the two Design Parts takes place via the already present *natural gas grid*, in The Netherlands.

Feedstock

As stated above, on different locations different biomass feedstocks will be used to produce bio-gas. In principle, almost all sources of biomass can be digested towards methane. However, some of the feedstocks offer better opportunities for closing material cycles than others. The fertilizer coming out of the process can immediately be used on the land where the biomass is harvested in the case of grown wood or grass as feedstock. This is of course not possible in the case of demolition wood or municipal organic waste.

The largest problem with digestion of wood is the conversion of lignin. Lignin is a branched aromatic structure and mostly occurs in cell walls. In wood, up to 40% dry weight consists of lignin and therefore, biological processes cannot easily degrade it (Klass 1998).

In grass there is less lignin present, so less problems will occur during digestion. In the design worked out in this report, the design for one feedstock, verge grass is worked out. This feedstock is chosen because of its availability, it is possible to bring back the fertilizer, and a good worked out case study (Smith and Frank 1988) (further denoted as the Smith-case) could be found in which grass is used as the feedstock. The latter argument is important, because of the low level of detail of this design.

Pretreatment of biomass

The feedstock *verge grass* includes water, sugars, nitrogen sources, mineral salts, and growth factors such as vitamins and amino acids. The grass is shredded in order to make retention times in the digester shorter. The small grass particles (a few mm) are diluted with water. The harvesting of verge grass is in the climate of The Netherlands limited to the period starting in April and ending in September. So half of verge grass produced in these six months will be in stock at the first of October. To convert the lignin, alkaline pretreatment is required; therefore lime (CaO) is added together with the biomass. The reference process *Napier Advanced* (Smith and Frank 1988) uses 0.25 ton CaO per ton methane. It has two functions: to control the pH and to improve digestibility. In the line of these duties it may form salts like, $\text{Ca}(\text{HCO}_3)_2$, CaCO_3 or for instance calcium acetate. This CaO should be reused or recycled, because of the SBDCC approach. A possible use is as a fertilizer on the verge grass, but this implies continuous neutralization of the soil. From the Smith-case it is derived that this can be done, without destruction of the soil culture. However, there is no a priori reason to expect that this situation is a sustainable one, so the alternative is to recover the lime from the digestion waste. That would imply a solid liquid separation step (a filter press for instance) and recovering the Ca salts from the cake or from the liquid phase.

Digestion of biomass to methane

The conversion is done by anaerobic digestion. Anaerobic digestion, also denoted as ‘microbial gasification’ or ‘methane fermentation’, is a biological process that

converts biomass in absence of oxygen into methane and carbondioxide. Methane fermentation of biomass also occurs naturally in many ecosystems such as river muds, lake sediments, sewage and marshes (Klass 1998).

A two-phase digestion system could be used, consisting of a leaching bed biomass hydrolysis reactor followed by a packaged bed methane digester. Chopped biomass with a 35% total solids content is put in large open tanks. Water is sprayed over the material and as the grass is hydrolyzed by acid-phase bacteria; soluble products (including volatile acids) are removed by the liquid leaching through the bed. The leachate is then transferred to a packed bed digester operated at an solids retention time of three days, where solubilized organic matter is converted to an 85% methane gas product. Operating temperatures are 25-30°C, so in the summer no extra heating is necessary. In order to obtain optimal yields, digestion must be carried out at constant temperature (Klass 1998; Smith and Frank 1988).

Anaerobic digestion consists in four steps: i) *hydrolysis* degrades the proteins, carbohydrates and lipids to amino acids or sugars; ii) then *acidogenesis* converts these products, together with some kinds of lipids to fatty acids; iii) from the fatty acids, acetate and hydrogen is formed by *acetogenesis*, and, iv) the methane synthesis from acetate is done by *methanogenesis*. All steps can take place in the same reactor, simultaneously (Schomaker, Boerboom, Visser, et al. 2000).

The overall nutrient ratio in waste materials is of major importance for the microbial biodegradation process. The C:N-ratio in wastes can vary in a considerable wide range between 6 (manure) and more than 500 (wood). For optimal degradation a C:N-ratio of 20 is recommended, which is foremost the case in grasses. The byproducts like NH_3 or H_2S may gradually cause increasing inhibitory effects.

Purification of methane

Because the specifications for the biogas are the same as for the natural gas, the methane has to be purified, i.e. the H_2S and CO_2 must be removed. It is favorable to do the CO_2 -removal with membranes, instead of pressure swing adsorption. The major reason for that is that in general membranes are cheaper at low capacity, while a technology like pressure swing adsorption is more convenient for higher capacities. It is assumed that the process takes place in the low capacity range, since the purification takes place at location.

The H_2S removal can be done by a biological caustic scrubber, in which the spent caustic solution is continuously regenerated in a bioreactor. In the scrubber, the H_2S containing gas is contacted in counter current mode with a scrubbing liquid. Absorption of H_2S in the scrubber occurs under slightly alkaline conditions (pH 8-9) and a chemical reaction with hydroxide ions takes place. These kinds of scrubbers are commercially available and can be applied on local scale.

Transport of methane

The methane is transported by the Dutch natural gas grid. The requirements for that gas grid are summarized in Table 5.6 (Schomaker, Boerboom, Visser, et al. 2000); the gas is compressed to a pressure of approximately 80 bar.

TABLE 5.6 BIOGAS REQUIREMENTS FOR THE DUTCH NATURAL GAS GRID

Parameter	Dimension	Value
Pressure	bar	80
Caloric Value	MJ/m ³	34.7 – 34.9
Wobbe-Index	MJ/m ³	43.5 – 44.4
H ₂ S	mg/m ³	< 5
H ₂ O (dew point at 1 bar)	°C	-35

In the case the heating value of the biogas is 37.3 MJ/m³ (Smith and Frank 1988) this can be lowered by adding CO₂ to the gas.

Mass balance

For the calculation of the mass balance, the case study ‘Advanced Case Napier Grass’ (Smith and Frank 1988) is taken and assumed that this would be the same for verge grass. In this case, the exact mass-flow of the methane is not given, only as a gas flow of 85850 m³, at standard conditions with a heat value of 3200 GJ. After some calculation, it can be said that 265 ton Napier grass produces 61 ton methane per day, while using 49 ton water and 14 ton lime. The process further has two waste streams of 146 ton CO₂ (in the first reaction step 116 and the second 30 ton) and of 121 ton fertilizer, that can be used for land application. This all on a continuous base, calculated for a production per day.

The methane leaves the process in a purity of 97%, of which 3% is water. It is assumed that this 3% also can be removed and can be replaced by CO₂ to meet the gas grid conditions in the Netherlands better. The lime leaves with the fertilizer, but can in a further design be replaced by other pretreatment methods. There is also unreacted biomass present in the fertilizer and all the other elements, which are not mentioned in our mass balance; it is assumed that all these other elements (Fe, Ni, Al, etc.) leave the digestion step in solid form, in the fertilizer. Only S can be a problem, because the digestion H₂S can be formed from solid S. Therefore, it is recommended to use a biological caustic scrubber together with the CO₂-membrane.

The methane is used for two purposes, the steam-reforming in the the methanol plant (assumed to be 40%), second the real methanol synthesis (requires 60%). In the furnace for the heating, the methane is burned with air to CO₂ and H₂O. The methanol synthesis consists of two steps; the steam reforming of methane to syngas (3H₂ + CO), and the methanol synthesis with a efficiency of 87.5 mol%.

The total amount of verge grass that is needed is 1036 kt/a, with a biomass-yield of 30 ton/ha, this equals a area of 345 km²; which is a scale up factor of 10 regarding the Smith-case (Smith and Frank 1988). It is assumed to have 11 digesters all over the country, which can be run by the verge grass in the neighborhood or other feedstocks.

Possibilities for optimization and integration

For the fermentation step also some energy is needed for shredding, mixing and compression and also for heating of the digester. In the Smith-case no heating of

the digester is needed, because the digestion is done in Central Florida, where the ambient temperature is significant higher than in The Netherlands. The methanol plant is self-sufficient by burning part of the feedstock; the ratio of 40/60 can be improved by further process integration.

5.5.6 *SBDCC-approach of the process*

The different process streams can be described in a closed cycle model, see Figure 5.9. In this model, the streams are considered coming in and going out the process. In this way, it is proved that no polluting streams are produced. All the rare elements, present in the biomass leave the process in the fertilizer stream, together with the lime. Also some water is present in the fertilizer stream, besides the water that is going from the process in pure form. Sulfur is separated from the biogas flow in solid form and therefore presented as a independent stream, but mostly this stream can be mixed up with the fertilizer stream. Hydrogen and carbon dioxide leave the process as gas flows. Methanol is the final product. Both the fertilizer stream and the biomass stream are mix flows, containing a lot of elements. The other flows represent pure compounds.

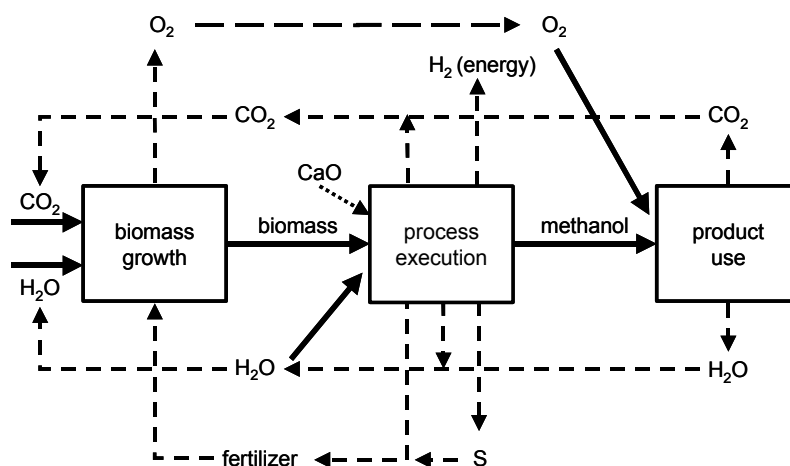


FIGURE 5.9 CLOSED CYCLES MODEL OF THE BIOMASS-METHANOL ROUTE

5.5.7 *Economic evaluation*

It is not the main goal of this case study to perform a rigid economic evaluation and it must be emphasized that the method followed above is not accurate enough. However, the conclusion can be drawn that the bio-gas produced in our case can have a price that is in the price-competitive range. The economic evaluation is also divided into two parts: i) the production of methane, and ii) the production of methanol. The methanol plants is commercially available and price competitive. The only thing that has to be proven here is that the methane price is in the competitive range.

The Smith-case was carried out in 1982, therefore a interest factor for 21 years is used; this index number is derived from Coulson and Richardson (Sinnott 1993). In the book the price for the gas produced is calculated to be 5-6 \$/GJ, that is equivalent with 18-22 USDcent/m³. For these calculations, an economic plant life of 30 years is assumed. The natural gas prices in the Netherlands are around 0,10 euro/m³ for the industry and 0,20 euro/m³ (according to the ECN-website) for the households, so with a dollar to guilder rate of about 2, the conclusion can be drawn that the price of the biological produced natural gas is in the price competitive range.

Factors influencing the real price in the design presented in this report include: i) the number of plants and as a result of this, the sizes of the different plant, ii) the amount of the different feedstocks used, iii) the prices of these feedstocks, iv) the level of automatisaton and the number of personnel, v) available subsidies for clean technology. When the design is carried out with a higher level of detail, the factors mentioned above can be filled in and a more accurate price estimation can be made.

A remark with respect to the final methanol price is the introduction of a possible CO₂ tax. In a design like this, this tax does not have to be paid, because the source of the CO₂ waste in the methanol plant is the biomass fed to the digestion plant. The amount of CO₂ that is discharged during the methanol synthesis, this is 1.2 ton CO₂ per ton CH₃OH. On yearly basis, this implies a CO₂ production of 300.000 ton and therefore the cost reduction with respect to this tax can be millions of dollars (assuming that the CO₂-tax will be somehow like 10-20 dollar per ton CO₂).

5.5.8 *Concluding remarks on the SBDCC case study*

The mass and energy balances of the process are correct; all material cycles are closed including the feedstock exploitation and the use of the final product; in this way the process is driven by sunlight only on a short temporal scale. The presented process setup is economically profitable and price competitive, due to the low price of the feedstock, the low transport costs, and the avoidance of a CO₂-tax. All processing steps use well-known technology and meet HES-requirements. The design is presented to a forum consisting of NGOs, government, industry, and local public. It is possible to explain the process to a non-experienced public and clarify its sustainability.

5.6 **Concluding remarks**

The problem definition and the definition of system boundaries is described with three elements: 1) goal and scope definition, 2) criteria determination, 3) knowledge mapping. These three elements give the designer the opportunity to define the design problem in a coherent and structured way, while incorporating sustainability issues. Two tools are developed in this Chapter, the decision sequence ranking tool (DSR) and the system boundaries and closed cycles tool (SBDCC); the validity of the tools are illustrated by case studies:

- The newly developed decision sequence ranking tool (DSR) gives a hierarchical approach to problem definition and solving. The industrial case study shows that this method indeed can structure decision-making. The tool

used the experience and knowledge of the members of the design team and it reflected their intuitions well.

- The system boundaries and closed cycles tool (SBDCC) focuses the design to the fixed input-output scheme. In this way the final design has closed system boundaries and closed cycles as defined in the design problem definition. The case study shows that all material cycles are indeed closed including the feedstock exploitation and the use of the final product; in this way the process is driven by sunlight only on a short temporal scale. The design, in the form of a simple basis of design, is presented to a forum consisting of NGOs, government, industry, and local public. It is possible to explain the result of the design to a non-experienced public and clarify its sustainability.

Chapter 6

SUSTAINABLE PROCESS DESIGN METHODOLOGY, PART II: *GENERATION OF ALTERNATIVES STAGE*

Summary *The heart of every design is the stage in which the alternatives are generated. This is the creative part of the design, where integrative and innovative solutions are developed. In this Chapter, the generation of alternatives is more explored by dividing it into three elements: 1) creativity stimulation, 2) function identification, 3) concept integration. After that tools are discussed to improve the generation of alternatives by stimulating creativity. Then a chemical route selection tool (CRS) is described together with a design case. Design guidelines are becoming increasingly important as the complexity of the design methods increases, this leads to the guidelines for process synthesis tool (GPS).*

6.1 Generation of alternatives (see also Chapter 4)

Now that needs have been assessed and the design problem is defined, the various alternatives are generated. The generation of alternatives is more or less the heart of the design activity, because in this stage the creativity of the designer is the most important factor. The somehow quantitative and sometimes vague needs are translated into exact process specifications. Decisions are made on many different topics, like *identification of possible feeds*, the *identification of possible synthesis routes*, the *investigation of reactions and separations with corresponding options and thermodynamic data*, etc. As discussed in Chapter 4, the generation of alternatives consists in three elements: 1) *creativity stimulation*, 2) *function identification*, 3) *concept integration*. In Chapter 4 an introduction was given to these concepts; here these steps are discussed in more detail, and after that some design tools are introduced and evaluated.

6.1.1 Creativity stimulation

It is emphasized here that it is impossible to logically derive a design solution from the design problem, this follows from the discussion about design methodologies in Chapter 4. This statement implies that the description of a technical design problem is subject to a multitude of demands. Some of which are, or seem to be, in conflict with one another. The designer's task is to create a solution that is optimal in terms of all these demands. The designer tries to convince the stakeholders of the design in many ways that the presented solution is feasible and reliable. The description of the design problem is a *rational* activity, and the analysis of the design solution is also a *rational* activity, but the generation of alternatives is a *partly irrational* activity.

Stating that the synthesis activity of the design procedure is the most *creative part* can summarize the paragraph above. Creativity in this context is seen as *all kind of activities that enable the designer to bridge the gap between the description of the problem and the analysis of alternatives*. This is the reason that the stimulation of creativity can be seen as an integral part of the design activity. In general three categories can be distinguished as mechanisms of idea generation (Roozenburg and Eekels 1995): *Associative*, *Creative*, and *Analytic-systematic* methods.

Associative methods: the theories on association methods describe the ability of human beings to connect unexpected thoughts with the problem in a sensible way in order to increase new and useful ideas. Training can teach this skill; a common tool to do this is brainstorming.

Creative confrontation methods: decision-making and problem solving is a common human activity; a design problem can be solved when a similarity is drawn between, for example, daily life and the technical problem at hand.

Analytic-systematic methods: after a decomposition of the design problem, alternatives can be investigated and developed. The combination of partial solutions delivers a new solution. This solution is found by comparing the design problem to an existing design with a related design problem.

6.1.2 Function identification

Process synthesis based on function engineering offers great opportunities for designing within the concept of sustainable and technological development. The method is not restricted by levels of design (like unit operations based methods) and will only focus on the synthesis phase of the design methodology. Given the states of raw materials and product streams, process synthesis involves the selection of processing operations to convert the raw materials into products. Put in other words, each operation can be viewed as having a role in eliminating one or more of the property differences. The conceptual designer, thinking directly in terms of equipment, would consider reactors, separators or mixers etc. Unlike the common conceptual design approach, property differences are not resolved directly in terms of equipment. The incorporation of an explicit task identification step provides the designer with fundamental insight into the chemical and physical phenomena that occur in the process.

After the identification of the functions, the functions have to be integrated to a process flowsheet. This step does not logically follow from the identification step, but is mainly based on creativity and intuition. To help the designer, guidelines or heuristics are very useful that give direction to the generation of alternatives, see the description of the GPS tool in this Chapter.

The raw materials undergo a number of physical treatment steps to put them in the form in which they can be reacted chemically. Then they pass through the reactor. The products of the reaction must then undergo further physical treatment - separations, purifications, etc.- for the final desired product to be obtained, see Figure 6.1.

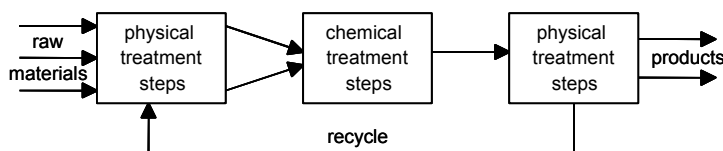


FIGURE 6.1 SIMPLIFIED SCHEME OF CHEMICAL PROCESS FUNCTIONS

The functional identification approach for chemical engineering is described by some authors (Chakrabarti and Bligh 2001; Harmsen and Chewter 1999) (Pohjola, Alha, and Ainassaari 1994; Tanskanen 1999). Here, the articles written by Siirola (Siirola 1995; Siirola 1996) are used as main reference. The Siirola-approach differs from traditional chemical engineering in the sense that it is not based on unit operations design, but on the idea that a chemical process is a combination of functions that deal with manufacturing of substances (see also Chapters 3 and 4). The change in physical and chemical properties of materials and streams is the focal point of a conceptual design, since a chemical process has the function to eliminate property differences, which exist between the incoming and outgoing mass and energy flows.

A functional engineering approach attacks the design problem in a hierarchical manner, as a natural hierarchy among property differences exists: i) identity, ii)

amount, iii) concentration, iv) phase, v) temperature and pressure, vi) shape and form. Combining this hierarchy and the fact that obvious methods for reducing or eliminating property differences exist (as can be seen in Table 6.1), lead to an approach for the systematic generation of a conceptual process flow sheet. Preconditions for property changing methods can be met, if necessary, by adjusting properties lower in the property hierarchy, e.g. identify separations in order to get appropriately pure feed conditions for reaction tasks, adjust temperatures in order to get better conditions for executing separation tasks. However, the procedure would never consider changing the identity to get better conditions for separation.

TABLE 6.1 PROPERTY DIFFERENCES HIERARCHY

Property difference	Property changing operator
Molecular identity	Chemical reaction
Amount	Mixing / splitting
Composition / Purity	Separation
Phase	Enthalpy modification
Temperature / Pressure	Enthalpy modification
Form	Various methods

Property differences are not resolved directly in terms of equipment, but the incorporation of an explicit task identification step provides the designer with fundamental insight in the chemical and physical phenomena that occur in the process. More specifically, important questions in task identification could be:

- *Operation of reactions*: What are the possible or desired product mixtures? What is the operating window with respect to pressure and temperature?
- *Separation methods*: What methods can be used? What are the energy requirements of the methods? What are the operating windows with respect to pressure and temperature?
- *Heat integration*: What is the quantity and quality of heat produced and required?
- *Critical features*: What problems can be expected, e.g. difficult separations, expensive equipment, high-energy requirements, etc.?

Function identification can be used as a hierarchical process design method consisting of the following steps (Siirola 1996): i) *construction of a reaction network* and ii) *species allocation*.

Construction of reaction path and plant network (see chemical route selection tool). This is done considering only the molecular identity property. Identity-changing blocks are specified, which convert raw materials into a desired property (namely identity) while ignoring all other properties. These blocks are placed strategically like islands on the flow sheet. It is known that they will be required, but at first it is not known exactly how they will be connected to the raw materials, the product, or to each other.

Species allocation, plant connection and recycle determination. Reactor interconnections are determined considering only the role of each species and the amount property. Also target mass flows among raw materials, reactions, products

and wastes are determined including possible recycle of incompletely converted reactants.

The layout of a chemical process, seen from a function engineering point of view, starts by the input of raw materials that has to undergo a number of physical treatment steps to put them in the form in which they can be reacted chemically. Then they pass through one or more chemical treatment steps, see also Figure 6.1. In these treatment steps, the physical and chemical properties of the materials are changed. The property differences, as presented in Table 6.1 can be assigned individually to a treatment step. Of course, a change of identity is accompanied by a (physical) change in temperature, phase, purity and amount of chemical, but here these changes are taken as the result of a change of identity. These physical changes of temperature, phase, purity and amount will be eliminated in the physical treatment steps after the chemical treatment step (as well as they will be changed before the chemical treatment step to meet the required pre-conditions of the input stream).

Combining Siirola's property differences hierarchy with the chemical process layout as was presented in Chapter 3, results in a function engineering approach as is given in Figure 6.2. The heart of the chemical process is defined by the chemical reaction. Therefore, the synthesis of the chemical process starts with the identification of all identity changes, meaning the determination of reaction kinetics and the reaction phase. Sometimes reaction kinetics is difficult to determine, but for a basis of design it is enough to estimate temperature, pressure, phase and the chemical conversion.

Now, having defined the physical properties of the reaction the property differences between the input of the process and the input of the reaction section can be identified and a decision hierarchy can be defined by Siirola, as shown in Figure 6.2. Following a line, e.g. representing chemical A, first the amount has to be changed (most of the times by adding the recycle stream), then the purity, often not necessary for the input, then the phase and eventually the temperature and pressure, resulting in the right input for the chemical treatment steps. The same could be done for the output physical treatment steps.

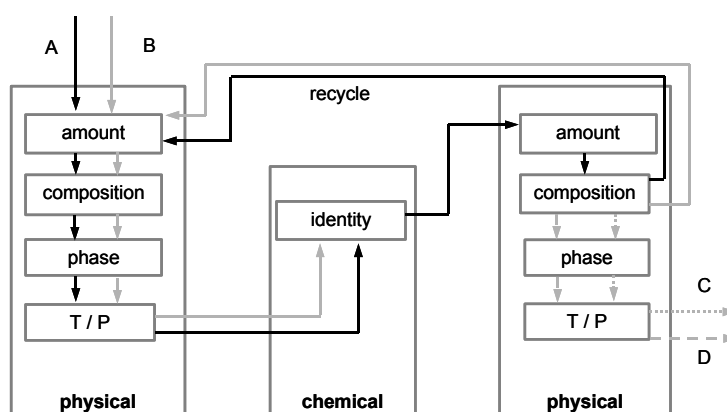


FIGURE 6.2 PROPERTY HIERARCHY AND A CHEMICAL PROCESS LAYOUT

Until now the main source for functional engineering is literature provided by Siirola. In this thesis, knowledge is obtained about the rigor and validity of the method. The idea of function identification and concept integration as two different steps is useful, but the use of the method described by Siirola delivers specific problems during application. The method is only useful in a well-defined design space; for an ill-defined design solution the method can not be applied. Improvements are given to make the tool more generally applicable.

6.1.3 *Concept integration*

Although the decomposition of the problem is one of the possibilities for design synthesis, it is assumed here that a complex design activity like chemical engineering design always consists of various design concepts. These design concepts have to be integrated in such a way that the combination of the parts delivers the solution to the entire design problem.

Very important here is already the set of criteria. In some way the designer has to present a solution that is the answer to the problem definition, the final answer will be given after the analysis and evaluation step. However, here the concept has to be integrated in such a way that the assessment and evaluation can be carried out against the defined criteria.

6.2 **Creativity and the generation of alternatives**

In this section creativity tools applicable for the generation of alternatives are discussed. The creativity techniques are not classified into various stages of the design or the type of problem. The described methods are only to stimulate creativity in any stage of the design process. Problem solving and decision-making need relevant knowledge *and* creativity. The role of scientific knowledge becomes more important towards the latter stages of the design. The creativity is mainly needed in the earlier stages of the design, but is necessary for every synthesis step that has to be taken.

Considering the *decision-making sequence* (see Chapter 4) there are no strict rules to perform the synthesis phase. The designers have almost unlimited methodical freedom ending with reporting the ideas. The step from *function* to *form* during the design is performed by reductive reasoning. Algorithmic rules would block that reasoning process. The degree of feasibility is validated afterwards, in the analysis step.

The psychological argument for methodical freedom is the space required for creative flashes of inspiration. Restrictions by strict methodical rules narrow down that space. Besides that, ideas are generated all the time and often take place just at that moment the designer is not consciously occupied with generating alternatives. Still, there are methods to help the designer to generate more or better alternatives. The choice which method is best applicable is strongly dependent on the composition of the design team or the existing expertise.

It is mentioned already that three categories for creativity stimulation exist (Roozenburg and Eekels 1995): *associative methods*, *creative confrontation methods*, and *analytic-systematic methods*. This division of categories will be used here for the presentation of creativity tools. All tools presented here are used in the

designs that are elaborated during this research, comments and experiences are based on those design activities; this is rather personal and the vision of others can differ.

6.2.1 *Associative methods*

Brainstorming is the associative method that is used in general. This method is based on a discussion of a small group of people. The method prescribes certain rules for the discussion, which everyone has to obey: i) criticism is forbidden, ii) generate ideas unrestrainedly, iii) associate on other ideas, iv) try to think by association as much as possible. Brainstorming is applicable for relatively easy, open formulated problems. If brainstorming is applied to complex problem solving the problem owner could best divide the problem into partial problems. Brainstorming is not suitable for specialized problems that require experts to solve it.

The composition of the group influences the outcome of the brainstorm. Groups that do not work together intensively as a team generate more, and sometimes better, ideas. The following should be kept in mind when preparing a brainstorm, training and careful composition of the group may prevent such blockades: i) participants can react too much on formerly mentioned ideas; this blocks radical new inspirations, ii) participants are inclined to stay with the field, which they feel competent with, iii) participants of lower standing may feel hindered in the presence of their superior, iv) verbal violence of one person may strongly influence the whole session, v) the high speed of the brainstorm can frustrate secondary reacting people.

Associative methods as variants on brainstorming are: iii) *brainwriting*, *individual-associative methods*, *associations checklists*.

Brainwriting; Ideas are written down on papers, which are shared by the other team members. The idea is that every person generates ideas by associating on the ideas written on the paper. Advantage of this method is that generation of ideas is not disturbed by the group process. The paper is anonymous so no one is hindered; ideas can be sketched, and become more detailed and qualified than in brainstorming.

Individual associative methods; Excursions are made on individual basis. The rules are generic, but every person comes up with other thoughts.

Associations Checklists; This is an individual method as well, it can consists of words like substitute, combine, adapt, modify, put-to-other-use, eliminate or rearrange (the so-called SCAMPER list, developed by Osborn in 1963). These words force one to think in a solution direction.

6.2.2 *Creative confrontation methods*

Creative confrontation methods are characterized by the connection of ideas that are not related to each other in the first place. This is also true for association methods, but in the case of creative confrontation, the connection is forced based on analogy or serendipity. Examples of analogies are: family relationship, form similarity, technical functional analogy, etc.

A commonly used method for creative confrontation is the synectics-method, developed in the 1960s by Gordon. Synectics is derived from the Greek words *syn* and *ectos* which suggest *bringing diversity together*. The method combines the problem definition with situations which have nothing or barely nothing to do with the problem at first sight. This principle results in surprising ideas. The method consists of two phases: i) the problem defining phase (*becoming familiar with the strange*), ii) the creativity phase (*becoming unfamiliar with the familiar*).

The Synectics method elaborates the idea generating people by so-called excursions: i) *personal analogy*, e.g. how would you solve a similar problem in your daily life, ii) *direct analogy*, e.g. find an analogue problem in another field, like nature, iii) *symbolic analogy*, e.g. find words, schemes, proverbs to describe the problem, iv) *fantasy analogy*, e.g. define an imaginary solution and describe the threats for its implementation

Many more excursions tools are possible to stimulate the creativity: i) *random stimulus*, e.g. choose an arbitrary word in a paper and use that for a problem redefinition or a solution description, ii) *intermediate impossible*, e.g. think of the ideal solution by wishful thinking or idealised design and define the oppositions to such a design. iii) *concept challenge*, e.g. formulate a judgement about a proposed solution, which can be accepted by everyone; the designer attempts to undermine this judgement in order to find new solutions.

6.2.3 Analytic systematic methods

Analytic systematic methods are based on the analysis and systematic description of the problem. Alternatives for partial problems are investigated and developed in a rational way; the combination of partial solutions delivers a new solution. In practice three kinds of methods exist: i) *function analysis*, ii) *morphologic methods*, iii) *decisions trees*.

Function analysis starts with an empty black box, for which the boundary conditions are known. The designer gives an overview of all functions that have to be considered to come from the defined input to the defined output. Due to the structural approach, the problem is decomposed into partial problems. The function structure gives insight into the problem, but it does not give tools for solving the problem.

Morphologic methods are characterized by the separation between the phase of generating alternatives and the selection of one of them. The method delivers a so-called *morphologic chart* that consisting of parameters and combinations of these parameters. This chart has the following properties: i) the parameters are independent; ii) the definition and selection of parameters are done by specialists and strongly based on the engineering field the design is made for; iii) every combination of parameters can deliver an alternative solution.

Decision trees deliver a hierarchical classification, by an evolutionary approach. Depending on the problem the designer categorizes the decisions that have to be made in an iterative way. Actually this method is more an analysis method, because decision tree explains how to make a classification of decisions, but it does not describe how to make the decisions.

6.3 Chemical route selection tool

This section describes the Chemical Route Selection tool (CSR). Although this method can be used both for the generation of alternatives and the analysis of alternatives, it is placed in this Chapter, because the tool is created exclusively for the generation of a sustainable chemical route structure. New in this tool is the application of exergy concepts during the process synthesis. The methodology helps to deal with the following questions that arise during this selection process: 1) which basic reactions produce the desired chemical, 2) what are the alternative supply chains of the corresponding feedstocks, 3) which supply chain has the least exergy loss.

The supply chain is defined as the whole of processes that is required to produce the desired chemical. The analysis can also be extended to include life cycle steps as re-use, recycling, storage, etc., but these issues are not considered in this work. Furthermore, the methodology can be used as an analysis tool for both new and existing chemical routes. The life cycle concept is based on taking a holistic view of a product or service, from raw materials through production to distribution and final disposal of all wastes. This approach has its beginnings in the 1960s and many studies have followed since; see also Chapter 2 and 3.

6.3.1 Background and objectives

This methodology elaborates on the Exergetic Life Cycle Analysis (ELCA) introduced in the dissertation of Cornelissen (Cornelissen 1997), by using it for the generation of alternatives instead of the analysis of alternatives. In the ELCA approach, energy streams are valued according to their exergy content. In this section the method is described, which is illustrated in the following Chapter with an example case on the production of monopropylene glycol (MPG).

The purpose of the methodology is to support the selection of a chemical route during the first stages of the innovation process. The objective of the methodology is to quantitatively assess the supply chains with respect to their renewability and efficiency, i.e. the amount of exergy input in relation to the output of useful products. The first aspect is important for the closing of cycles and the depletion of scarce resources. The second aspect provides insight in the efficiency of the supply chain and could form a basis for improvements.

6.3.2 Short introduction to life cycle thinking

At present, companies increasingly use LCA methodologies to help them make better business and environmental decisions. Accordingly, principles and guidelines of LCA have been included in the ISO 14000 series of environmental management standards in 1995. The corresponding framework is taken as the starting point for chemical route analysis and consists of the following components (Tibor 1996): i) goal definition and scoping, ii) Life cycle inventory (LCI) analysis, iii) impact assessment, iv) Improvement assessment.

Goal definition and scoping

This stage of LCA defines the purpose, the expected outputs, the boundary conditions and the assumptions for the study. The first step is to clearly understand

why the study is performed and which questions are to be answered. The second step is to determine the scope of the study in terms of breadth and depth to achieve the stated goals. The scope should include (Tibor 1996): 1) the function(s) of the system, 2) the functional unit, 3) the system(s) to be studied, 4) the boundaries of the system, 5) data requirements, 6) assumptions and limitations.

The LCA study should clearly define the function of the system it is going to study. When performing a LCA it is necessary to break down a complex system into unit processes for which the investigator can actually gather input and output data. An overall system boundary is defined to limit the analysis. Note that the individual unit processes also have system boundaries. A feasible LCA study clearly states the criteria for setting the system boundaries.

Once the system and boundaries are defined, the system is outlined using a process flow diagram to show the relationship between the unit processes. A listing can be made of the inputs and outputs to each unit process; inputs include raw materials and energy, outputs include waste heat, solid waste, air emissions, water emissions, and usable products.

Life cycle inventory

The main task of the inventory analysis is to collect data to measure the inputs and outputs of the system. Data collection is a resource-intensive process and will vary depending on the scope, the system, and the application of the study. During the data collection process, the system boundaries are often finalized on a cut-off criterion that limits the analysis of unit processes, e.g. when values are below a certain threshold. Calculation procedures are necessary to generate the inventory of results for the unit processes and for the overall system. The following steps are necessary: 1) prepare the data and make calculations within each subsystem, 2) analyze the data to identify problems, gaps, inconsistencies, or data that is non-detectable, 3) aggregate data from different sources, if necessary, for communication between the LCA practitioner and the user or for external purposes, 4) connect the subsystems to allow calculations of the complete system, 5) relate functional units of each system when comparing products or service systems.

Impact assessment

The purpose of impact assessment is to understand and evaluate the magnitude and significance of environmental impacts based on the inventory analysis. This stage consists of three steps: i) *classification*, ii) *characterization*, iii) *valuation*.

Classification, the grouping and sorting of the inventory data into impact groups, such as Global Warming, Acidification, and Toxicological Impact.

Characterization, the analysis and quantification of the impact in each category. An important component is the use of relevant physical, chemical, biological, and toxicological data that describe the potential impacts.

Valuation, the integration across impacts categories through weighting and ranking in order to determine the overall impact.

Improvement assessment

The improvement assessment component of the LCA is a systematic evaluation of the needs and opportunities to reduce the impacts associated with energy and raw material use and waste emissions throughout the life cycle of a product or process. The analysis may include both quantitative and qualitative measures of improvements.

6.3.3 From life cycle thinking to CRS

The chemical route selection tool (CRS) is based on the LCA framework, but is adapted to the analysis of chemical routes. It consists in the following 7 steps, in analogy to the ELCA method (Cornelissen 1997), which are further discussed and elaborated below: 1) define goals and scope, 2) identify alternative supply chains, 3) streamline the analysis, 4) conduct the inventory, 5) perform an exergy analysis, 6) assess the results, 7) report

The selection of chemical routes is very different from the analysis of existing designs. This brings the following two considerations in mind. Firstly, the chemical routes are typically still in development, which limits the *availability and reliability of data*, e.g. the formation of by-products and the energy requirements of the process. It is imperative that *assumptions* are made and that these are thoroughly checked afterwards. In other words, the selection of chemical routes is a design activity. Secondly, the identification of supply chains is characterized by a *large degree of freedom*, since the process has to be designed and all process-related decisions are made later in the design trajectory. For example, hydrogen can be made from at least three different feedstocks: natural gas (via steam reforming), water (via electrolysis) and biomass (via gasification). Therefore, *scenarios* should be defined in order to explore the implications of the different supply chains.

Define goals and scope

This stage defines the purpose of the study and identifies the questions that are to be addressed. The types of decisions can be divided into four types: 1) *Baseline*: the evaluation of existing routes or entirely new routes, 2) *Baseline versus baseline*: the evaluation and comparison of existing routes, 3) *Baseline versus new*: the evaluation of an existing route and an entirely new route, 4) *New versus new* analysis: the comparison of entirely new routes.

The chemical routes are identified in accordance with the type of analysis and as much as possible information within the time constraints is collected. If vital information is lacking, assumptions are made and documented. It is important that the practitioner clearly defines which resources are considered renewable and which other criteria/constraints are important (including metrics). When dealing with renewable resources the following criteria should be included: i) *the net CO₂ emission* - the overall emission of the entire supply chain minus the amount of CO₂ that is recycled or fixated. This criterion is important in the sustainability debate and also provides insight in the extent to which renewable carbon is used. It can be measured in tons per unit of product (ton/ton). ii) *The ecological impact required for the production of renewable resources* - if this criterion exceeds a certain limit,

the route could turn out to be practically infeasible. It can be measured in acres per year per unit of product (ha/yr/ton).

Two other aspects are absolutely crucial for this type of analyses and should be addressed as soon as possible: ii) *the system boundary* - the system boundary should be in accordance with the purpose of the study and should comprise the extraction of resources, energy conversion (e.g. production of electricity), replenishment of renewable resources (e.g. biomass growth), and the chemical processes (Figure 6.3). The system boundary can be streamlined with respect to the most important processes (see step 3). Sufficient information should be available after the identification of the supply chains. From a life cycle perspective, the scope of the analysis should be from 'cradle to grave'. For practical reasons this is very difficult, since base chemicals are typically used in a large variety of applications. The system boundary should thus define the limits of the analysis. ii) *the allocation methods* - if a process has multiple outputs, an allocation problem exists. The reliability of LCA studies highly depends on the allocation methods that are used to deal with this problem. Step 5 discusses the allocation on the basis of exergy values.

Identify alternative supply chains

In this step the production of the feedstocks is traced back to the extraction of resources. Along the way, decisions have to be made whether certain production processes should be considered or not. Criteria are defined to select among alternative routes, such as fastest, shortest, cheapest, etc. Accordingly, the following procedure is suggested: 1) define *engineering criteria* on the basis of which unit processes are considered, e.g. technical feasibility, availability, 2) identify the *tree of production processes* (see example case), 3) define *screening criteria* on the basis of which supply chains are selected, e.g. the smallest number of unit processes, availability of resources, 4) identify alternative supply chains. The information needed in this step can often easily be found in common literature sources, such as *Kirk-Othmer Encyclopedia of Chemical Technology* (Kirk and Othmer 1998) and *Ullmann's Encyclopedia of Industrial Chemistry* (Ullman 2000). Of course, in a business situation the existing research and development data are used.

Streamline the analysis

Practitioners seek ways to reduce the time and resource intensity of this type of studies. Streamlining generally can be accomplished by limiting the scope of the study or by simplifying the modeling procedures, thereby limiting the amount of data needed for the assessment. Methods of streamlining may include the following: i) limiting or eliminating life cycle stages, ii) using of estimations and assumptions, iii) establishing criteria to be used as *knockouts*, iv) limiting the constituents studied to those meeting a threshold value.

Streamlining allows the practitioner to tailor the goals and constraints to a subset that is directly applicable to the specific decision and narrows the scope of the analysis to the relevant constituents that influence the decision. An example of streamlining is the elimination of terms relating to the production of equipment. In

bulk processes the lifetime of equipment is very long (>20 years) and the throughput high, which reduces the significance of this contribution. In the assessment step, the use of the streamlining methods should be validated.

Conduct the inventory

This step is identical to the life cycle inventory of the LCA framework, as discussed above. There are, however, some points of attention in the case of chemical processes: 1) Data on chemical processes outside company borders are scarce: encyclopedias provide rough data on yields and selectivities, but specific information on for example energy requirements is not readily available. 2) Data on common operations are typically available in many varieties: if the differences are small there is no problem, if they are large one could consider to use scenarios, e.g. the use of fertilizers in agricultural operations. 3) Chemical processes can be complex: the unit processes should preferably be treated as a black box, since the inside structure is often unknown. Refineries, for example, are very complex with many chemical processes that are all intertwined. Assumptions are inevitable in this step. 4) The mass balances must be correct, the heat balances as much as possible. 5) All inventory data should be normalized per unit of end product.

If gaps occur in the inventory data and if plausible assumptions cannot be made, the corresponding unit processes must be analyzed individually. Needless to say, all gaps, assumptions, etc. must be clearly documented.

Perform an exergy analysis

The exergy analysis forms the core of the CRS tool and its purpose is to quantify the use of resources and the efficiency of the supply chain. These concepts and the procedure to calculate them are discussed with help of Figure 6.3.

Again it must be clearly defined what is considered a renewable resource, as the production of biomass and the conversion of energy is within the system boundary. This means that besides non-renewable resources only renewable energy and materials, so-called building blocks, enter the system. Unfortunately, the magnitude of the energy stream is not easily determined. The amount of non-renewable resources is therefore considered as the most practical indicator for the renewability of the supply chain, i.e. the less non-renewables the better. During the inventory analysis, the streams were normalized per unit of product (typically per ton). The use of non-renewable resources can then be expressed in $\text{GJ}_{\text{exergy}}$ per ton of product. Insight in the efficiency of the entire system is obtained by determining the total amount of exergy lost, which can be expressed as:

$$Ex_{\text{lost}} = Ex_{\text{total},\text{in}} - Ex_{\text{useful},\text{out}} = \sum_n Ex_{\text{lost},n} \quad \text{Equation 6.1}$$

The analysis of the system is nothing more than the accounting of streams: the exergy loss is the difference between what goes in and what goes out the system. This overall loss must equal the addition of the losses in all unit processes (also expressed in $\text{GJ}_{\text{exergy}}$ per ton of product). The analysis requires the exergy values of

all streams, including export heat and power, wastes and emissions and especially useful by-products.

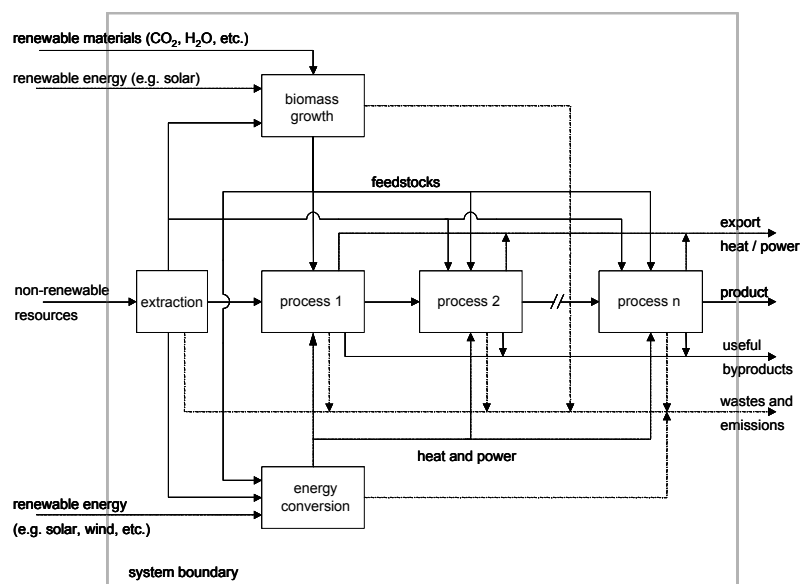


FIGURE 6.3 SCHEMATIC REPRESENTATION OF A SYSTEM

The purpose of the ELCA is to assess the performance of the supply chain of the desired end product. Accordingly, the use of resources and the loss of exergy must be allocated to this product. Otherwise the useful by-products would be produced for free, which is obviously not the case. This can be accomplished by first dealing with all unit processes through allocating the inputs to the corresponding useful products. The total non-renewable exergy input resources can then be allocated to each of the products (see method below).

In conclusion, the exergy analysis consists of the following steps: 1) define useful products and waste streams, 2) calculate the exergy content of all useful streams, 3) determine the allocation factors of the useful products in each unit process, 4) determine the exergy loss of each unit process and the overall loss, 5) allocate the non-renewable resources and the exergy loss to the useful products.

Steps 3 and 4 can be used as a consistency check by comparing the overall results and the results by adding the outcome of all unit processes. The procedure to calculate the exergy content of streams is discussed in Appendix B, possible allocation methods below. The exergy losses associated with renewable energy are typically difficult to assess, e.g. the exergy of wind, and probably provide little insight in possible improvements. Furthermore, this loss is not relevant since the renewable resources are “free” from an exergetic point of view. It can therefore be decided to consider the losses associated with the use of non-renewable resources only.

Allocation of multiple products

When a process has multiple outputs an allocation problem exists. This problem is common in this type of analyses and is inherently controversial. It should therefore be clearly defined which allocation method is used and how it is applied. In this methodology two types of typical multi-product processes are distinguished: *homogeneous* and *heterogeneous* processes.

A homogeneous process is defined as a process in which the origin of the products cannot be determined, i.e. the exergy available in the feeds is homogeneously distributed among the products. An example of this type is the production of hydrogen and carbon monoxide from natural gas; it cannot be said that a certain part of the exergy in the fuel or in the natural gas is stored in one of the products. Accordingly, the inputs are allocated on the basis of the exergy content of the products:

$$Ex_{in,n,m} = Ex_{in,n} \cdot \frac{Ex_{out,m}}{Ex_{out,total}} \quad \text{Equation 6.2}$$

In words, the exergy available in feed n is allocated to product m proportional to its exergy-weighted contribution to the total exergy output of products. The ratio is also called the allocation factor. Note that, the outputs can be both material and energy streams.

A heterogeneous process is a process in which the origin of the products can be determined, e.g. the co-production of styrene and propylene oxide in which the feeds are ethyl benzene and propylene, respectively (see the CRS case study). Obviously, it cannot be said that part of the ethyl benzene is stored in the propylene oxide. Unfortunately, there is no standard method to solve this allocation problem. The suggested approach is to divide the unit process in sub-systems, which are then allocated separately: homogenous sub-systems are dealt with as discussed above; the remaining heterogeneous sub-systems are dealt with as defined by the practitioner.

Assess the results

In this step the performance with respect to the other criteria (required areas, CO₂ emission, etc.) should be determined. Conclusions can then be drawn with respect to the goal of the ELCA study, i.e. which supply chain requires the least non-renewable exergy input per unit of product and which are possible areas of improvement. Furthermore, it must be checked whether the constraints are not violated, e.g. the area required.

Very important in this step is to perform sensitivity analyses. These analyses are required to check to which extent the conclusions are influenced by the assumptions made during the goal definition and streamlining steps. It is inevitable that many assumptions are made in this type of studies, which makes LCA-studies extremely sensitive (Copius Peereboom, Kleijn, Lemkowitz, et al. 1999).

The sensitivity analyses must be in accordance with the goals of the analysis. After all, a comparative study requires a different approach than a baseline analysis. The

following procedure is suggested: 1) list all inventory data and assumptions (should be readily available), 2) choose variables of sensitivity analysis, e.g. suspicious inventory data, 3) define a metric that determines the sensitivity, e.g. the ratio of the deviations, 4) perform sensitivity analysis, 5) determine which variables are important, 6) repeat step 4 in more detail with the important variables (if necessary), 7) assess the validity of the results and conclusions.

Report

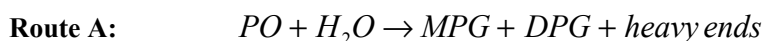
It is of crucial importance that the assumptions made during the ELCA are clearly documented. The report should contain at least the following items: ii) *Introduction* - describe the goals and scope of the CRS-study, including information on the chemical routes studied, ii) *alternative supply chains* - describe which supply chains are studied and why, iii) *approach* - describe the approach to the analysis, i.e. the decisions that are made in the streamlining step and the allocation methods used, iv) *results*: describe the results of the exergy analysis and the sensitivity analyses, v) *conclusions* - this Chapter discusses the conclusions and their validity, vi) *appendices* - these should contain all relevant information on assumptions, modeling, data of inventory analysis, data of exergy analysis, etc. The practitioner is strongly advised to use appendices for information that is not directly required in the corresponding Chapters. The example case in the next Chapter is outlined in accordance with these guidelines.

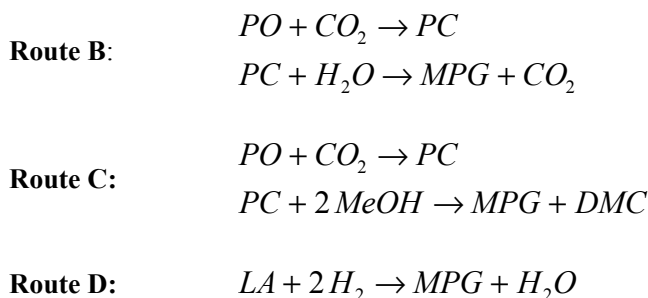
6.4 CRS case study: Monopropyleneglycol synthesis

The purpose of this example case is to illustrate the CRS methodology; the case deals with the production of MonoPropylene Glycol (MPG, $C_3H_8O_2$), a common base chemical used as a monomer in polymer production; some information is presented in. It can be produced via several chemical routes, among which are both fossil fuel and biological routes. The corresponding supply chains are not analyzed in great detail, as the objective is to illustrate: i) how to identify alternative supply chains, ii) how to conduct the inventory and exergy analyses, iii) how to present the results. The results of the case do provide useful insight in the sustainability of MPG production. The syngas case described in Chapter 7 (EA Case Study) provides more information on the analysis of individual processes.

6.4.1 Introduction

This case investigates the production of MPG from PropyleneOxide (PO) and from Lactic Acid (LA). The former feedstock is entirely produced from fossil resources; the latter can be produced from biomass containing carbohydrates (all types of biomass are considered renewable in this study). The following chemical routes are investigated:





Route A is used on a commercial scale in industry and produces the by-product DiPropylene Glycol (DPG) with a MPG/DPG ratio of 10 (Kirk and Othmer 1998). The reaction also produces heavy ends, such as TriPrpylene Glycol (TPG), but these are not taken into account. Excess water is required in order to reach this selectivity, which leads to an energy intensive separation step.

Route B avoids this excess of water, as MPG is formed via Propylene Carbonate (PC). The PO reacts in the first step with carbon dioxide and then forms MPG in the second step as water is added. This step is issued in a patent by Mais and Buysch (EP 0543234A2, 1993). The patent also describes *Route C*, which is a co-production of MPG and DiMethyl Carbonate (DMC), a promising industrial solvent. It is assumed that both routes do not form unwanted by-products.

Route D is interesting from a sustainable perspective, since MPG can be produced via *green* lactic acid. However, route D also requires hydrogen, which is not necessarily renewable. The patent issued by Zhang (WO 030744A1, 1999) describes a production process with a 90% yield of MPG with respect to LA.

The objective of this study is to compare the three alternative routes (B, C, and D) with the conventional route A (new vs. baseline analysis) from a supply chain perspective. The alternatives are analyzed with respect to the use of non-renewable resources and the quantity and origin of the exergy losses (both in GJ per ton of MPG). Furthermore, the study considers the net CO₂ emission and the area required for biomass growth, in ton/tonMPG and ha/yr/tonMPG, respectively. The results are presented separately; it is left to the reader to judge which alternative performs best.

6.4.2 *Alternative supply chains*

The *tree of production processes* is shown in Figure 6.4, in which the unit processes were selected on the basis of their technical feasibility and industrial application. Propylene oxide, for example, can be produced via several routes of which the co-production with styrene monomer is applied on an industrial scale in the Netherlands. The structure of the tree is entirely based on information as found in *Kirk-Othmer, Encyclopaedia of Chemical Technology* (Kirk and Othmer 1998).

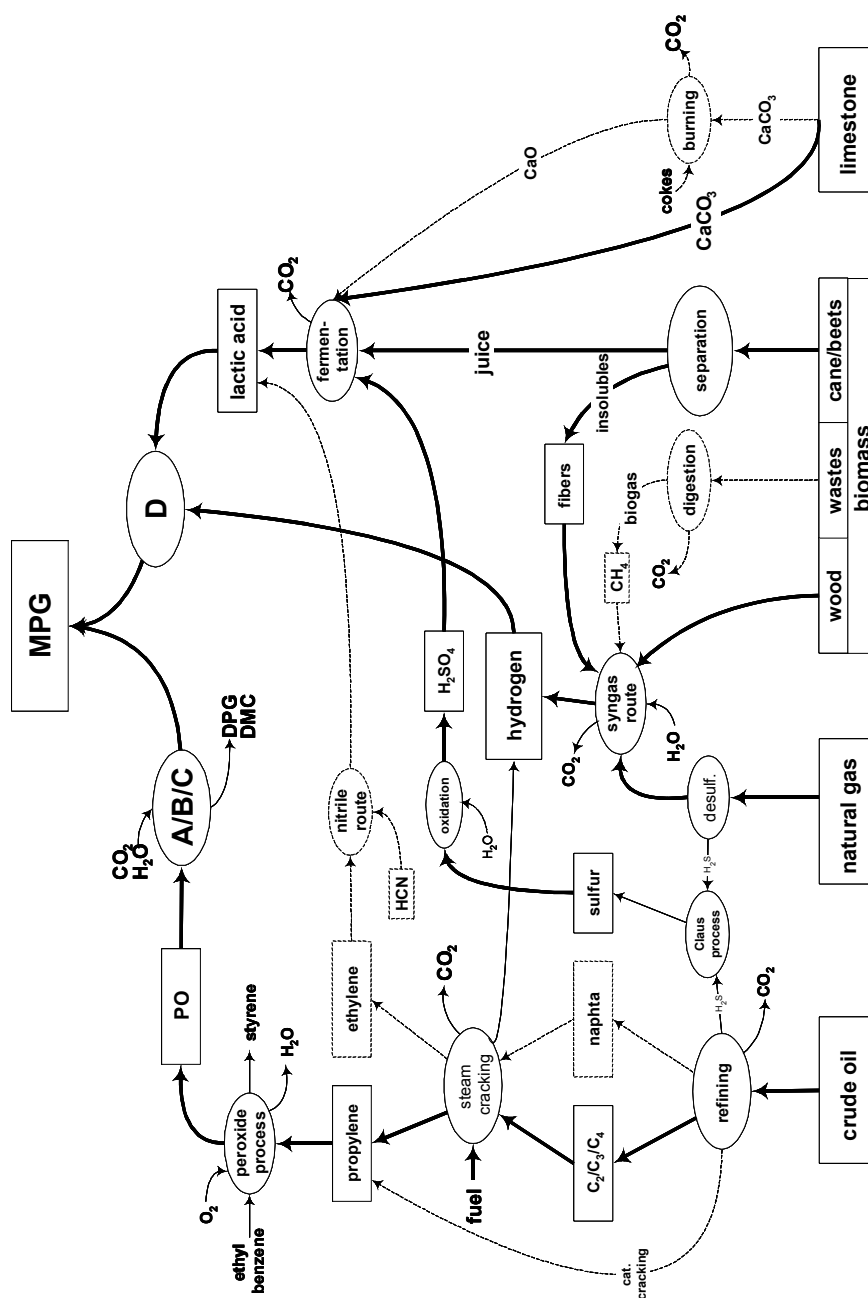


FIGURE 6.4 TREE OF PRODUCTION PROCESSES FPR MPG PRODUCTION

Many combinations of processes are possible to produce MPG. The ones with dotted lines in Figure 6.4 are not considered due to the following reasons: 1) it would be little efficient to produce lactic acid from ethylene, 2) steam cracking of

naphtha was considered to be too complicated, 3) the digestion of beet waste is not necessary when a gasification process is already available to process wood, and 4) it was assumed that CaCO_3 could be used directly in the fermentation process. As a result, six supply chains were selected in this study (shown in Figure 6.5A-D):

Supply chain 1: from crude oil as scarce resource via refining, thermal cracking of propane, the peroxide process, and finally route A (baseline)

Supply chain 2: same as Supply chain 1, but via route B

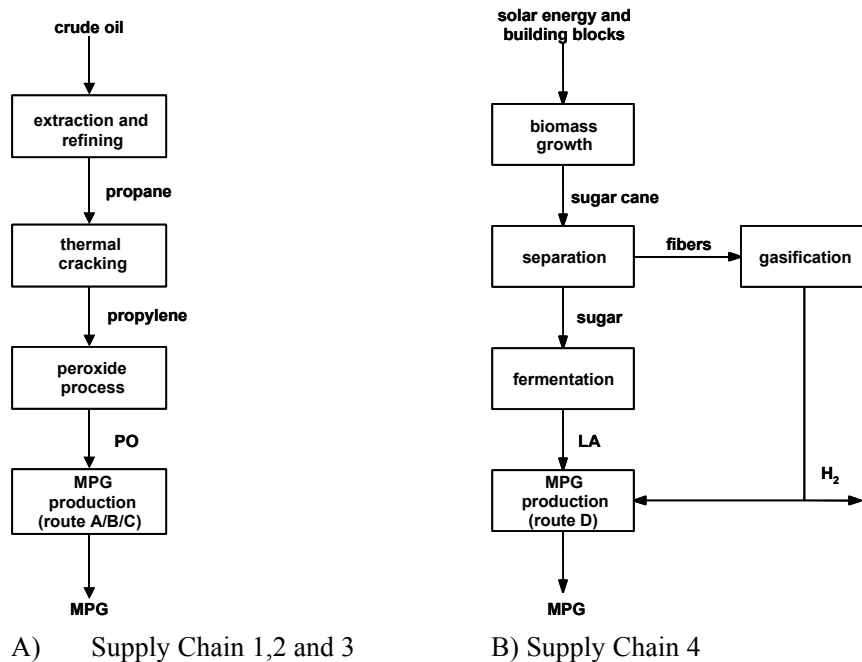
Supply chain 3: same as Supply chain 1, but via route C

Supply chain 4: from sugar cane as renewable resource via fermentation of sugar, gasification of fibers (via route D)

Supply chain 5: from sugar beets as renewable resource via fermentation of sugar and gasification of fibers and additional wood (via route D)

Supply chain 6: from sugar beets as renewable resource via fermentation of sugar, gasification of fibers and partial oxidation of natural gas for hydrogen production (via route D).

The sugar cane in Supply Chain 4 is grown in Brazil; the MPG is produced locally and shipped to Europe. The other supply chains are located in Europe. The purpose of the figures is to show the most important unit processes and do therefore not contain all streams, see Appendix C. Note that the production of sulphuric acid is not shown, but is taken into account.



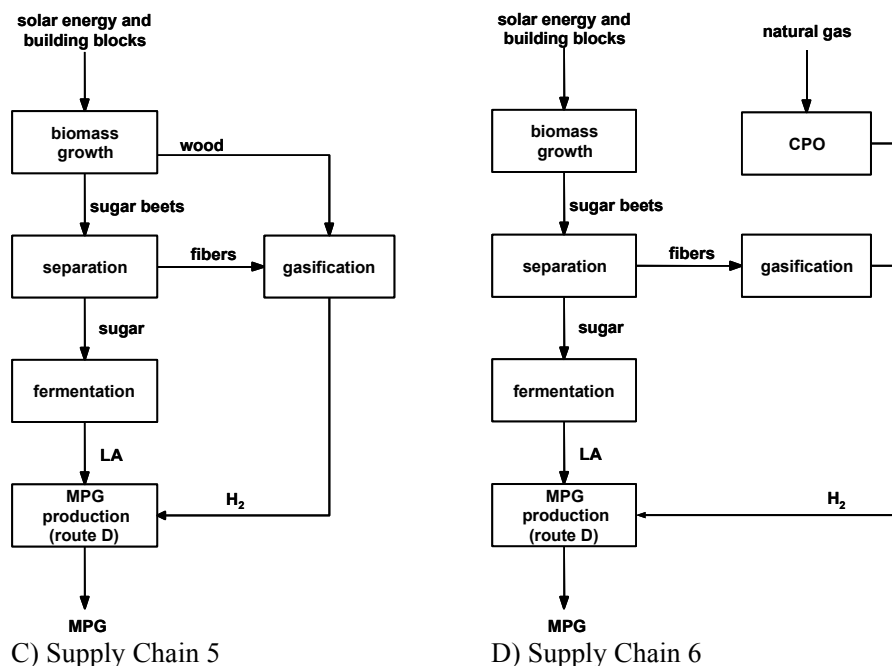


FIGURE 6.5 SIX ALTERNATIVE SUPPLY CHAINS FOR MPG

6.4.3 Approach

The analysis has been streamlined by neglecting the physical energy requirements of the unit processes, i.e. separations, pumps, compressors, etc. This assumption is made due to i) the scarcity of data, ii) the time intensity of modeling those energy streams, and iii) their relative small contribution to the total energy consumption (see methanol case). The energy requirements that are associated with chemical conversions are taken into account, e.g. furnace fuel for thermal cracking. If the differences between the alternatives turn out to be small, this assumption should be reconsidered. During the analysis, many other estimations and assumptions were made on unit process level. These can be found in Appendix C.

The homogeneous allocation method is used during the exergy analysis, except for the peroxide process. In this process, it was defined that the oxidation step of propylene to PO provides part of the exergy contained in styrene. In this case there is not an actual useful product, but more a useful contribution to styrene. This contribution was then treated as if it were a useful product. The exergy inputs and losses were allocated to the useful products on unit process level employing an allocation factor. In order to allocate the resources to the final product, the allocation factors of all unit processes can be aggregated into a cumulative allocation factor (homogeneous processes). In this way the resource consumption per unit of final product can be easily determined.

For example in the case of supply chain 4, in which the hydrogen produced is partly used again in the MPG production, the total cumulative allocation factor is calculated by adding the cumulative allocation factors of the parallel sub-chains, i.e. those of the chains to sugar and to the part of hydrogen used.

6.4.4 Results

This section discusses the final results of the exergy analysis. The results of the inventory analysis, including the exergy values of streams and allocation factors, can be found in Appendix C. Figure 6.6 shows only the overall results of Supply Chains 1 and 4. The results of the other alternatives can be presented in a similar way.

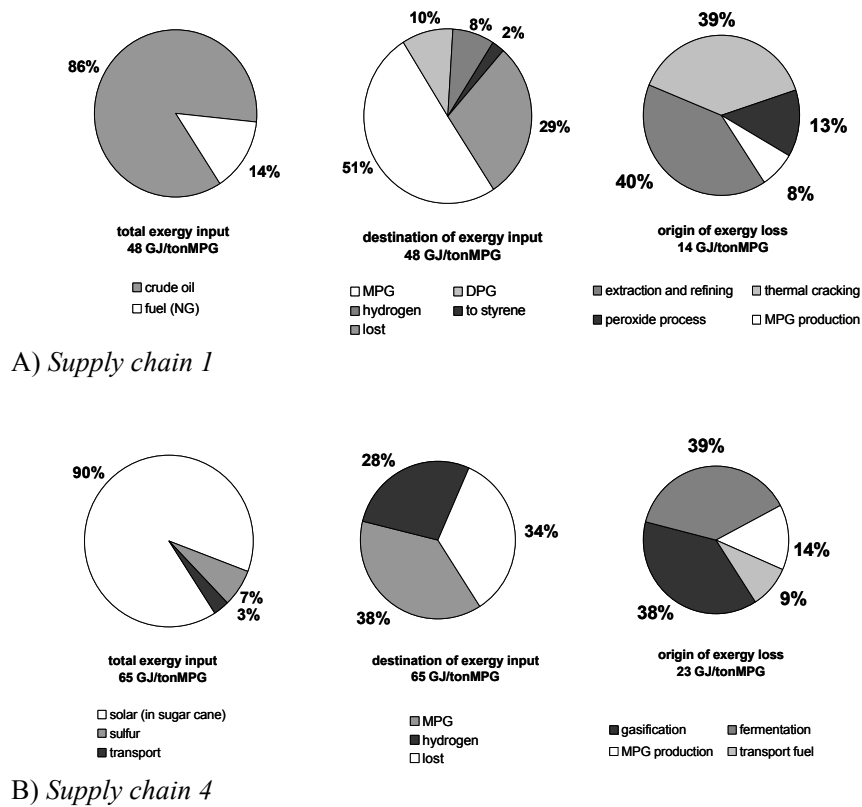


FIGURE 6.6 OVERALL RESULTS OF SUPPLY CHAINS 1 AND 4

The first pie-diagram shows the resources used and their total input of exergy and directly provides insight in the use of non-renewable resources. The second diagram shows the destination of the exergy input. Figure 6.6A shows that the largest part of the input is stored in the desired product and that a substantial part is

destroyed. The third diagram shows the origin of this loss, which provides insight in the performance of each of the unit processes. In order to compare the supply chains, the exergy input, losses and other criteria should be allocated to MPG. The results are shown in Table 6.2.

TABLE 6.2 RESULTS OF THE CRS (ALLOCATED TO MPG)

Supply chain	Total exergy input (GJ/ton)	Non-renewable exergy input (GJ/ton)	Net CO ₂ emission (ton/ton)	Area use (ha/yr/ton)
Chain 1a	34.7	34.7	0.5	-
Chain 1b ¹⁾	41.6	41.6	0.6	-
Chain 2	34.7	34.7	0.5	-
Chain 3	34.7	34.7	0.4	-
Chain 4	40.6	7.1 ²⁾	-1.6	0.13
Chain 5	38.8	5.9 ²⁾	-1.6	0.19
Chain 6	48.8	15.9 ²⁾	-1.0	0.17

¹⁾ When DPG is considered a waste.

²⁾ Including sulphur for production of sulphuric acid.

Supply Chain 1 and 2 show the same results, because the exergy content of DPG is similar to that of MPG. If the DPG is considered a waste, then route 2 significantly requires less non-renewable exergy input per ton of MPG. One could argue that the MPG has to be produced anyway and that the DMC produced in Supply Chain 3 should therefore only get the penalty of *additional* exergy input and CO₂ emission, 35.6 GJ/ton of DMC (natural gas in methanol production) and 0.22 ton/ton of DMC, respectively. The results of Supply Chain 3 are therefore also equal to Supply Chain 1.

The renewable Supply Chains (4 and 5) require similar amounts of exergy input, but the non-renewable part is significantly smaller. Supply Chain 6 requires natural gas for the production of hydrogen, which doubles the non-renewable input compared the Supply Chains 4 and 5. The sulfur needed for sulphuric acid production is responsible for 60-75% of this non-renewable exergy input. This sulfur, however, is a waste from refineries and natural gas production. One can argue that this should therefore not be considered.

The CO₂ emission in Supply Chains 4 to 5 is negative, because more CO₂ is fixated during biomass growth (approx. 3 ton/ton of MPG) than is emitted in the total supply chain. The area required is in the order of magnitude of 0.2 ha/yr/ton of MPG, which comes down to 300 km² for a MPG production rate of 150 kt/yr. The area for chain 4 is smaller, because a part is allocated to the excess hydrogen that is produced.

A sensitivity ratio (SR) has been used in order to determine which parameters have the largest influence on the final results:

$$SR = \frac{\text{Deviation in result}}{\text{Deviation in parameter}} \quad \text{Equation 6.3}$$

TABLE 6.3 SENSITIVITY RATIOS OF PARAMETERS FOR SUPPLY CHAINS 1-3

Parameter ¹⁾	Total exergy input	Non-renewable exergy input	Net CO ₂ emission
MPG/DPG ratio in route A	0.4	0.4	0.0
Selectivity of propylene production	1.2	1.2	1.2
Furnace efficiency (steam cracking)	0.1	0.1	0.6
Refining efficiency	1.0	1.0	4.4

¹⁾ The parameters were varied by 10%

TABLE 6.4 SENSITIVITY RATIOS OF PARAMETERS FOR SUPPLY CHAINS 4-6

Parameter ¹⁾	Total exergy input	Non-renewable exergy input	Net CO ₂ emission
Yield of MPG production from LA	1.1	1.1	1.1
Yield of fermentation of sugar	0.3-0.4	0.8-1.4	0.0
NR input of biomass growth	<<1	0.1-0.8	<<1
Yield of H ₂ production from cellulose	0.1	0.0	0.2

¹⁾ The parameters were varied by 10%

The efficiencies of propylene production and refining are the most important parameters in Supply Chains 1 to 3, i.e. the SR is larger than unity. Especially the latter has a profound influence on the CO₂ emission of Supply Chains 1-3. The yields of MPG production from LA and of the fermentation of sugar have the most influence on the results of Supply Chains 4-6. The ratios in Table 6.4 vary as a result of the differences in hydrogen production in the chains. The table shows that these differences do not have large influence on the ratios.

The differences between the chains with respect to the three criteria, as shown in Table 6.2, are considerable. It is not expected that reasonable deviations in yields and efficiencies have any influence on the comparison of the results. Furthermore, the assumption to neglect physical energy requirements seems to be justified.

6.4.5 Concluding remarks on the CRS case

The objective of this study was to compare the three alternative routes (B, C and D) with the conventional route A (new vs. baseline analysis) from a supply chain perspective. Accordingly, the following conclusion are drawn:

- The supply chains associated with chemical routes A, B and C require significantly more non-renewable exergy than the ones associated with route D.
- Due to their high selectivity, routes B and C require less scarce resources per ton of MPG than route A (if DPG is considered to be a waste).
- Compared to route B, DMC can be produced with an additional exergy input (non-renewable) of 35.6 GJ/ton and an additional net CO₂ emission of 0.22 ton/ton.
- The green supply chains associated with route D fixate CO₂ whereas the other chains emit approximately 0.5 ton/ton of MPG.

- Sensitivity analyses show that the influence of the assumptions is too small to undermine the comparison.

6.5 Guidelines for process synthesis tool

Design methods in general are essential to approach and solve design problems, but are useless when no effective strategy is at hand. Guidelines can help the designer to develop and implement such a strategy. Obviously, the design of chemical processes requires guidelines due to its complex nature. This Chapter focuses on guidelines that can contribute to the design of sustainable processes. Guidelines must be an integral part of synthesis methods that can be divided in four categories (Herder 1999, 1999]: i) *learning on the job* methods, ii) *optimization-based* methods, iii) *knowledge-based methods*, iv) *hierarchical methods*. In the common chemical engineering literature (like the teaching books discussed in Chapter 4), many guidelines appear, but here the emphasis is on the development of guidelines for energy efficient engineering.

Learning on the job guidelines are based on individual experiences and, as a result, no documented methods of structured thinking are available. The *optimization-based methods* and the *knowledge-based methods* are more technological and case-specific methods, such as pinch techniques and specialist software tools, respectively. It is expected that these methods are little supported by general applicable guidelines and are for this reason not discussed in this Chapter. As background literature, reference is made to articles by Cano-Ruiz (Cano-Ruiz and McRae 1998) and Yang (Yang and Shi 2000), which give a nice review of current developments in the field of optimization and knowledge engineering related to environmental constraints.

Hierarchical methods are used in almost every design process, because the human mind simply cannot consider all details at the same time. During the design process a hierarchical approach helps to decide which factors are important and which are not. Accordingly, this Chapter discusses guidelines from a hierarchical point of view.

Hierarchical design methods can actually be considered as a collection of strategic and practical guidelines. The former type helps the designer to structure the generation of alternatives and should enlarge the chances of success. The latter are *heuristics* or *rules of thumb* that quickly help the designer to find an optimal solution. For example, Douglas' hierarchical approach (Douglas 1988) is well-known and widely used in chemical process design (as already discussed in Chapter 3 and 4). Many design methodologies have adopted this strategy and elaborated it in various ways. For example, the textbook by Seider et al. provides many guidelines (Seider, Seader, and Lewin 1999); although they consider some environmental and safety issues, a truly sustainable approach is not discussed.

6.5.1 Existing guidelines for process synthesis

More guidelines on the individual sustainability issues can be found in literature. Needless to say, there is an inevitable overlap between the separate issues, but this is considered to be of minor importance. Below some categories of guidelines are

provided: i) intensification opportunities, ii) recycle structures, iii) energy integration, iv) economics, v) environment, vi) safety and health.

Intensification opportunities

- If an endothermic reaction is driven by an exothermic reaction, investigate one tube processes (e.g. CPO)
- When using an exothermic reaction investigate chemical heat recovery (e.g. using a pre-reformer in syngas production)

Recycle structure

- Minimise inerts and non-reacting components.
- Best reactor is counter-current.
- The best process is the one in which energy/mass is withdrawn over the full length of the apparatus.
- If the reaction is exothermic increase temperature.
- If the reaction is endothermic decrease temperature.
- It is not necessary to fully convert the reactants, recycling is better.
- The larger the recycle, the larger the losses.

Energy integration (Sama 1995)

- Heat (or refrigeration) is more valuable the further it its temperature is from the ambient.
- Minimise mixing of streams with differences in P, T and composition.
- Do not heat refrigerated streams with hot streams or with cooling water.
- Heat exchange between two streams is more efficient if the flow heat capacities are similar. If there is a large difference, consider splitting the larger.
- Minimise the use of intermediate heat transfer fluids.
- The economic optimum ΔT at a heat exchanger decreases as the temperature decreases and vice versa.
- Minimise throttling.
- The larger the mass flow, the larger the opportunity to save (or waste) exergy.

Economics

All teaching books on process design contain guidelines and heuristics that are usually implicitly based on economic considerations. Besides that for many, the essence of conceptual process design is a cost estimation based on heuristics for economic calculation of process equipment, such as compressors and vacuum pumps, cooling towers, crystallization, etc.

There is a growing need for a life cycle approach in process synthesis from an economic perspective. This approach could improve the performance of the process with respect to operability, maintainability, flexibility, reliability, availability, capacity, etc. Unfortunately, it is beyond the scope of this work to discuss the progress on each subject. To get an impression, an article by Ishii (Ishii 1997) is

recommended for further reading, because it is a good example of a life cycle approach towards economic considerations.

Environment

During the last few decades the attitude towards the environment has been shifting from end-of-pipe waste treatment to source reduction, recycle and reuse. Examples of this development are *Waste Minimization* and *Pollution Prevention* (see also Chapter 2), two approaches with different names but similar goals. The first objective is to look for opportunities to minimize waste at the source. If that is not possible, the next option is to recycle the material or reuse it. This reuse can be facilitated by collaboration between companies. The third option is to treat the waste and if all options run out than the last resort is safe disposal. Here, a sample set of heuristics for minimization and prevention of waste is provided:

- Wherever possible eliminate waste materials at their source. This can sometimes be achieved by switching raw materials.
- Recycle waste materials within the process. Where not possible, explore the possibility of using these materials within other processes.
- If wastes are formed reversibly, recycle to extinction.
- Look at the product – can another product that generates less waste fill the same customer need.
- Review chemistry alternatives including catalysis.
- For all heating duties use the utility with the lowest practical temperature.
- Minimize the total number of main equipment items and minimize piping connections.
- Look at changing set points or tightening control variations of key variables. Modifying single equipment items (like changing column internals) can also yield significant improvements with little capital expenditure.
- Pollution prevention and control are generally more difficult and costly in batch operations than in continuous processes.
- The inherent flexibility of batch plants makes raw material product substitution simpler.
- Don't buy waste – in raw materials, packaging, etc.

A good source of guidelines is the journal *Chemical Engineering Progress* published by AIChE and often contains articles on this subject. Berger (Berger 1999), for example, discusses heuristics that apply to pollution prevention and control decisions in multi-product plants.

Safety and health

Kletz ((Kletz 1999) is a well known author in the field of *inherent safer design* and discusses the characteristics of a friendly plant in a hierarchical way and provides design guidelines accordingly. Kletz wrote this book in 1990 and much progress has been made since then, especially in the hard- and software of process control. However, many of his guidelines are still generally applicable.

- *Intensification*; friendly plants contain low inventories of hazardous materials. The amount is so little that it does not matter if it all leaks out.

- *Substitution*; if intensification is not possible then an alternative is substitution: using a safer material in place of a hazardous one.
- *Attenuation*; another alternative is to use a hazardous material under the least hazardous conditions.
- *Limitation of effects*; if friendly equipment does leak, it does so at a low rate that is easy to stop or control.
- *Simplification*; simple plants are friendlier than complex plants because they provide fewer opportunities for error and contain less equipment that can go wrong.
- *Avoiding knock-on effects*; friendly plants are designed so that those incidents that occur do not produce knock-on or domino effects.
- *Making incorrect assembly impossible*; friendly plants are designed so that incorrect assembly is difficult or impossible.
- *Making status clear*; with friendly equipment it is possible to see at a glance whether it has been assembled or installed incorrectly or whether it is in the open or shut position.
- *Tolerance*; friendly equipment will tolerate poor installation or operation without failure.
- *Ease of control*; when possible, physical principles should be used for control rather than added-on control equipment.
- *Software*; errors are much easier to detect and correct in some programmable electronic systems than in others.

6.5.2 *Towards sustainability guidelines*

Design guidelines are increasingly becoming important as synthesis methods rapidly grow in number. There is a huge amount of literature available on guidelines, but still no synthesis step is attempted to integrate these with sustainability perspectives. This is without doubt a difficult task, because on the one hand the guidelines must be accessible in a user-friendly manner and on the other hand they should cover a broad range of applications with a high level of detail. Definitely, an opportunity lies in the development of design supporting software tools that could be integrated with flowsheeting simulators.

Guidelines that improve the exergetic performance

This section provides and discusses a selection of guidelines that help the designer to deal with the abstract second law of thermodynamics. There are many authors who argue that the complex problem of sustainable development could be tackled with the second law of thermodynamics or exergy approach, e.g. Cornelissen (Cornelissen 1997) and (Dewulf, Van Langenhove, Mulder, et al. 2000). The concept of exergy can, for example, help to obtain quantitative and qualitative insight in the use of resources. However, it is not always clear how and when to use this concept in the development of new chemical processes, because mainly the tool is used for the analysis of existing processes and not for the generation of process innovations. In Appendix B a short introduction is given to the concept of exergy and the ways to perform an analysis.

Chemical reactions

Chemical reactions are typically responsible for large exergy losses; during an exothermic reaction, chemical exergy is converted into physical exergy. This conversion inevitably leads to exergy losses as shown in Figure 6.7 (Hinderink, Kerkhof, Lie, et al. 1996b; Hinderink, Kerkhof, Lie, et al. 1996a). The same principle applies to an endothermic reaction, in which physical exergy is converted into chemical exergy.

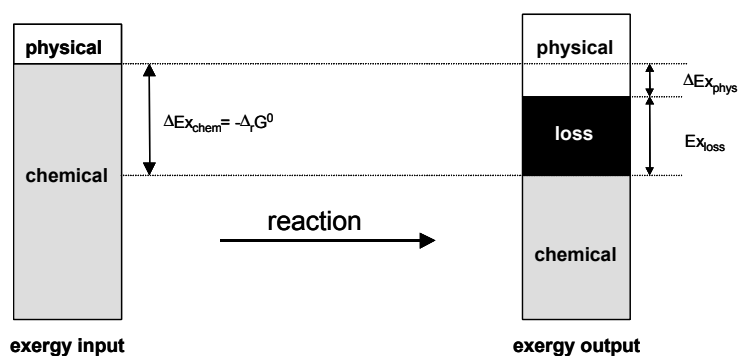


FIGURE 6.7 CHANGES IN EXERGY DURING AN EXOTHERMIC REACTION

The differences in chemical exergy of a single reaction cannot be avoided, since the difference in molecular identity must be resolved. This drop in chemical exergy can be used to drive an uphill reaction ($\Delta G^0 > 0$) through direct or thermal coupling. Direct coupling can, for example, be accomplished in electrochemical cells with special catalysts. The exergy losses are then reduced dramatically, as the driving force (=overall Gibbs energy of reaction) can in theory be reduced to almost zero. However, this is still not applied in industry and is therefore not discussed here. Thermal coupling can be found, for example in the production of syngas case, in which the combustion of natural gas drives the reforming reaction ($\Delta G^0 > 0$). The overall difference in the Gibbs energy of reaction can then be reduced, but a certain loss is unavoidable (Hinderink, Kerkhof, Lie, et al. 1996a; Hinderink, Kerkhof, Lie, et al. 1996b).

Since the basic chemistry is typically fixed in this stage of the design, this section deals with maximizing the return of physical exergy in exothermic reactions and minimizing the investment of physical exergy in endothermic reactions. Guidelines 1-3 help the designer to minimize the associated exergy losses, background and arguments are given below:

- Guideline 1** *In the case of exothermic reactions, heat must be withdrawn at the highest possible temperature.*
- Guideline 2** *In the case of endothermic reactions, heat must be supplied at the lowest possible temperature: investigate chemical heat recovery.*
- Guideline 3** *If the reaction is run in the gas phase and the number of molecules increases; it must be operated at the highest possible pressure and vice versa.*

The guidelines are derived as follows. The Denbigh relation shows that one has to look at both the reaction temperature and the Gibbs energy of reaction to minimize the exergy losses (Hinderink, Kerkhof, Lie, et al. 1996a):

$$Ex_{loss} = -\frac{T_0}{T_r} \cdot \Delta_r G(P_r, T_r) \quad \text{Equation 6.4}$$

In which T_r is the temperature at which the reaction proceeds isothermally. The relation shows that the loss of exergy is a function of both the temperature and pressure of the reaction, since these directly affect the Gibbs energy of reaction. In the case of exothermic reactions it is beneficial to increase T_r , and thereby simultaneously reducing $\Delta_r G$ (Guideline 1). The opposite applies to endothermic reactions, as $\Delta_r G$ is then reduced (Guideline 2), which also applies to varying the pressure (Guideline 3).

In the case of highly exothermic reactions (large $\Delta_r H^0$), the temperature is usually limited by the formation of by-products, decomposition reactions, etc. In the case of slightly exothermic reactions (small $\Delta_r H^0$), the highest possible temperature is the equilibrium temperature. At this temperature the Gibbs energy of reaction becomes zero and the reaction does not proceed further. An optimal situation must then be found in order to minimize the exergy losses while obtaining a reasonable conversion. This can, for example, be accomplished by dividing the reaction in several isothermally operated segments; e.g. one at high and one at lower temperature. Figure 6.8 shows the reduction of the exergy losses represented by the areas with the *squares* pattern (Carnot factor $\times$ enthalpy difference). In an actual flowsheet this could be implemented by taking two reactors, or by developing one reactor with both a high and low temperature zone. Obviously, a trade-off must be made between exergy losses and costs.

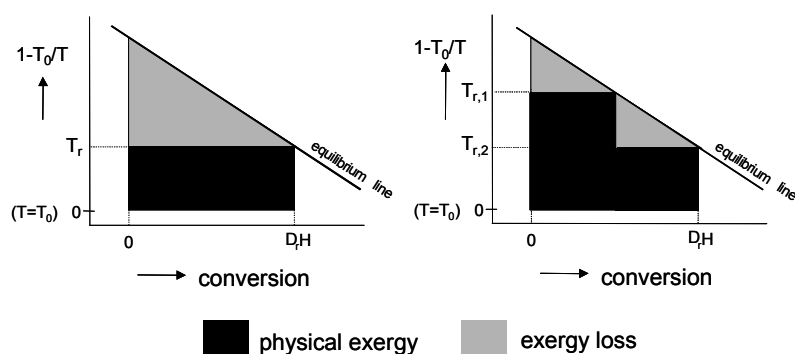


FIGURE 6.8 EXAMPLE OF USING GUIDELINE 1 IN EQUILIBRIUM REACTIONS

In the case of endothermic reactions, the designer can investigate chemical heat recovery (Guideline 2), i.e. driving the reaction with recovered heat of a sufficiently high temperature. An example is the use of a pre-reformer in synthesis gas

production (Hinderink, Kerkhof, Lie, et al. 1996b). Heat available in flue gases or hot product gases is then used to partly convert the natural gas. As a result, less high-temperature heat is required in the actual reformer.

A consequence of Guideline 1 is that the use of excess reactants and inerts (to reduce the reaction temperature) must be minimized. In the case of endothermic reactions this also applies, as exergy is always lost in the process of heating the reactants and cooling the products.

Guideline 3 seems to contradict the principle of *Chatelier*, which states that the pressure must be reduced if the number of molecules increases. This principle leads to an increased driving force and thereby to increased exergy losses. When a reaction has a large driving force, the pressure can probably be increased. In the case of a small driving force, however, the pressure could have a large influence on the conversion. The designer should then be aware of the drawbacks of applying guideline 3

Similar to the application of different reaction temperatures, the exergy losses can be reduced if the pressure is adjusted along the equilibrium line. However, reactors will then become increasingly complex and expensive. In the methanol case, the exergy losses in four different types of reactors are analyzed and discussed. The results illustrate the interpretation of the guidelines provided above.

Separations

This section discusses several guidelines based on those provided by King (King 1980), which can be used in the task identification stage when separation methods should be selected. Not all guidelines from these references seem to be useful, so only some are selected and some are taken together in the remaining part of this section.

The design of separations systems depends on the nature of the mixture(s) to be separated, which can be divided in (Schweitzer 1997): i) liquid-liquid mixtures, ii) liquids with dissolved solids, iii) gas (vapour) mixtures, iv) solid-liquid mixtures, v) solid mixtures, vi) gas-solid mixtures

Although each category has its specific approaches King (King 1980) shows generally applicable heuristics that should provide a basis for this stage of the design process. However, King's heuristics do not provide any insight in the synthesis strategy that should be followed. Therefore, the following design strategy is suggested: i) determine the requirements of the separation system as a black box (In/output, purity, recovery, etc.), ii) identify possible separation techniques and the corresponding steps, which typically do not depend on energy-related criteria, iii) estimate typical exergy requirements of the techniques, iv) synthesize an initial flow sheet with minimal exergy consumption while employing the 2nd law guidelines.

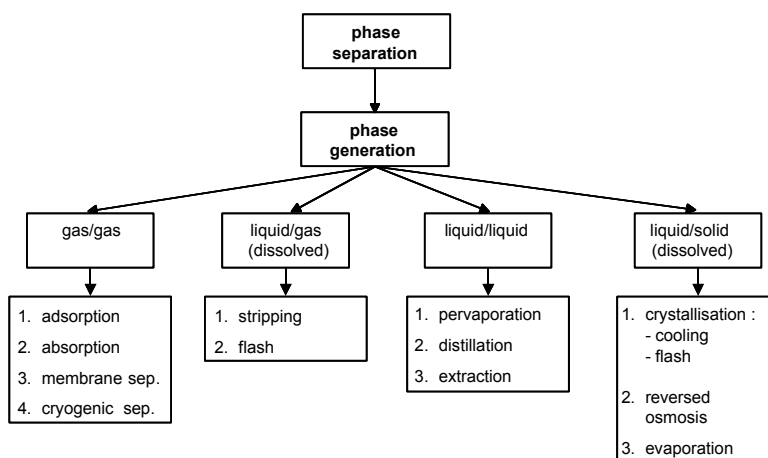


FIGURE 6.9 IMPORTANT SEPARATION METHODS IN CHEMICAL PROCESSES

In Figure 6.9, a decision diagram is sketched for the choice of separation systems. The tree starts with phase separation, because mechanical separations (filtration, centrifugation, etc.) generally require much less energy than separation processes for homogeneous mixtures:

Guideline 4 *Perform mechanical separations first if more than one phase is present in the feed mixture.*

Guidelines 5-8 then help the designer to select and develop a method for separating the resulting homogeneous mixture:

Guideline 5 *Favour separation processes transferring the minor component(s) between phases.*

Guideline 6 *Look at the quantity and quality of the energy that is required (exergy and temperature level); endeavour to use the full temperature difference between heat source and sink efficiently.*

Guideline 7 *For separations driven by heat throughput over relatively small temperature differences, investigate possible use of mechanical work in a heat pump.*

Guideline 8 *If phase changes are required, favour those processes with a lower latent heat of phase change.*

The energy consumption of a separation process is often directly related to the amount of material that must change phase. Particularly when a dilute solution is to be separated, it is often effective to choose a process, which will transfer the low-concentration component(s) between phases rather than the high-concentration component (Guideline 5). For example, ion exchange has an energy advantage over evaporation for desalting slightly brackish water (King 1980).

Then looking at alternative separation methods, it is important to look at both the quantity and quality (Carnot factor) of the energy that is required (Guideline 6). For example, both distillation and eutectic freeze crystallization can be used to separate liquid/liquid mixtures. However, the latter uses electric power with high quality for refrigeration purposes whereas distillation requires heat at relatively low

temperatures. It is therefore possible that distillation requires less exergy than crystallization although it uses more energy. Furthermore, it is important that the quality of heat is kept high. This can be accomplished by using the temperature difference between source and sink as much as possible. For example, heat applied to a reboiler can be re-used in the form of condensation heat when the temperature-drop over a distillation column is small, e.g. multi-effect distillation or is multi-effect evaporation.

Energy-separating-agent processes (evaporation, distillation, etc.) that do not involve too large a temperature difference between heat source and heat sink (typically <50 K) can also be operated through a *heat-pump principle* (Guideline 7). Heat pumps use mechanical work, as in a refrigeration cycle, to withdraw heat from a low temperature and to supply it at a higher temperature. For example, heat pumps can be used in the distillation of a mixture of propane/propylene. The vapor from the top is recompressed in order to use the heat of condensation in the reboiler.

In separation processes that exploit phase changes (e.g. distillation), the energy requirements for a given separation factor are directly proportional to the latent heat of phase change. Obviously, the energy consumption is reduced when agents with lower latent heats are transferred (Guideline 8). However, the incentive is reduced somewhat when multi-effect configurations are possible, in which the invested heat can be recovered more effectively.

Mixing and enthalpy changes

Sama (Sama 1995) provided a set of guidelines that are related to mixing and changes in enthalpy. The following guidelines are considered to provide insight in the associated exergy losses and to be generally applicable:

Guideline 9 *Minimize the mixing of streams with differences in temperature, pressure or chemical composition.*

Guideline 10 *Do not discard heat at high temperatures to the ambient or to cooling water.*

Guideline 11 *When exchanging heat between streams, the exchange is more effective if the flow heat capacities of the streams are similar. If there is a large difference between the two, consider splitting the flow with the larger heat capacity.*

Guideline 12 *Minimize the use of intermediate heat transfer fluids when exchanging heat between two streams.*

Guideline 13 *Minimize the throttling of steam, or other gases.*

Exergy is always destroyed when mixing streams, because driving forces are typically large and completely unrestrained (guideline 9). Quenching, for example, is a quick and cheap solution to cooling a hot stream, e.g. by using cold-shots in an exothermic reaction. However, it can be seen in the methanol case that the quench reactor shows the highest exergy losses compared to the other reactor types. If the hot streams were counter-currently exchanged with a cold stream, the heat could be recovered at higher temperatures. The same principle applies to the mixing of streams with differences in pressure or chemical composition.

Guideline 10 seems deceptively obvious, but learning from experience this type of mistake is often made in process design. Guideline 11 can be used when optimizing a heat exchanger network. The idea behind this guideline is that higher temperatures are obtained when exchanging streams with similar flow heat capacities (FC_p). For example, when a hot stream is exchanged with a cold stream with a higher FC_p , the heat is recovered at a relatively low temperature.

Exergy is inevitably lost in each step of heat transfer, because a minimum temperature difference is required in order to make it happen. When intermediate heat transfer fluids are used, this temperature drop is suffered at least two times. Hence, their use should be minimized (guideline 12). For example, it is better to heat cold process streams with hot streams than to generate steam.

Throttling is another useless destruction of exergy (guideline 13): physical exergy is converted into potential energy of the molecules through expansion, but instead of using this to perform work it is converted into low quality heat. For example, if flashing cannot be avoided, it should be performed in several steps in order to obtain vapor flows with higher pressure. Another option is to use turbines, which convert part of the physical exergy into electricity.

6.6 *GPS case study: Methanol synthesis*

Four alternative reactors for methanol synthesis are investigated in this case. Its purpose is to provide insight in the exergetic performance of individual reactors and in the performance of the overall process. In this way the validity of the guidelines presented in the description of the GPS tool can be provided. First, background information on the reactions is provided, alternative reactors, and the general flowsheet of the synthesis loop are discussed, then the performance of the individual reactors is discussed, and finally the performance of the entire loop is dealt with. Some background information on the methanol case is provided in Appendix D.

6.6.1 *Process background*

Methanol is typically synthesized in the gas phase over a heterogeneous catalyst from a gas that contains a combination of hydrogen, carbon monoxide, and carbon dioxide. Methanol is formed according to the following reactions:



$$\Delta_r H^0 = -90.5 \text{ kJ/mol}$$

$$\Delta_r G^0 = -25.1 \text{ kJ/mol}$$

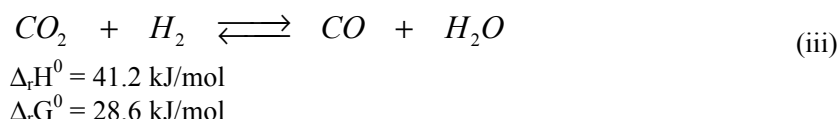


$$\Delta_r H^0 = -49.3 \text{ kJ/mol}$$

$$\Delta_r G^0 = +3.5 \text{ kJ/mol}$$

The reactions show that the synthesis gas should preferably contain as much carbon monoxide as possible, as an excess amount of carbon dioxide lowers the methanol

yield per unit of hydrogen. Although the first reaction (i) is thermodynamically favored above the second one (ii), a considerable amount of carbon dioxide is converted at operating conditions (approx. 260 °C, 60 bars). A reverse water-gas shift is also promoted over catalysts that promote methanol synthesis and must therefore also be considered. This reaction proceeds according to:

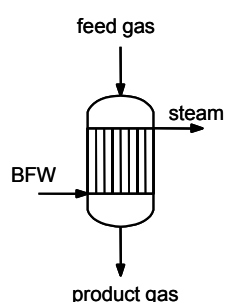


During methanol synthesis by-products are formed, such as higher alcohols, ethers, ketones, etc. These reactions are not considered in this case.

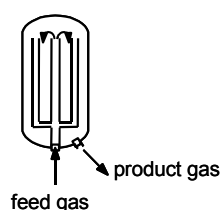
6.6.2 Reactor alternative

Four alternative reactors can be distinguished for the production of methanol, which are considered in this case (Cheng and Kung 1994): 1) Lürgi tubular converter, 2) ICI tube-cooled converter, 3) ICI quench converter, 4) Kellogg spherical intercooled reactors.

The Lürgi isothermal converter is a shell-and-tube unit in which catalyst is contained within relatively small diameter tubes. Reaction heat is transferred to the shell side, which contains boiling water. The shell side is connected to a steam drum, where normally 40 bars steam is generated. Figure 6.10A shows a schematic representation of this type of reactor. Figure 6.10B shows the ICI tube-cooled reactor, in the which reaction temperature is controlled by transferring heat to the incoming feed on the inside of the tubes. This reactor is actually adiabatic and was modeled accordingly. ICI also offers a quench reactor, which is shown in Figure 6.10C. The reactor consists of several beds between which fresh feed is introduced in order to cool the reaction gases. Figure 6.10D shows the Kellogg spherical reactor system consisting of several adiabatic reactors. The hot reaction gases are intermediately cooled through steam generation.



A) Lürgi tubular converter



B) ICI tube-cooled converter

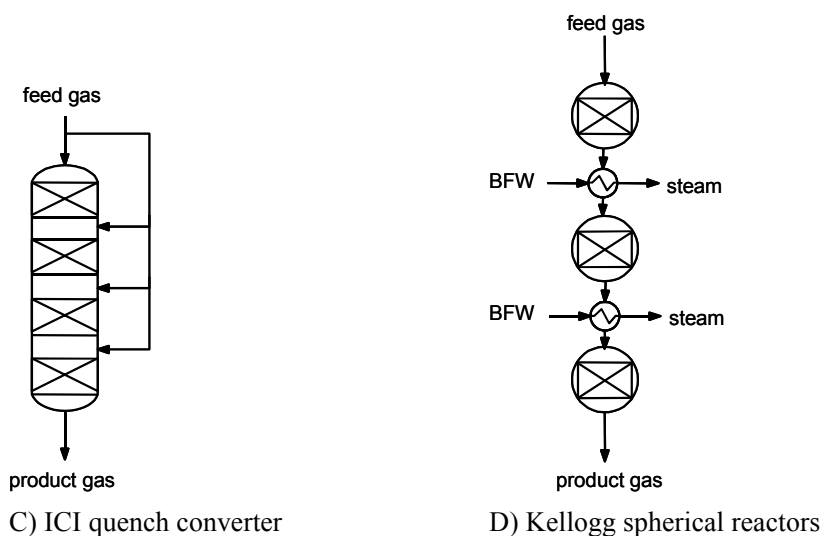


FIGURE 6.10 FOUR METHANOL REACTORS

These alternative reactors are generally incorporated into a synthesis loop, which is shown in Figure 6.11. Because of the relatively low conversion, a recycle is required in order to achieve a reasonable yield on feedstock. The syngas is compressed and mixed with the recycle stream after which it is preheated to reaction temperatures (typically in a feed/effluent heat exchanger). After reaction and heat exchange, the effluent is led to a crude condenser, where methanol and water are condensed out of the recycle gas. The recovered crude product then passes to the distillation train in order to meet specifications. Inerts and excess reactants are purged between the condenser and recycle compressor. In conventional processes, this purge contains large amounts of hydrogen and is used as furnace fuel.

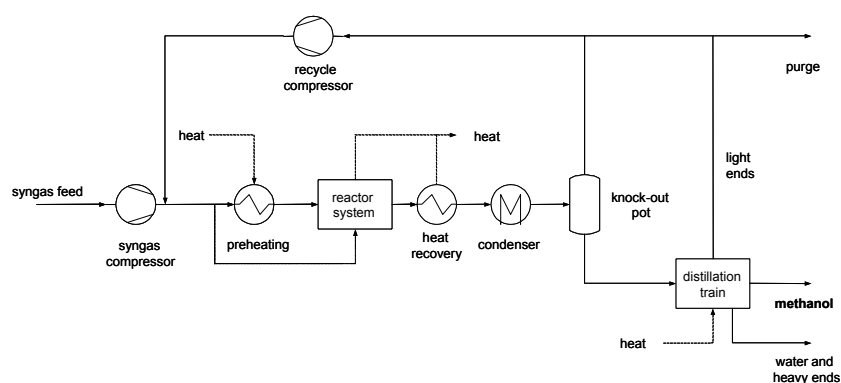


FIGURE 6.11 GENERAL FLOWSHEET OF METHANOL SYNTHESIS

The reaction and recovery sections produce heat whereas the preheating and distillation sections require heat. It is assumed that the compressors use electric power. In the case of the ICI quench reactor, part of the feed bypasses the preheater and is directly fed to the reactor.

6.6.3 Performance of the individual reactors

The reactors were first simulated individually to obtain insight in the exergetic performance of the different types. Table 6.5 shows a typical feed composition taken from Cheng and Kung (Cheng and Kung 1994).

TABLE 6.5 TYPICAL FEED COMPOSITION

Component	Mol %
H ₂	78.70
CO	4.33
CO ₂	3.48
Methanol	0.31
CH ₄	12.29
N ₂	0.85
H ₂ O	0.04

The reactors were modeled to produce the same amount of methanol in order to make a fair comparison. This implied that the reactor effluents should have the same temperature (265 °C), as this parameter is directly coupled to the equilibrium composition. Table 6.6 shows the exergy losses in each reactor both excluding and including losses due to heat transfer.

TABLE 6.6 EXERGY LOSSES IN THE REACTORS

(GJ/ton of methanol)	Lürgi	ICI tube	ICI quench	Kellogg
Excluding heat transfer	0.13	0.33	0.41	0.11
Including heat transfer	0.60	0.55	0.62	0.56
Reactor ¹	0.38	0.33	0.41	0.34
Heat transfer ²	0.22	0.22	0.22	0.22

¹) Heat transfer to steam (20 bars) with $\tau_{\text{ex}}=0.78$

²) Heat transfer to process stream with $\tau_{\text{ex}}=0.74$

The results show that the Kellogg and Lürgi systems have the lowest exergy losses when the contribution of heat transfer is excluded. However, the differences in losses between the alternatives become smaller due to heat transfer. In the isothermal Lürgi converter, for example, reaction heat is transferred to boiling feed water in order to generate steam, which leads to an exergy loss of 22%. The overall losses in the adiabatic reactor now become smaller than in the isothermal operation.

6.6.4 Performance of the entire synthesis loop

The alternatives were integrated in the synthesis loop as discussed above. The results of the exergy analysis are shown in Table 6.7.

TABLE 6.7 RESULTS OF THE EXERGY ANALYSIS OF THE SYNTHESIS LOOPS

(GJ/ton of methanol)	Lürgi	ICI tube	ICI quench	Kellogg
Total exergy input	37,17	37,12	36,66	35,23
Syngas	36,03	35,95	35,44	34,20
Power	0,81	0,81	0,79	0,76
Import heat	0,34	0,36	0,43	0,27
Exergy output	34,48	34,41	33,91	32,72
MeOH	22,38	22,38	22,38	22,38
Purge	12,10	12,03	11,53	10,34
Exergy losses	2,69	2,71	2,75	2,50
Compressors	0,21	0,21	0,20	0,19
Mixing	0,49	0,49	0,47	0,45
Reactor	0,38	0,39	0,50	0,43
Recovery	0,22	0,23	0,18	0,08
Separation	0,70	0,70	0,70	0,70
External	0,69	0,69	0,68	0,64

First of all, it can be seen that the exergy losses in the reactors are relatively modest compared with the overall losses. Furthermore, the results show that the exergy losses in the integrated reactors are again different among each other. This time the isothermal reactor comes out best. However, it must be said that the differences are very small and do not form a firm basis for comparison. The overall performance of the Lürgi and ICI tube-cooled reactors are nearly the same. When the purge is considered a loss (it actually is an undesired product), the ICI quench and Kellogg systems perform better. This is mainly caused by the higher conversions of hydrogen, which leads to reduced purges. The purge and conversion of hydrogen (influenced by the reactor conditions) are the most important design variables when optimizing the performance of this type of synthesis loops. Sensitivity analyses were conducted to investigate their impact on the performance.

6.6.5 Concluding remarks on the GPS case

The results of the exergy analysis already showed that the exergy losses in the reactors are relatively small compared to the overall loss, which mainly consists of the chemical exergy present in the purge and less of losses that are associated with compression, mixing, cooling, and so on. As a result, the exergetic performance is much more sensitive to changes in the magnitude of the purge than to manipulation of the reactor conditions. It is therefore recommended that the loop is first optimized with respect to the purge and losses in the recycle (at reactor conditions that are optimal for synthesis). Then sensitivity analyses can be used to investigate potential improvements by varying the reactor conditions. Especially when reaction heat is required in other sections of the process. Note that the minimization of

exergy losses is analogous to the economic balance between purging and recycling. Although many authors describe the method of exergy analysis, it is still not fully integrated in chemical process design methodologies (as in textbooks). The methanol case deals with the performance of four types of reactors and the overall performance of the synthesis loop. It shows that the designer should be careful in applying the guidelines provided in this part.

6.7 Concluding remarks

The generation of alternatives is described in three elements: 1) creativity stimulation, 2) function identification, and 3) concept integration. The explicit stimulation of creativity gives the opportunity to come up with innovative design alternatives. The identification and integration of functions urge the designer to define the design space in a conceptual way, so the design is not bound to existing solutions but there is also a large freedom for innovation. For the generation of alternatives phase, two tools are developed: the chemical route selection tool (CRS) and the guidelines for process synthesis tool (GPS).

- The chemical route selection tool (CRS) compares alternative processing routes based on exergy analysis. In this way, in a early stage of the design, routes can be compared and the route with the lowest exergy loss can be preferred. The use of the exergy theory in this stage of the design, during the generation of alternatives, is new. The case study shows that such an exergy calculation can be obtained in a reasonable time with reliable outcomes.
- The set of heuristic guidelines for process synthesis (GPS) gives the designer a tool for the use of exergy during the generation of alternatives stage. Although many authors describe the method of exergy analysis, it is not integrated in the synthesis of chemical process designs. The translation of exergetical insights in guidelines is a new way of integration of exergy and process design, which is developed during this thesis research. The case study shows that the use of guidelines improves the design in an exergetical way, but that the designer should be careful in applying the guidelines for separation design.

Chapter 7

SUSTAINABLE PROCESS DESIGN METHODOLOGY, PART III: *ANALYSIS OF ALTERNATIVES STAGE*

Summary *The analysis of alternatives consists in three elements: 1) concept simulation, 2) concept reliability analysis, and 3) concept feasibility analysis. These elements are explored in this Chapter. Sets of checklists and metrics are described that help the designer to focus on sustainability during the analysis of the design. Furthermore a design method is discussed relating to the analysis of design alternatives. The exergy analysis (EA) tool compares the exergy loss within a given set of design block schemes. The exergy loss is a measure for the primary energy required and the efficiency of mass use.*

7.1 Analysis of alternatives (see also Chapter 4)

The analysis of alternatives is the decision step where design solutions have to be compared and a choice has to be made about which one will be further developed. The alternatives are analyzed against the criteria set in the problem definition phase. Technological feasibility and profitability are of course important here, but in a sustainable design a concept should also be judged on its environmental and societal merits. The analysis of design alternatives is a scientific assessment of the reliability and the feasibility of the design options that are generated in the former decision step: *the generation of alternatives*. Many existing tools are available for the analysis of design alternatives in the chemical engineering field, like all kinds of flowsheet simulators. That is the reason that the analysis of alternatives gets less attention in this thesis; however, this is not a sign of less importance.

The tools for the analysis of the design are strongly related to the tools that are chosen in the synthesis phase, in the sense that the analysis tools and synthesis tools are two sides of the same phenomenon. That is the reason that in this Chapter not that much emphasis is on the development of tools for the analysis of alternatives. The emphasis of the discussion here is to stress the important points of the analysis phase on an abstract level, as in practice the designers have to determine at forehand which tools they will need during their analysis of the alternatives.

It is further emphasized here that a strong division should exist between the generation of alternatives and the analysis of alternatives. Designers must be aware of the problems that could arise when the synthesis and the analysis are done together. In practice this means that useful ideas are immediately dismissed, because of some instant or implicit decision-making. In this way, the designers do not value incomplete design ideas and do not give them a chance for further development. A strong division between the analysis and the generation of alternatives can prevent this, because for every idea, a clear argument should be given for acceptance or denial.

In Chapter 4, it was already discussed that the analysis of alternatives consists in three elements: 1) *concept simulation*, 2) *concept reliability*, and 3) *concept feasibility*. In Chapter 4 an introduction was given to these concepts. Here these steps are discussed in more detail, and after that some design tools are introduced and evaluated.

7.1.1 Concept simulation

In some way the designer should represent the design by common knowledge, which ensures the design is performing well. The representation of the design is called here the *concept simulation*. Of course the use of the term simulation can be confusing, but it is taken here in the most general meaning: every presentation by which the working of the concept is simulated and is proven to be valid. This concept simulation is the first step of the analysis of the alternatives, because it gives insight in the internal integration within the concept and it also stimulates the designer to deliver and rethink the integrative and innovative aspects of the concept.

In practice, concept simulation strongly depends on the level of detail of the final decision. In the first stages of the design, e.g. the need identification, a rough sketch of the design can be enough to do an analysis on the validity of the concept. In latter stages, e.g. the conceptual process design, a flowsheet simulation is needed along with the calculation of unit operations properties.

It is emphasized here that it is important that the designer or the design team chooses a kind of representation that gives the best opportunities for the design analysis. Mainly this depends on three issues: i) the common practice in the design organization (e.g. company, agency, or institute), ii) the scope and goal of the chosen design criteria, iii) the level of detail that is needed to prove the reliability and the feasibility of the concept.

7.1.2 *Concept reliability*

Many assumptions and decisions are made during the design of technical artifacts; this is true both for large-scale chemical processes and small-scale chemical products. Those decisions must be communicated to the principal of the design, the colleagues of the designer, etc. The way this has to be done is just like the *concept simulation*, i.e. dependent on the details that are required. In the first stages of the design, a simple mass balance can be enough; in the latter stages a complex mathematical model must prove the reliability of the decisions that are made.

Many tools exist in the chemical engineering discipline, like sensitivity analysis, decision trees, mass and heat balances, flowsheet simulation, waste minimization algorithms, etc. All kinds of tools are developed and still under development and they all are focused on the demonstration of the validity of the design against the given criteria. Here some tools are categorized: i) *economic analysis*, ii) *risk analysis*, iii) *thermodynamic analysis*, and iv) *environmental impact analysis*.

Economic analysis; mainly used to estimate capital investment costs and profitability. They can be found in nearly all teaching books.

Risk analysis; comprising the ‘What if’/Checklist method, the HAZard and OPerability (HAZOP) method, the Failure Mode and Effect Analysis (FMEA) method, the Fault-Tree Analysis (FTA) method, and finally safety index methods, e.g. DOW’s Fire and Explosion Index.

Thermodynamic analysis; comprising ‘Lost Work Analysis’, and ‘Exergy Analysis’, which is a more modern version of the former. Both aim to analyze the thermodynamic efficiency of the process and to point out possible improvements.

Environmental impact analysis, i.e. indicators and indices, many environmental impact indices have been developed, but these usually do not represent absolute measures and aim to support the selection among alternatives (Hertwich, Pease, and Koshland 1997).

7.1.3 *Concept feasibility*

The feasibility of the design is mainly strongly determined by practical considerations, like the available knowledge (may be limited by licensing), the innovation that is required, the time-to-market, etc. The *concept reliability* is a scientific approach to assess the validity of the design, and the *concept feasibility* is a definition of practical limitations, derived from the problem definition.

7.2 Exergy analysis of chemical processes

The analysis of process alternatives in general has to do with the following questions: i) which alternative performs best, ii) what are the areas of possible improvement, iii) to what extent can the design(s) be improved?

The third question is relevant when selecting among designs that are not fully optimised. In that case, insight is required in the impact of potential improvements. This section does not intend to provide a comprehensive methodology, because it is based on existing methods. It is presented here as illustration of analysis of process alternatives from the viewpoint of exergetical insights.

With the aid of exergy the heat integration of a process can be qualified and quantified. This is important related to the reduction of energy consumption of the process, which is directly linked to the CO₂-emission. In Chapter 6 (the CRS tool) and Appendix B exergy analysis is introduced; the calculation method for the analysis of processes is the same and here this is not elaborated in detail.

7.2.1 Introduction to exergy analysis

Although the method of exergy analysis is described extensively already for application in chemical and mechanical engineering design, e.g. by Szargut (Szargut, Morris, and Steward 1988), it is still not fully integrated in chemical process design methodologies. In the commonly used textbooks in this field (see Chapter 4), only Seider (Seider, Seader, and Lewin 1999) discusses the use of a second law analysis. Possible explanations of this phenomenon could be: i) the concept of exergy is abstract and the benefits of using it are not always clear, ii) literature on exergy analysis mainly focuses on existing processes, iii) little guidance is provided in dealing with the outcome of the analysis.

This Chapter therefore approaches the method of exergy analysis from a designer's perspective and provides a framework that can be applied when design alternatives are available after the generation of alternatives phase in the task integration stage. The objective of the method is to quantify the performance of designs with respect to their exergy consumption and irreversibility, i.e. the amount of exergy lost internally. The first aspect is important when selecting among alternatives, the latter forms a basis for improvements.

The framework is similar to that of the CRS tool, yet with different objectives and scope. It is briefly discussed below and important elements are discussed separately. The analysis method is illustrated in an example case on the production of synthesis gas; see the next section.

7.2.2 Exergy analysis of chemical process alternatives

The integration of exergy analysis in the innovation process requires a systematic approach to dealing with design alternatives and their inherent uncertainty. The corresponding framework consists of the following steps: 1) goal definition and scoping, 2) modelling of alternatives, 3) inventory analysis (simulation), 4) exergy analysis, 5) improvement assessment, 6) assessment of results, 7) documentation. In practice, the analysis is a comparison of some block schemes.

In this type of analysis it is important to define the nature of the study, i.e. is the analysis part of an *analyse and improve* strategy, or is it a comparison between

alternatives, or both. Obviously, these objectives require different approaches in the other steps of the analysis. For example, if alternatives with different feedstocks or energy requirements (e.g. steam and power) are compared, it may be necessary to increase the scope. This is illustrated in the EA case study.

In the second step the alternatives are modelled in a flowsheeting simulator such as *Aspen Plus* (licensed by Aspen Technology, Inc.). In order to guarantee an equal comparison the same unit operations must be used or they must be modelled in a similar way. Furthermore, the practitioner should anticipate on heat recovery and integration, as the design is probably not sufficiently elaborated in this phase. One of the benefits of performing an exergy analysis in an early stage is that it provides quantitative insight in the heat balance of the process. Therefore, an approach to heat recovery and integration is discussed separately.

In the third step, the inventory data are generated through simulation. It is important that consistent mass and energy balances are obtained. These inventory data form the basis of the exergy analysis in the subsequent step, which is discussed below. The areas of possible improvement are then identified and further investigated in the improvement assessment. Sensitivity analyses play a key-role in all three steps, which are also discussed below. They can be used to assess uncertainties in the analysis and to identify the major contributors to the performance, which is important when optimizing the design.

7.2.3 *Approach to heat recovery and integration*

Prior to modelling and simulating the design, the approach to heat recovery and integration must be defined. After all, one has to account for the exergy losses that are associated with heat transfer. This section therefore provides a generally applicable approach to dealing with this issue. The approach can also be used in the analysis of existing processes for which little data are available. The approach aims to: 1) *quantify the exergy output*, with this information the import or export of exergy can be determined, 2) *provide qualitative insight* in the heat integration: what is the amount of heat required and available at certain temperature levels.

The approach to quantifying the recovery of exergy is discussed first, because it determines how the exergy input should be dealt with. Furthermore, a procedure is recommended for modelling the heat transfer. The syngas case provides an example on how to interpret the results.

Recovery of exergy

It is inevitable that part of the exergy is lost during recovery. In order to take the associated losses into account, an exergetic efficiency τ_{ex} of heat transfer is used (Hinderink, Kerkhof, Lie, et al. 1996b; Hinderink, Kerkhof, Lie, et al. 1996a):

$$t_{ex} = \frac{Ex_{recovered}}{\Delta Ex_{cooled\ medium}} \quad \text{Equation 7.1}$$

This equation can be used to estimate the amount of recovered exergy that is directly available for heating purposes (this is equal to the exergy input). However,

the exergetic efficiency is typically not constant over the entire temperature range of heat transfer. Distinct temperature levels are therefore defined in which the exergetic efficiencies is assumed to be constant. For example the following three levels could be defined: high (>600 °C), medium (300-600 °C) and low (150-300 °C). For each of those temperature levels an average efficiency can then be determined.

When performing the analysis the practitioner should define the destination of the exergy output, i.e. production of steam or heating other process streams. Reaction heat, for example, is typically transferred to steam while the reactor effluent is used for heating the other process streams, e.g. the reactor feed. Heat available at high temperatures is typically transferred to High Pressure Steam (HPS), of which the exergetic efficiency can be calculated as follows:

$$t_{ex} = \frac{\text{Carnot factor}_{\text{steam}}}{\text{Carnot factor}_{\text{source}}} = \frac{Ex_{\text{steam}} / Q_{\text{transferred}}}{1 - T_0 / T_{\text{source}}} \quad \text{Equation 7.2}$$

in which the Carnot factor of the heat source is calculated with the absolute temperature in Kelvin. The Carnot factor of the steam is calculated by dividing its exergy value by the amount of energy that is required to produce the steam. Figure 7.1 shows the outcome of the equation given above for a temperature range of 150-1000 °C (heat source). The temperature difference between the heat source and the steam is between 40 and 50 °C for all three conditions of the steam. Figure 7.1 also shows the exergetic efficiency of heat transfer from a hot stream to a cold process stream, which is calculated as follows:

$$t_{ex} = \frac{\text{Carnot factor}_{\text{sink}}}{\text{Carnot factor}_{\text{source}}} = \frac{1 - T_0 / T_{\text{sink}}}{1 - T_0 / T_{\text{source}}} \quad \text{Equation 7.3}$$

The temperature difference between the source and the sink is assumed to be 50 °C. Of course the practitioner is free to define other temperature levels with other temperature differences. The exergy output can then be estimated by using the *average* value of the exergetic efficiencies, which can be calculated or determined from Figure 7.1. For example, the exergetic efficiency of producing HPS (50 bars) by cooling a hot stream from 1000 to 600 °C is 0.57, since the efficiencies at 600 °C and 1000 °C are 0.53 and 0.61, respectively.

Exergy input

The exergy input of a process is rather easy to determine, as the exergy loss of heat transfer is already accounted for in the exergetic efficiency. Insight in the heat integration can be obtained by defining temperature levels at which cold streams are heated. Obviously, these levels should correspond to the output levels that are defined earlier, i.e. with a certain temperature difference.

It is recommended that the practitioner pays attention to the boiling temperature of components. For example, if process steam at 50 bars is produced, a considerable

amount of heat is required at 263 °C. When this heat comes available again through condensation it cannot be used to produce HPS again. It may therefore be convenient to adjust the temperature levels in order to account for this inherent mismatch. For example, the heat of condensation is recovered in the low temperature level while the same heat is required in the medium temperature range when producing the steam. This approach provides a more realistic insight in the amount of heat recovered and required.

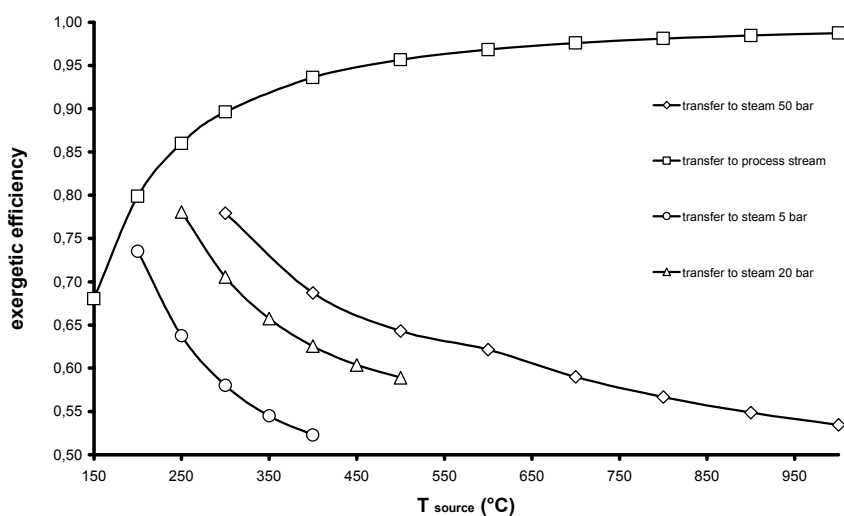


FIGURE 7.1 EXERGETIC EFFICIENCIES OF HEAT TRANSFER

The approach must be dealt with in the modelling step, as the simulation model of the flowsheet requires additional unit models. The recommended procedure of modelling is as follows: 1) define temperature levels at which heat is recovered, 2) define the nature of heat transfer, e.g. to steam or to other process streams, 3) define temperature levels at which heat is required, i.e. the temperature difference, 4) include relevant heaters in the simulation model.

7.2.4 Exergy analysis

In this step the exergy input per unit of product and the corresponding irreversibility are quantified. In accordance with the ELCA methodology, the criteria are expressed in GJ_{exergy}/ton of product. The approach to the analysis is discussed with help of Figure 7.2.

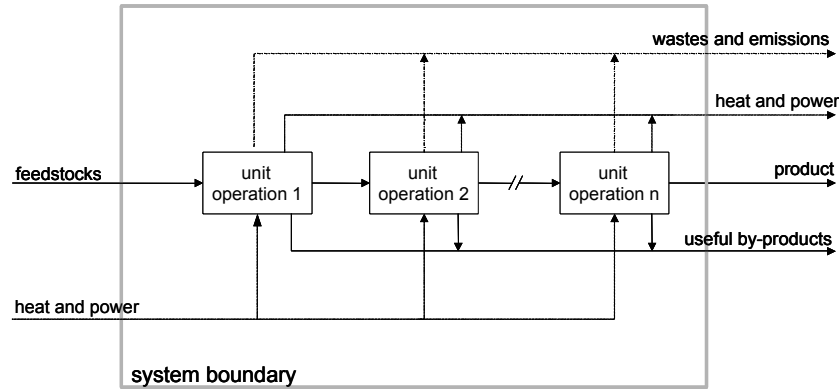


FIGURE 7.2 SCHEMATIC REPRESENTATION OF A PROCESS

The exergy input per ton of product is determined in a similar way as discussed in the CRS methodology: through allocation of the exergy of the feedstocks and import exergy (heat and power) to the desired product. The irreversibility of the processes is defined as the amount of internally lost work per ton of product. The exergy losses are therefore divided into *external* and *internal* losses. The former losses are associated with useless heat and material streams leaving the system boundary, e.g. heat discarded to cooling water and stack gases. The internal losses are associated with irreversible processes such as heat transfer and combustion. The exergy losses can be determined as follows:

$$Ex_{loss, overall} = Ex_{input, total} - Ex_{output, useful} = Ex_{loss, internal} + Ex_{loss, external} \quad \text{Equation 7.4}$$

With:

$$Ex_{loss, external} = \sum Ex_{wastes\ and\ emissions} + \sum Ex_{useless\ heat} \quad \text{Equation 7.5}$$

$$Ex_{loss, internal} = \sum Ex_{loss, process\ segments} \quad \text{Equation 7.6}$$

In order to identify the origins of internal losses the process must be divided into segments, which can consist of one or more unit operations. Since these losses represent process irreversibilities, the analysis provides quantitative hints on where to look for possible improvements.

In conclusion, the following procedure is recommended for performing the exergy analysis: 1) calculate the exergy values of all streams (including heat transfer), 2) define useful and useless streams leaving the system boundary, 3) determine the total exergy input, external losses and the overall exergy loss, 4) divide the process into relevant segments, 5) determine the internal losses per segment, 6) allocate the exergy input and overall losses to the desired product.

7.2.5 *Sensitivity analysis*

Sensitivity analyses can be used in order to assess the uncertainties in the analysis and the impact of improvements. The sensitivity of assumptions can be investigated with the procedure described in the CRS methodology. The assessment of the improvement potential, however, requires a more fundamental approach: 1) identify the process segments with major exergy losses, 2) determine the nature of the exergy losses, 3) identify the most important design variables through sensitivity analyses, 4) investigate the effect of these variables on the performance, 5) estimate the improvement potential.

The results of the exergy analysis form the starting point of the iterative process of improvement. The practitioner should focus on the process segments with major exergy losses, as these have the highest priority and highest possible impact of improvements. The first step is to determine the nature of the losses: i) what are the driving forces that cause the losses (e.g. differences in temperature, pressure or chemical potential), ii) are large driving forces required or can they be reduced, iii) which design variables influence the driving forces?

It is important to understand what causes the exergy losses, since this knowledge directly provides insight into which design variables are relevant. However, some driving forces can be unavoidable or even required in order to guarantee small unit operations. In that case, the solution must be found elsewhere. If the driving forces can be reduced, the most important design variables must be identified through sensitivity analyses.

When relevant design variables are identified, their influence on the performance should be investigated. This can be described as a second round of sensitivity analyses, of which the objective is to quantify the potential improvements. These results help the practitioner to make a fair comparison between alternatives. Furthermore, if it turns out that only minor improvements are possible, the answers to the questions above could lead to more fundamental improvements when repeating the process synthesis step.

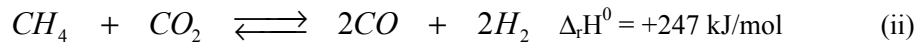
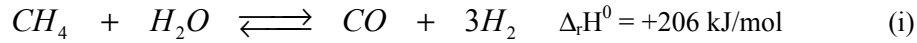
7.3 *EA case study: production of synthesis gas*

Five alternative production processes of synthesis gas (syngas) are investigated in this case. Exergy analyses are performed and the results are used as a basis for an ELCA in which the alternatives are compared. Three alternatives are then used to illustrate that the results of the exergy analysis can provide more insight in the performance of alternative designs and possible improvements.

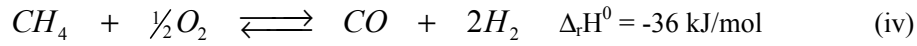
The production of synthesis gas (syngas) has been selected as topic for the case study, since the corresponding processes are large energy consumers. Moreover, syngas is a key feedstock for the production of a large variety of base chemicals, such as hydrogen, ammonia, methanol, etc. In this work it is assumed that the syngas is used for methanol production. This methanol process is divided into two individual cases: the production of syngas and the production of methanol (see Chapter 6). The results in this case are normalized to the maximum amount of methanol that can be produced from the syngas, which guarantees a consistent approach in comparing the different production processes.

7.3.1 Introduction

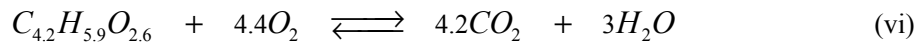
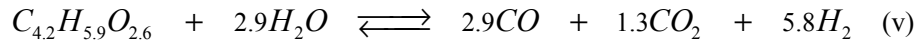
Synthesis gas can be produced from hydrocarbons such as natural gas and naphtha by either steam reforming or partial oxidation (autothermal reforming). The principle reactions during steam reforming of methane are (Hinderink, Kerkhof, Lie, et al. 1996a; Hinderink, Kerkhof, Lie, et al. 1996b):



The overall reaction of partial oxidation is:



This overall reaction is a combination of the combustion of methane and reactions i, ii, and iii. Syngas can also be produced from biomass through steam gasification. Biomass (poplar) is gasified according to the following principle reactions:



Reaction v is endothermic (estimated to be 5.6 GJ/ton biomass) with an assumed H_2/CO ratio of 2 (Klass 1998). The second reaction is the combustion of biomass with a lower heating value of 18 GJ/ton (Roeterink and Stikkelman 2000). In both partial oxidation and biomass gasification the heat for the endothermic reaction is provided by combustion of a part of the feedstock. Therefore, the energy efficiency can be improved by lowering reaction temperatures, i.e. by using catalysts. Catalytic Partial Oxidation (CPO) is an example of this principle. The synthesis gas composition for methanol synthesis is best described by the so-called stoichiometric number (SN):

$$SN = \frac{n_{H_2} - n_{CO_2}}{n_{CO} + n_{CO_2}} \quad \text{Equation 7.7}$$

Steam reforming of methane produces syngas with a SN of approximately 3, partial oxidation results in a SN below 2, and steam gasification of biomass yields a synthesis gas with a SN of approximately 0.4.

7.3.2 Alternative production processes

Five alternative production processes are investigated, of which steam reforming of natural gas is considered to be the reference process:

- Steam reforming of natural gas (SR)
- Catalytic Partial Oxidation of natural gas (CPO)
- Biomass gasification (BM)
- Steam reforming of natural gas with additional carbon dioxide (SR+CO₂)
- A combination of steam reforming of natural gas biomass gasification (SR+BM)

Alternative 4 is used in industrial production of methanol to increase the yield per unit of natural gas. Syngas is then produced with a SN of two, which avoids the inefficient combustion of the excess hydrogen. The same applies to alternative 5, in which CO₂-rich syngas is added to the syngas from steam reforming. This option was suggested and investigated by Interduct (Roeterink and Stikkelman 2000). Although different routes are applied, syngas can be produced using the basic process scheme shown in Figure 7.3.

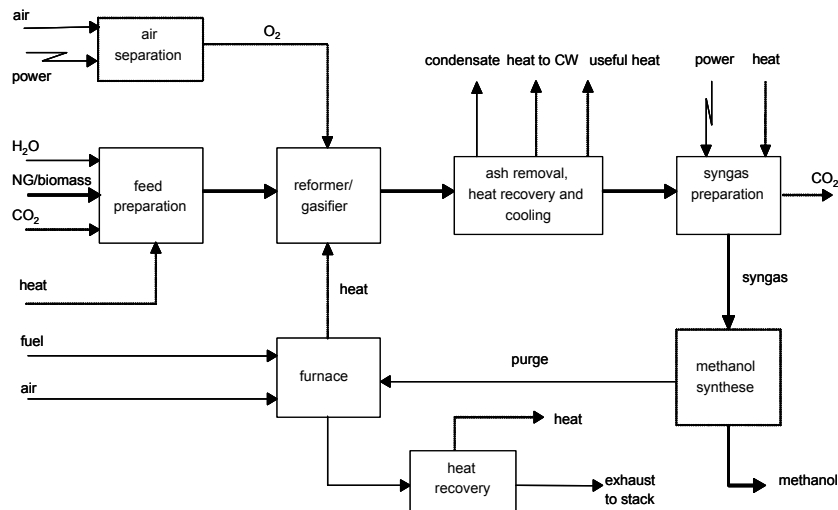


FIGURE 7.3 BASIC PROCESS SCHEME OF SYNGAS PRODUCTION

The general process can be described by the following steps:

- *Preparation of the feeds*; i.e. mixing, heating and pressurizing of the reactants. In the case of route 4, CO₂ is recovered from flue gases through absorption techniques
- *Separation of air* when partial oxidation is applied (CPO and BM)
- *Generation of crude syngas* in a reactor corresponding to the five routes: 1) reformer with external furnace, 2) autothermal fluidised bed reactor, 3) autothermal reformer, 4) reformer with external furnace, 5) Both 1 and 3 after which the streams are mixed
- *Cooling of the crude syngas* in order to separate condensate while recovering heat; ash is removed first in the case of biomass gasification
- In the case of biomass gasification, *excess CO₂ must be removed* in order to obtain a SN of 2

- *Methanol synthesis*, which is not considered here. However, all processes purge inerts, such as N_2 and CH_4 , and excess reactants. This purge is combusted in the reformer furnace together with the fresh fuel or, in the case of CPO and biomass gasification, is combusted in an external furnace in order to recover the corresponding heat.

In this case study, it is assumed that the maximum amount of methanol is produced, which is not the case in reality. The methanol synthesis loop is discussed in detail in Chapter 5.

7.3.3 System boundaries

Figure 7.4 shows the systems boundaries that are defined in this case. System boundary I is used in the analysis of the alternative production processes, system boundary II could be used in a CRS.

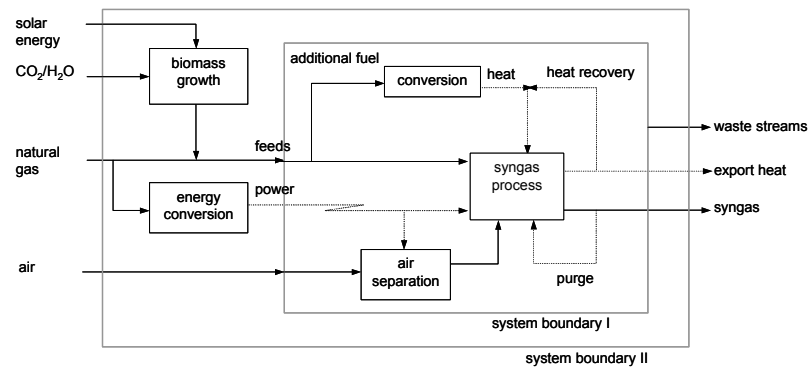


FIGURE 7.4 SYSTEM BOUNDARIES DEFINITION FOR THE SYNGAS CASE

Figure 7.4 shows that only power and feeds enter System Boundary I, which implies that the production process must be self-sufficient in heat requirements. The gasification of biomass, for example, requires the combustion of additional biomass in order to generate sufficient steam for the removal of CO_2 . The export exergy is the difference in requirements and recovery. The purge is also accounted for within System Boundary I.

System boundary II can be used in a CRS. It is assumed that power is generated from natural gas with an efficiency of 40% on low heating value basis. The efficiency of natural gas production and the CO_2 emission factor are taken as 92% and 0.055, respectively (see CRS case study, Chapter 6).

TABLE 7.1 RESULTS OF SIMULATION (PER TON METHANOL)

Section	SR	CPO	BM	SR+CO ₂	SR+BM
<i>Input</i>					
Total natural gas (ton)	0.78	0.58	-	0.73	0.59
Total biomass (ton)	-	-	1.98	-	0.23
Water (ton)	1.98	0.71	2.03	1.49	1.59
CO ₂ (ton)	-	-	-	0.33	-
<i>Output</i>					
Syngas (ton)	1.32	1.25	1.07	1.26	1.29
SN	3.0	1.8	2.0	2.0	2.0
CO ₂ (ton)	0.68	0.13	2.67	0.89	0.71
Condensate (ton)	1.21	0.65	1.68	0.99	1.05
<i>Reformer</i>					
Temp. in/out (°C)	500/900	600/1000	600/850	500/900	-
Pressure (bara)	20	35	20	20	-
Absorbed duty (GJ)	9.4	-	-	7.4	-
Steam ratio (molH ₂ O/molC)	3.5	1.2	1.25	3.5	-
Oxygen (molO ₂ /molC)	-	0.56	0.31	-	-
<i>Furnace</i>					
Fuel feed (GJ _{LHV})	10.6	-	6.3	15.0	11.6
Purge feed (GJ _{LHV})	9.0	1.2	1.0	1.3	1.3
Temp out (°C)	1000	-	1365 ¹	1000	1000
<i>Air Separation</i>					
Compressor duty (GJ)	-	0.86	0.91	-	0.20
Pressure in/out (bara)	-	1/35	1/20	-	1/20
Temp. out (°C)	-	105	86	-	86

¹) Temperature of adiabatic combustion of biomass

7.3.4 Simulation results

Table 7.1 shows the simulation results with respect to System Boundary I and have been validated against literature data in Table 7.2, in which several key data were used. In Appendix E background data on the case study are shown, like the assumptions made during the simulation, the way the biomass gasifier was modeled, and the mass and enthalpy balances of the alternatives.

Worth mentioning is the small difference in natural gas (NG) consumption between conventional steam reforming and steam reforming with CO₂ addition: In order to compensate for the H₂-poorer purge, considerably more NG must be combusted in the furnace. Even though the absorbed duty is less, the decrease in total NG consumption is rather modest.

TABLE 7.2 VALIDATION AGAINST LITERATURE DATA

Process	Simulation result	Literature value	Error (%)
<i>Conventional Steam Reforming</i> ¹			
NG consumption (LHV) (GJ/tonMeOH)	37.2	33.2	11
<i>Biomass</i> ²			
H ₂ required for SN=2 (ton/tonBiomass)	0.13	0.14	5
Methanol production (ton/tonBiomass)	1.3 ³	1.2	8

¹) Cheng (Cheng and Kung 1994)

²) Roeterink (Roeterink and Stikkelman 2000)

³) Without additional biomass for heat requirements.

Table 7.2 shows that the simulation of conventional steam reforming has a maximum error of approximately 10%. Sensitivity analyses at the end of this case study, however, show that this error can be reduced to 3% by preheating the air in the furnace. The errors in the biomass process are in the same order of magnitude. Furthermore, it must also be noted that the errors are based on single literature values, but these are considered typical.

7.3.5 Exergy analysis of the production process only

The temperature levels were defined as High (>600 °C), Medium (220-600 °C), and Low (150-220 °C) with τ_{ex} -values of 0.57, 0.94, and 0.56, respectively. It was assumed that exergy at high temperatures is transferred to HPS, at medium and low temperatures to process streams. In the case of CPO, the medium temperature level was defined as 250-660 °C. External losses are associated with useless heat and material streams leaving the system boundary: i) stack gases at 150 °C, ii) process condensate at 50 °C, iii) exergy lost through external cooling.

Table 7.3 shows the exergy input and output of the processes in GJ/ton methanol. It is recommended that the absolute values are used, because exergetic efficiencies can be defined in numerous ways and are therefore inherently ambiguous. The export of exergy is the difference between the exergy input and output, cumulative over all temperature levels. Table 7.3 also shows that there are large differences between the alternative processes. The exergy losses can be substantially lower (CPO) and higher (biomass gasification) than conventional steam reforming. Steam reforming can be improved through addition of carbon dioxide and through combination with biomass gasification.

TABLE 7.3 RESULTS OF EXERGY ANALYSIS

(GJ/ton methanol)	SR	CPO	BM	SR+CO ₂	SR+BM
Input					
Total natural gas	39.0	29.0	-	36.7	29.3
Total biomass	-	-	38.5	-	5.6
Power	-	0.9	0.9	-	0.2
Total	39.0	29.9	39.6	37.0	35.0
Output					
Syngas ²	23.9	23.9	23.8	23.7	23.6
Export exergy	3.5	0.9	1.1	2.8	2.2
Total	27.4	24.8	24.9	26.5	25.8
Lost work					
Internal	10.3	4.4	12.1	9.4	7.9
External	1.3	0.7	2.5	1.1	1.3
Total	11.6	5.1	14.6	10.5	9.2

¹) The water, air and CO₂ streams are included in the totals.

²) Real value of syngas minus value of purge.

More insight in the nature of the exergy losses is obtained when looking at the process segments of the alternatives:

- *Feed preparation*; depressurization of natural gas, pressurization of water, mixing of reactor feeds, feed preheating and steam generation (losses are allocated to heat transfer).
- *Reaction section*; steam reformer tubes, reformer furnace, biomass gasifier, external furnaces for combustion of biomass and purge (CPO and BM).
- *Heat recovery*; cooling of hot combustion gases and hot product gases.
- *Air separation*; compression of air, separation of air in a useless nitrogen-rich stream and a desired oxygen-rich product.
- *CO₂ removal*; stripping of crude syngas from biomass gasifier (BM), stripping of flue gases (SR+CO₂).

Table 7.4 shows that in each process the major losses originate in the reaction section and in heat recovery. The external losses are mainly caused by cooling of the hot product gases in order to remove condensate and by emitting the hot flue gases. Furthermore, the table shows that exergy losses are reduced if external heat transfer in furnaces is avoided (CPO). This benefit, however, is completely lost in the gasification of biomass, as additional biomass must be combusted in an external furnace to generate steam for the removal of CO₂.

As a result, heat is generated at high temperatures while it is only required for low temperature applications. The process now exports exergy while biomass is combusted in order to close the heat balance. The heat recovery method can reveal these kinds of heat integration issues. Note that the overall exergy export is rather optimistic, because additional losses are unavoidable when exergy is transferred across temperature levels. This would be the case if the process is self-supporting.

It would therefore be better to import low temperature heat than to combust additional biomass.

TABLE 7.4 SUBDIVISION OF THE EXERGY LOSSES

(GJ/ton methanol)	SR	CPO	BM	SR+CO ₂
Feed preparation	0.27	0.17	0.00	0.30
Reaction section	7.41	2.81	7.10	6.57
Reformer tubes	0.64	-	-	0.48
Gasifier	-	2.38	4.20	-
Reformer furnace	6.77	-	-	6.09
External furnace	-	0.43	2.90	-
Heat recovery	2.58	1.14	2.70	2.17
Air separation	-	0.24	0.30	-
CO ₂ removal	-	-	2.00	0.40
External losses	1.28	0.72	2.52	1.08
Total	11.6	5.1	14.6	10.5

The data for the SR+BM alternative were not determined, because the data of the individual process provide sufficient insight. However, it must be noted that the combination of the two has a synergetic effect, as the removal of CO₂ is no longer necessary, and the combustion of valuable hydrogen is avoided.

7.3.6 Exergy analysis including ecological system

Table 7.5 shows the results of the exergy analysis for System Boundary II. It was assumed that the input of non-renewables (fertilizers, pesticides, etc.) in the production of biomass was 0.95 GJ/ton (as in the MPG case, see Chapter 6). The corresponding CO₂ emission factor was taken as 0.067 ton/GJ. The exergy input and CO₂ emission were allocated to syngas, because steam is considered an undesired by-product.

TABLE 7.5 RESULTS OF THE EXERGY ANALYSIS OF SB II

(per ton of methanol)	SR	CPO	BM	SR+CO ₂	SR+BM
Total exergy input (GJ)	42.4	34.0	43.0	40.3	38.2
NR exergy input (GJ)	42.4	34.0	4.5	40.3	32.7
Net CO ₂ emission (ton)	0.87	0.41	-0.71	0.75	0.37

It is clear that all other alternatives perform better than conventional steam reforming with respect to the input of non-renewable exergy. Furthermore, the results show that the emission of CO₂ directly corresponds with the use of non-renewable resources. Hence, one should be careful when using both criteria,

because they are directly related. Note that CPO is a very efficient process and that its performance is almost as good as the partly renewable SR+BM process. This is a good example of the improvement of conventional processes. Although non-renewable resources are still used, the performance is substantially improved. It can be therefore argued that reaching for green resources does not always have to be the only right answer.

7.3.7 Sensitivity analyses

The purpose of the sensitivity analysis is to show that results of the exergy analysis provide insight in which areas have the largest improvement potential. Obviously, the largest improvements can be made when choosing better technologies and equipment. This type of decisions, however, is considered to be part of process synthesis and is therefore not dealt with in this section. This section deals with improvements that can be obtained when varying design variables, such as pressures, temperatures, recycles, etc. This analysis supports the selection of alternatives and simultaneously forms the basis of further optimization.

The subdivision of the exergy losses revealed that the reaction section and the heat recovery are responsible for the major losses in the production of syngas. The latter origin of losses is a consequence of decisions in other process segments and can therefore not be influenced directly. The losses in the reaction section mainly originate in the uncontrolled combustion of natural gas or biomass. This combustion cannot be avoided, but the furnace duty can be influenced by the following design variables: i) the *temperature in the reformer tubes*, ii) the *temperature of the combustion air*, and iii) the *pressure in the reformer tubes*.

- *The temperature in the reformer tubes*; when the temperature is lowered the duty of the furnace is reduced. But as a result, the conversion of natural gas decreases, which leads to reduced methanol production and a methane-rich purge.
- *The temperature of the combustion air*; when the air is preheated the temperature rises in the furnace, which leads to reduced fuel consumption. This can only be achieved when sufficient heat is available.
- *The pressure in the reformer tubes*; when the pressure is reduced, the conversion of natural gas increases and hence the fuel requirements decrease. This option, however, is not investigated in this study.

There are other variables such as the steam ratio and temperature of the reformer feed, but these are considered of minor importance. Table 7.6 to Table 7.8 show the results of sensitivity analyses of the SR, CPO, and BM alternatives. The other alternatives show similar results, since these are the same types of processes with small differences.

Table 7.6 shows that the consumption of natural gas can be reduced by at least 10% through varying T_{ref} and T_{air} . Reducing the reformer temperature has a small influence on the performance and is probably less economic, as the fuel is led through the entire process before entering the furnace as purge. This results in an increased consumption of feedstock and a reduced consumption of fuel, as can be seen in Table 8.6. The temperature of the combustion air, however, has a large

effect on the fuel requirements: a reduction of 8% is already achieved when the air is preheated to 220 °C. Note that the same trend applies to the exergy losses.

TABLE 7.6 SENSITIVITY ANALYSIS OF SR

(GJ _{ex} /ton methanol)	T _{ref} 800°C	T _{ref} 850°C	T _{ref} 900°C (basecase)	T _{ref} 950°C	T _{air} 220°C
Natural gas input	38.0	38.4	39.0	39.7	35.9
Feedstock	34.1	30.0	27.8	26.8	27.8
Fuel	3.9	8.4	12.2	12.9	8.1
Exergy losses	11.21	11.30	11.55	11.93	9.41
Feed preparation	0.33	0.29	0.27	0.26	0.27
Reformer tubes	0.54	0.58	0.64	0.72	0.64
Reformer furnace	6.52	6.63	6.77	6.95	4.99
Heat recovery	2.48	2.50	2.58	2.71	2.33
External losses	1.33	1.29	1.28	1.28	1.18

TABLE 7.7 SENSITIVITY ANALYSIS OF CPO

(GJ _{ex} /ton methanol)	T _{gas} 800°C	T _{gas} 900°C	T _{gas} 1000° (basecase)	T _{gas} 1100°	T _{ox} 300°C
Exergy input	51.0	34.5	29.9	29.5	29.7
Natural gas	50.2	33.7	29.0	28.6	28.9
Power	0.8	0.8	0.9	0.9	0.8
Exergy losses	18.04	7.94	5.05	4.85	5.00
Feed preparation	0.29	0.19	0.17	0.16	0.17
Gasifier	2.38	2.33	2.38	2.51	2.30
External furnace	7.58	2.10	0.43	0.10	0.44
Heat recovery	6.11	2.22	1.14	1.10	1.14
Air separation	0.22	0.23	0.24	0.26	0.24
External losses	1.46	0.88	0.69	0.72	0.71

In the case of CPO, varying the amount of oxygen has a larger effect than varying its temperature. The more oxygen is fed to the gasifier, the higher the temperature becomes. As a result, the conversion of natural gas is increased. The results of the sensitivity analysis show that 1000 °C is near optimal. If the temperature is further increased the natural gas consumption is little reduced. If the temperature is reduced, the consumption rises exponentially. Moreover, the maximum temperature is around 1000 °C as the catalyst deactivates at higher temperatures.

TABLE 7.8 SENSITIVITY ANALYSIS OF BM

(GJ _{ex} /ton methanol)		T _{gas} =850°C (basecase)	T _{gas} =1000°C
Exergy input		39.44	39.79
Biomass feedstock	31.66		33.81
Biomass fuel	6.87		4.90
Power	0.91		1.08
Exergy losses		14.56	15.13
Feed preparation	0.00		0.00
Gasifier	4.21		4.79
External furnace	2.94		2.27
Heat recovery	2.72		3.24
Air separation	0.27		0.29
CO ₂ removal	1.96		2.04
External losses	2.52		2.57

It was expected that the consumption of biomass would be reduced if the temperature was increased, because the gasification of biomass was believed to be more efficient than combustion. The results show that this is not the case. However, it must be noted that this is probably caused by the assumptions in the model of the gasifier. The influence of the temperature of the oxygen is expected to be as small as in the CPO process.

7.3.8 Concluding remarks on the EA case

Five alternative production processes of synthesis gas were investigated in this case. Exergy analyses were performed from both a process perspective (System Boundary I) and from a CRS perspective (System Boundary II). Furthermore, sensitivity analyses were conducted in order to assess the improvement potential of the three basic processes (SR, CPO and BM). The following conclusions can be drawn for each of the three types of analyses.

Exergy analysis of system Boundary I – production process only

CPO requires the smallest input of exergy per ton of methanol whereas the biomass gasification process requires the most: In the CPO process, large temperature differences are avoided between the hot flue gases and reformer tubes. In the BM process, the relatively high exergy losses are caused by the inefficient combustion of additional biomass, which is needed to close the heat balance. In all processes, the major exergy losses originate in the reaction section and in the recovery of heat.

Exergy analysis of system Boundary II – including ecological system

Although the process is relatively inefficient, biomass requires the smallest amount of non-renewable exergy per ton of methanol and fixates 0.71 ton CO₂ per ton of methanol. The combination of SR and biomass gasification is a substantial improvement compared to conventional steam reforming. CPO performs almost as

well as the SR+BM alternative, although it is entirely based on natural gas consumption. The addition of carbon dioxide in conventional steam reforming is only a minor improvement.

Sensitivity analyses

The consumption of natural gas in steam reforming can be reduced by at least 10% through preheating the combustion air (which corresponds better with literature data). Given the models, the sensitivity analyses show that the biomass gasification and CPO alternatives cannot be improved significantly. The ranking of the alternatives was not influenced by the sensitivity analyses in either exergy analyses (SB I and II).

7.4 Concluding remarks

The analysis of alternatives is described with the following three elements: 1) concept simulation, 2) concept reliability analysis, 3) concept feasibility analysis. It is important that a distinction is made between the generation of alternatives and the analysis of alternatives. The first is a creative part and the origin of innovation, the second is the validation of the ideas against the problem definition. In the analysis part the design solution is described in such a way that the feasibility and the reliability of the design become clear. Checklists are helpful means to ensure that the design team considers every relevant item.

In this Chapter a tool is described for the analysis of design alternatives focused on sustainability: the exergy analysis tool (EA).

- The Exergy Analysis tool (EA) gives the possibility to compare different block schemes for the basis of design level on the degree of exergy loss. The exergy analysis tool in itself is not new. In this research however it is used specifically for the comparison of two system boundaries on which conclusions to support the incorporation of exergy insights early in the design phase.
- In the case study for the EA tool, five alternative production processes of synthesis gas were investigated. Exergy analyses were performed from both a process perspective (System Boundary I) and from a CRS perspective (System Boundary II). A distinction can be made between basic processes (CPO, BM, and SR). In all processes, the major exergy losses originate in the reaction section and in the separation section.
- The outcome of the exergy analysis tool depends strongly on the system boundary that is defined for the analysis. In the case of a system boundary including the ecological system, it becomes clear that the use of biomass for a feedstock is the best option from the perspective of minimized exergy loss. Focusing only on the process level, the biomass processes turn out to be relatively inefficient.

Chapter 8

SUSTAINABLE PROCESS DESIGN METHODOLOGY, PART IV: *DESIGN EVALUATION STAGE*

Summary *The design evaluation of the proposed solution consists in three elements: 1) goal and scope satisfaction, 2) criteria satisfaction, 3) concept communicability. After the exploration of those issues, various tools are presented that can stimulate the carrying out of the evaluation phase. Primarily the stakeholders, aided by the designer, do the evaluation. The sustainability ranking tool (SRT) is a method that enables the evaluation of a set of rough ideas based on sustainability criteria. This method is developed in this Chapter and illustrated with an industrial case study.*

8.1 Design evaluation (see also Chapter 4)

In the evaluation phase, a trade-off is made between the criteria and considerations that are made during the decision-making procedure. The evaluation is more value-laden than the analysis phase. In the *analysis of alternatives*, feasibility and reliability of the alternatives are considered based on the insights of the engineering field. In the *design evaluation* phase a final choice is made, in which all criteria are weighed. Important here is that primarily the stakeholders, aided by the designer, do the evaluation.

In Chapter 4, three elements are presented that are relevant during the evaluation of the designs: 1) *goal and scope satisfaction*, 2) *criteria satisfaction*, 3) *concept communicability*. After that a decision can be made and the design can go to a next more detailed level of design, or if the goal of the design and its criteria are not met, the decision-diagram is iterated, until the desired result is reached.

8.1.1 Goal and scope satisfaction

In the synthesis of alternatives and the analysis of alternatives, design solutions are created and synthesized to integral design proposals, and their feasibility is analyzed. In the evaluation step, these solutions are checked against the goal and scope, which are defined in the first step of the decision diagram. It is a free choice for the designer or the design team to do this in some consistent way. Mainly, some iteration is possible between this step and the problem definition step to get a coherent set of evaluation criteria that shows clearly the extent to which the expected design result is reached. As discussed in Chapter 5, three main items are important in the goal definition: 1) the main drivers, 2) the level of innovation, 3) the market or target group. The scope definition and the boundaries of the final design solution, should match with each other.

The context of the design is of great importance to the final decision; this context cannot be influenced directly by the engineer within the scope of the design trajectory. However, incorporation of external factors belonging to the societal and economical context of the design makes the outcome more robust to changes; this incorporation can be by the application of a scenario set. All externalities influencing the process are incorporated into the scenario (market developments, environmental legislations, social transitions, etc.). The scenario set can be made in co-operation with a diverse panel of stakeholders. The main idea of a scenario set is that external effects can be determined and their influence on the design/project can be evaluated.

A scenario is an imagined or projected sequence of events, especially any of several detailed plans or possibilities (The Random House Dictionary of the English Language, 2nd edition, 1987). In this thesis, scenario sets are defined as tools for ordering one's perceptions about alternative future contexts in which today's decisions might be played out (as defined by the Global Business Network).

Scenarios do not aim to *forecast* the future. Their main purpose is rather to ensure that through the imaginative thinking stimulated by the scenario process the future design takes all the interests of the various stakeholders into account. At least two scenarios need to be constructed, which are both mutually consistent and exclusive.

The robustness of the design can then be tested in both scenarios, which gives insight into the performance of the design as viewed against different future developments. Scenarios contain trend discontinuities; so called high-impact/low probability events. Each scenario should be defined as internally consistent. It is important that a set of scenarios is developed which are very different from each other.

Although no scenarios are value free, it is often useful to distinguish between *normative* and *descriptive* scenarios. Normative scenarios are explicitly value-based, exploring the routes to desired or undesired endpoints. Descriptive scenarios are evolutionary and open-ended, exploring paths into the reality-based future options. Descriptive scenarios are built as descriptions of possible, rather than preferred, developments.

The purpose of the set of scenarios is to assess the particular technology in each scenario. If the technology has a positive outcome in all scenarios, then that technology is more robust for the future than a technology that has a positive outcome in none or in only one scenario. If the technology fails in some scenarios in some aspects it could be modified and assessed again with the scenario set.

In general, a scenario set is built by interviewing or brainstorming with various experts and various stakeholders. The following steps have to be taken to build a consistent set of scenarios: 1) *describe the problem*, 2) *identify variables and factors*, 3) *classify variables and factors*, 4) *build scenarios*, 5) *analyze scenarios*, 6) *apply scenarios*.

Describe the problem; describe the potential problems of the technology (and its use), describe the context of the technology and what decisions to take on your technology using the scenario set. Also define a time horizon; i.e. when the technology will be applied and for how long.

Identify variables and factors; Identify variables and qualitative factors for building the scenarios by describing the present situation and analyzing key variables and trends which determine success or failure of the technology. Include not only current trends, but also discontinuities; so-called “high impact/low probability events”. Include variables for ecology (e.g. emissions), society (e.g. equity, population development, use) economy (e.g. scarce resources, economic growth, external costs).

Classify variables and factors; classify the variables and factors into: i) constant variables in time, ii) predictable variables in time, iii) uncertainties (especially high impact low probability events)

Build scenarios; build at least two different story scenarios. Transform if necessary the variables into quantitative indicators. Decide which qualitative factors to include. Each scenario should be internally consistent as much as possible.

Analyze scenarios; analyze the scenarios on relevance, scope, insight, clarity, plausibility, validity, and reliability. Remove less useful scenarios. Give remaining scenarios a fitting name.

Apply scenarios; apply each scenario to the technology and draw conclusions on its fit. Draw overall conclusions on the robustness of the technology and provide hints for improvements.

8.1.2 Criteria satisfaction

In both Chapter 2 and 5, sustainability criteria are discussed extensively. The designers or the design team apply these criteria to the design and afterwards, the final decision is evaluated against the criteria from the *problem definition* step. The purpose of the criteria satisfaction is to investigate whether a design fulfils the design objectives. The design team should be able to assess the degree to which a design alternative meets the goal and the scope of the design in order to define when a final decision can be taken and the design can pass to the next design phase. Put in other words, what is the *quality* of the design in relation to its problem definition? After the evaluation of the design, the designer can select the best alternative, which as a result of this procedure is the one with the highest quality. In Chapter 5, the importance of a stakeholders investigation is discussed. It is stated there that a collectively reached sustainable solution has more legitimacy and is more efficient (Jansen 2003; Robèrt, Schmidt-Bleek, Aloisi de Larderel, et al. 2002). This leads to the statement that two kinds of practices are possible (see Figure 8.1). In the *common practice*, a negative assessment by the society can be large after the production is started, which can have a large effect. It is better to involve the society during or after the design stage, in such a way that a negative assessment by the society can be avoided (Harmsen 1999).

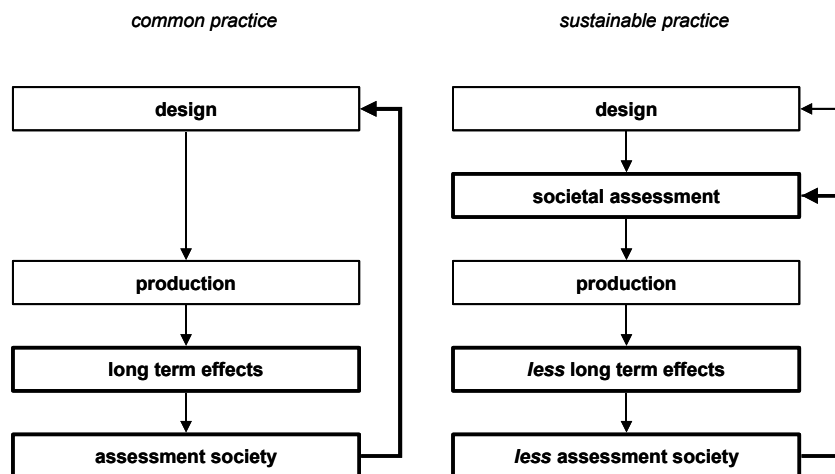


FIGURE 8.1 SUSTAINABLE DESIGN EVALUATION

The second approach is called the *sustainable practice*: a more democratic approach of design, in which the process or product is presented to as part of the design phase. This is done before the production starts, so that the design can be modified to meet society's criteria.

8.1.3 Concept communicability

The third issue in the evaluation is the communication of the final design result to the problem owner. It is important that the design solution is convincing and can be

communicated in a transparent and consistent way. Mainly, within a given company or institution a format is provided in which the design should be presented, although it is very helpful if the design is presented in the format of the methodology presented in this thesis. This provides a uniform format with enough freedom for the special design case, in this way the communication can be done in a structured way.

8.2 Checklists and metrics

During the evaluation of the design solution measures are needed to present the quality of the design in both a qualitative and quantitative way. This section discusses the background of some common sustainability checklists and metrics specifically suited for chemical process or product design. First some definitions are given, then some examples are discussed.

Checklists are compilations of relevant criteria; an advantage of checklists is that they can be used quickly without special methodological expertise. The quality of the outcome is dependent, apart from the quality of the checklist, on the user's knowledge and the availability of data. Usually checklists are based on existing and more or less generic knowledge.

One of the purposes of *metrics* is to support the comparison among design alternatives. It is therefore important to keep in mind that metrics do not necessarily have to be absolute measures, but should always be related to objectives stated during the problem definition. Accordingly, the term *sustainability metrics* is defined here as follows: *sustainability metrics are objective measures that help the parties involved in the design process to quantify economic, environmental, and societal issues in order to rationalise the evaluation and selection of design alternatives.*

8.2.1 Various kinds of metrics

All disciplines use their own specific metrics, varying in differences in *site-specificity*, *complexity*, *comprehensiveness*, *sophistication* and *uncertainty* (Pennington, Norris, Hoagland, et al. 2000). The metrics can be classified according to their level of aggregation, which results in the following hierarchy: 1) *inventory data*, 2) *indicators*, 3) *indices*.

Inventory data, which are physically measurable and not normalised against any reference point

Indicators that comprise certain effect categories in which the inventory data are normalised in order to determine the total contribution to the corresponding category

Indices, which are aggregated indicators of different categories based on weighting, valuation or other multi-objective decision-making theories.

Inventory data are easy to gather and understand, but do not provide insight in the impact. *Indicators* do attempt to estimate the impact, but are time intensive and often based on different methods and assumptions, which makes comparison even more difficult. *Indices* are based on decision-making theories with implicit weighting factors and therefore often loose meaning and insight. Moreover, it can

be argued that indices are actually analysis methods with one single numerical outcome.

The selection of appropriate metrics obviously depends on the availability of data, the nature of concerns and the required accuracy. According to Sharatt (Sharatt 1999) the following criteria should apply for the development of environmental performance measures (indicators and indices): i) the measure should be *unbiased*, with perfect input data the method will converge to a measure of the actual impact, ii) the measure should be *complete*; distortions that arise from ignoring some impacts and not others will give poor solutions and misdirect resource, iii) the measure should be *meaningful*; measures should be proportional to the effect on the environment, iv) the measure should be *relevant* to any regulatory constraints, v) the measure should be *transparent*; aggregated or highly complex measures that do not communicate clearly are likely to lead to misunderstanding and error, vi) the measure should be *applicable* in such a way as not to make the solution of the model excessively expensive or impossible

The Center for Waste Reduction Technologies (CWRT, as presented on their website in 2003: www.aiche.org/cwrt), an industry alliance of the American Institute of Chemical Engineers (AIChE) states that sustainability metrics must: i) be efficient and non-perverse (few, simple to collect, calculate and understand), ii) have both business and environmental value (relevant to business, drives continued improvement and right behaviour, related to economic criteria), iii) provide for growth (business value, standard of living, environmental quality). It is clear that CWRT's criteria are influenced by economic considerations and illustrate the gap between scientists (like Sharatt) and reality.

8.2.2 *System levels and metrics*

The application of metrics strongly depends on the system levels they are provided for. Veleva (Veleva and Ellenbecker 2001) distinguishes a hierarchy of five levels of indicators, varying from rather straightforward conformance indicators (level 1) to complex sustainable systems indicators (level 5): 1) facility compliance/conformance indicators, 2) facility material use and performance indicators, 3) facility effect indicators, 4) supply chain and product life-cycle indicators, 5) sustainable systems indicators.

Fiksel (Fiksel 1996) distinguishes high level metrics, which represent the overall performance of the manufacturing enterprise, and operational metrics, which represent observable and controllable measures associated with a product or process. He suggest the following types of metrics: i) energy usage metrics, ii) water usage metrics, iii) material burden metrics, iv) recovery and reuse metrics, v) source volume metrics, vi) exposure and risk metrics, vii) economic metrics.

Metrics should ideally be assessed with respect to the life cycle of the product or process being developed. A common practice in environmental quality assessment is to use scaling or weighting techniques to aggregate various specific performance measurements. Since metrics are quite specific most companies have developed their own metrics. Many institutions have also developed metrics for the use in a specific field of application.

8.2.3 *Checklists for sustainable process design*

Below examples of checklists are presented that help the designer to determine the sustainability issues related to the design: i) checklist for needs analysis, ii) checklist for system boundaries definition, iii) checklists for life-cycle approach. The checklists are based on various student design projects, carried out during this research.

Checklist for needs analysis

- How does the design actually fulfil social needs?
- What are the products main and auxiliary functions?
- Does the product fulfil these functions effectively and efficiently?
- What user needs does the design currently meet?
- Can the design be expanded or improved to fulfil users' needs better?
- Will this need change over a period of time?
- Can the design anticipate on changes through (radical) innovation?

Checklist for system boundaries definition

- What problems can arise in the production and supply of materials and components?
- Which components are used in the design?
- What are the functions of these components?
- Do these materials fulfil their functions effectively and efficiently?
- Are there alternatives for these components?
- What is the environmental profile of the components (production process, renewable raw materials, energy content, and toxicity)?

Checklists for life-cycle approach

- What problems can arise in the production process
- How many, and what types of production processes are used?
- Are these processes fully optimised?
- Are there alternatives for this production process?
- How much, and what types of auxiliary materials are needed?
- What is the level of the energy consumption?
- How much waste is generated?
- Are any toxic emissions released?
- What problems arise in the distribution of the design to the consumer?
- How much energy is required to transport the components?
- What problems arise when using, operating, servicing and repairing the product?
- How much, and what type of energy is required, direct or indirect?
- What and how much auxiliary materials are required?
- Is the product easy and safe to handle?
- What is the (technical and aesthetic) lifetime of the product?
- What problems can arise in the recovery and disposal of the design?
- How is the design currently disposed of?
- Where do the components end up?

- Do any components accumulate in nature?
- Are components toxic?
- Are components or materials being reused?
- What components could be reused?
- Are any (toxic) emissions produced during the disposal?

8.3 Sustainability ranking tool

In this section, the development of a Sustainability Ranking Tool is described, that can be used as analysis tool for the selection of criteria generated during a brainstorm. The tool is developed during an industrial design project at Shell Chemical, Amsterdam. The contents of the design project can not be presented here, because of confidentiality.

8.3.1 Goal and scope of the SRT

Within the industrial design project team, only the possibility exists to come to new process design options within the context of a given input and output (feeds/products). Many improvements are still possible in the current process design, considering the 150 ideas generated in various brainstorm sessions. Research has already started on some ideas, while others still have to be evaluated. A method to rank the ideas against the sustainability could be helpful to steer the study on the process design improvement.

The aim of this study is the development of a method for the evaluation of sustainability during the conceptual process design stage. To do this, three steps are taken: 1) the issues of sustainable development in a chemical production process are discussed and the effects on the development of a new process in this industrial project are reviewed, 2) an analysis method is developed to rank the various process design improvement proposals against the sustainability idea, 3) the current process design is studied from the perspective of sustainability and possible improvements in the process design as proposed are taken into account.

The method developed here takes into account the three well-known issues of sustainable development (people, planet, and profit) all divided into more specific measurement tools, both for *quantitative criteria* and *qualitative criteria*:

Quantitative criteria: Profit: capex (1), opex (2), and externals reduction (3)

Planet: renewables incorporation (4) and waste reduction (5)

Qualitative criteria: Planet: plant scale issues (6)

People: preferred technology (7) and knowledge resource (8)

The quantitative criteria are taken together in a calculated factor, and the qualitative criteria form a filter factor. Both factors are multiplied and give together with a chance of success the final sustainability score. The final ranking regarding sustainability issues, results in another outcome than the previous ranking done by the design-team, which was based on profitability only.

8.3.2 Basic assumptions

Keeping in mind all the preceding remarks about system levels and the three themes of sustainability, it is assumed that an analysis tool can deal with the following issues: i) social awareness of the engineers, ii) a possible negative social

assessment, iii) optimal utilization of technical experience, iv) explicit justification of all kind of decisions can promote the sustainability.

The SRT is specifically developed for the analysis and selection of brainstorm alternatives, generated during the one of the first stages of the design trajectory. The brainstorm phase is just an item in the start of the project, in which possibilities are investigated. The Sustainability Ranking Tool is made for this stage of the process, but it can also be used later in the process design, during the final sustainability evaluation.

The assessment has two phases, one quantitative (or calculated part) and one qualitative (or filter) part. The quantitative part is based on the following process data: i) average yearly production, ii) waste production, iii) capital and operational investments, iv) stoichiometry of the reactions, v) on stream time per year, vi) average price feedstock, vii) an assumption for a CO₂-tax, viii) costs of wastes disposal, ix) costs of energy, x) scale up factors.

The quantitative part is done by assessment scores, which are discussed below. The idea behind this is that part of the sustainable development problem can be calculated, but that another part of the problem is subjective, dependent on the judgement of the designer (which are related to the external communities). In this way, the intuitive knowledge of the design team is used, which may help to locate the design in a broader context.

The process is evaluated by 8 criteria, 5 of them are calculated, and for 3 of them, an assessment is defined. The *five* quantitative criteria are *Capex Reduction* (capital costs relative to target), *Opex Reduction* (operational costs relative to target), *Externals Reduction* (external costs relative to target), *Renewables Incorporation* (relative to product), and *Waste Reduction* (relative to product). The *three* qualitative criteria are *Plant Scale Issues*, *Preferred Technology*, and *Knowledge Source*.

8.3.3 *Quantitative criteria: profit*

Capex Reduction; for the Capital Investment or Capex, the total reduction of capital costs is taken in relation to the current Capex. Negative numbers indicate an increase of Capex. All process alternatives stay at the same production level.

Opex Reduction; the operational cost reductions (Opex) are calculated in the same way as the Capex reductions.

Externals Reduction; external costs are per definition the costs not included in CAPEX and OPEX (e.g. an assumed CO₂-tax, water use, land use, resource use, and scarcity). The calculation of external cost reduction consists of two parts: the calculation of the reduction of energy demand and the reduction of water consumption. Both are calculated relatively to the current energy intensity and the current water consumption.

8.3.4 *Quantitative criteria: planet*

In Table 8.1, the so-called LCA themes are summarized. These themes can be seen as the ecological impacts that a technology might have.

TABLE 8.1 GENERALLY RECOGNISED ENVIRONMENTAL IMPACTS

Depletion	Pollution	Disturbances
Abiotic resources Biotic resources	Ozone Layer Depletion Global warming Potential Photochemical oxidants Acidification Human toxicity Ecotoxicity Nutrification Radiation Thermal pollution Noise Smell Occupational health	Desiccation or Dehydration Ecosystem degradation Landscape degradation Human victims Animal victims

For this SRT tool, only two items are taken directly from this table for the assessment of ecological criteria: the renewable feedstock (is about the depletion of abiotic and biotic resources) and the waste reduction, which has to do with the waste water streams and thus with ecotoxicity.

Renewables Incorporation; for the calculation of renewables, the increase of renewability is taken as starting point. In the current process, no renewables as feedstock, energy source, catalyst and inhibitors resources, or construction materials are used. The score of renewability is given as a calculated score, because weighed percentages could be calculated, but this is not elaborated in this project. For that, the contribution of renewable energy and renewable feedstocks to the process can be presented in a number, like the weighed number for the external costs.

Waste Reduction; the waste streams of the process consist in flares, purges, wastewater streams, organic waste streams, and degraded catalysts. Per unit operation, the relative reduction can be determined, based on one of the mentioned items.

8.3.5 *Qualitative criteria: planet*

From now on, the evaluation of the criteria is done by the definition of scores between 0 and 100. All criteria are defined on the conceptual stage; for other system levels (see Chapter 2) the criteria can look different and have to be defined again. That is the reason that it is tried to describe as clear as possible how the criteria are derived, so the reader should be able to do the same derivation for other system levels. For each issue, guiding principles are given and a definition of the scores.

Plant Scale Issues point of departure for this item is the life cycle of the plant, the focus is not directl on the product life cycle. From the point of view of the designer, the demolition of the plant after use is important. From societal perspective, it is necessary to consider the complexity of the technology and the easiness to explain hazards and risks (both human and ecological). There is a trade-off between *process intensification*, *controllability/maintainability*, and *decommissioning*.

Guiding principles for the derivation of the assessment are: i) degree of maintainability and controllability, ii) use of process integration, iii) complexity of plant operation, iv) easiness of decommissioning, v) controllability of side effects.

Assessment values

0	uncertain; no decision possible
25	very complex plant construction
50	complex unit operations
75	no complexity; easy to maintain/dismantle
100	all life cycle issues are controllable within environmental constraints

8.3.6 *Qualitative criteria: people*

Preferred Technology; this item is derived from the *precautionary principle* (this principle advocates no inputs into the environment of substances with an unknown hazardous or toxic nature, especially where there is reason to believe that harmful effects are likely to occur). The reason for this is that society can refuse or forbid the technology based on precaution. Hence, the technology must fit in the current and future societal context. This means that the *feelgood* factor is important and the demands of society have to be taken into account.

From the perspective of the designer emission flows, waste streams, and assessment of effects should be known. For most designers innovative technology is a logical step for improvement of environmental unfriendly processes. From a societal perspective, communication is very important. Innovation does not automatically mean that processes are improved; due to misunderstanding and prejudices the society can ban very beautiful and elegant processes. Therefore, engineers should be able to avoid technological arrogance and should be oriented at serving society.

Guiding principles for the derivation of the assessment are: i) precautionary principle, ii) use of proven technology, iii) known emissions, iv) pollution prevention, v) responsible care.

Assessment values

0	uncertain; no decision possible
25	new technology; many unknown (side) effects
50	tested technology; unknown (side) effects
75	evolutionary approach (scale up/integration); most (side) effects are acceptable
100	proven technology; long term and large-scale (side) effects are known and acceptable

Knowledge Source; this item is derived from the *equity principle* (equity means a fair distribution of wealth power and knowledge). Sustainable Development is mainly discussed on the issue of *sustainability*, but often it is forgotten that the focus should be *sustainable development*. Sustainable Development is a development, which is advantageous for all people, for all nations, for all cultures. That is the reason that the issue of equity is very important in the sustainable development debate.

The question is now how a designer or design team can contribute to this debate on the level of chemical process design. From the viewpoint of different system levels

(see Chapter 2), the following can be stated: i) at the *functional level* (political, both management and government) *power-inequity* exists, ii) at the *market level* (economical) *wealth-inequity* exists, iii) at the *route and processing level* (technological) *knowledge inequity* exists.

From this a criterion is developed about the sources of the knowledge that is used during the process design. From the perspective of the designer all knowledge that is available (both confidential and public) is useful during the design. From the viewpoint of the society, company cultures should be open, knowledge should be public accessible, decision strategies should be transparent.

Guiding principles for the derivation of the assessment are: i) open company culture, ii) equity principle, iii) transparency of decision.

Assessment values

0	uncertain, no decision possible
25	exclusive technology
50	technology for specialised companies
75	common engineering knowledge
100	free accessible technology

8.3.7 *Concluding remarks on the SRT*

The main goal of this case study is to show that Sustainable Development can be made applicable at low system levels in the early stages of a design. There it is very important that the design team does the societal evaluation. Sustainability is translated into both qualitative and quantitative assessment criteria. The definition of the criteria strongly depends on the system level in which they are applied. For the conceptual design phase, the following considerations are made: i) *economical issues*: short and long term costs have to be internalized, this can be done quantitatively, ii) *ecological issues*: avoidance of wastes or emissions and use of renewable feedstocks, those factors can be calculated; also the consideration of the life cycle of processes and products is important, this is done qualitatively, iii) *social issues*: equity and precaution are main parts of the sustainability debate, they can only be valued by qualitative factors.

It is assumed that this method also can be applied to other system levels, which asks for other definitions of the criteria (economic, ecological, and societal). This can be done in a similar way as described, based on guiding principles and intensive discussions of what sustainability means in this case.

TABLE 8.2 PROCESS DATA SRT CASE

Name	Status	Unit	Target	Result	Unit
<i>Process data</i>					
Production of A	xxx	kt/year			
Production of B	xxx	kt/year			
Current CAPEX (SRI - scaled)	xxx	M\$	20%	xxx	M\$
Utilities	xxx	MW	20%	xxx	M\$/year
Ethylene + Benzene, D stoichiometric	xxx	t/t A	20%	xxx	M\$/year
Propylene, D stoichiometric	xxx	t/t B	20%	xxx	M\$/year
Current OPEX (Feedstock, Utilities, and Maintenance)				xxx	M\$/year
Waste water production	xxx	t/t B	50%	xxx	kt/year
Waste Na production	xxx	t/t B	50%	xxx	t/t B
Waste catalyst production	xxx	kg/t B	50%	xxx	kg/t B
<i>Fixed data</i>					
Total on stream time per year	8000	hours			
Average price C2, C3, Benzene	400	\$/t			
CO ₂ tax (20 \$ / ton C)	5,45	\$/t CO ₂		xxx	M\$/year
CO ₂ production	2,00	kt/MW			
Costs of waste water disposal	50	\$/t H ₂ O		xxx	M\$/year
Costs of energy, average	20	\$/MWh			
Scale up A Production	xxx	kt/year			
Scale up B Production	xxx	kt/year			

8.4 *SRT case study: ranking of brainstorm alternatives*

The industrial project, presented here is an innovative redesign of an existing chemical process. The process produces two products A and B from the same source.

8.4.1 *Reduction factors*

In Table 8.2, the process data are presented, which are used in this evaluation. In the early design stages of this project, brainstorms are performed, which resulted in a list of 150 process alternatives. The process alternatives differ largely in system level and implementation time, the Sustainability Ranking Tool gives a ranked overview of these process alternatives from different viewpoints. In the remaining part of this section, Sustainability Ranking Tool is followed as described in the previous section.

CAPEX reduction

Only some design alternatives are related to a scale up of the production of both product A and B to a level of 25% and including outer battery limits. Therefore the

capital investments of these design alternatives are related to the growth in production. So in this case the CAPEX Reduction is an upline reduction. For getting a more proportional number, the reduction of capital costs is calculated relatively to a target value.

OPEX reduction

The operational costs reductions are calculated in the same way as the CAPEX reductions. The scale up is treated as described previously. A targeted OPEX reduction is calculated relatively to a reference value.

External costs reduction

The calculation of external cost reduction consists in two parts: the calculation of the reduction of energy demand and the reduction of water consumption. Both are calculated relatively to the current energy intensity and the current water consumption.

Renewables incorporation

For the calculation of renewables, the increase of renewability is taken as starting point. In the current process, no renewables as feedstock, energy source, catalyst and inhibitors resources, or construction materials are used. In none of the proposed ideas, the direct replacement of an existing source by a renewable source is postponed. That is the reason that all alternatives get a score of 0. For every new application of this method, the design team should agree upon a calculation approach if renewables are used.

Waste reduction

The waste streams of the process consist in flares, purges, wastewater streams, organic waste streams and degraded catalysts. All purge gases and liquid wastes are fed into an incinerator for the generation of energy, so that in the calculation of the waste numbers only the catalyst degradation and the additives for the neutralization of wastewater are taken into account. Per unit operation the relative reduction can be determined, based on one of the mentioned items.

Qualitative criteria

The remaining criteria, *Plant Scale Issues*, *Preferred Technology*, and *Knowledge Source*, are filled in following the Assessment values presented in the description of the SRT. Those values are based on the intuition of the design team, which means that these numbers are strongly dependent on the persons that provided them. It was learned that it is very important to have much discussion on the numbers and that the scorecard must be filled in at once. By doing so, it seems that one gets a feeling for the relative influence of the various design possibilities and thus can do the trade-off between them. In such a way the scorecard gives insight in the non-technological impact, this is the main goal of this whole exercise.

8.4.2 Final scorecard

Using the numbers from the calculation sheet and the qualitative values, a Final Scorecard is created. This Final Scorecard can not be presented here, because it contains too much process-specific information. The format of such a Final Scorecard is as presented in Table 8.3.

TABLE 8.3 EXAMPLE OF FINAL SCORECARD

		quantitative						qualitative								
nr.	proposal	economic		ecological				social								
		capex reduction	opex reduction	externals reduction	renewables incorporation	waste reduction	quantitative score	plant scale issues	preferred technology	knowledge resource	qualitative score	economic score	ecological Score	social score	average score	filter score
1	Process Alternative I	48	5	0	0	0	11	50	75	50	58	18	17	63	29	6
2	Process Alternative II	23	64	0	0	-1	17	75	50	50	58	29	25	50	33	10
3	Process Alternative III	-15	25	28	0	34	15	75	75	25	58	13	36	50	31	8
4	Process Alternative IV	13	2	30	0	34	16	75	50	25	50	15	36	38	29	8
5	Process Alternative V	0	57	0	0	0	11	50	50	50	50	19	17	50	26	6
6	Process Alternative VI	12	9	44	0	0	13	75	75	75	75	22	25	75	36	10
7	Process Alternative VII	28	22	45	0	18	22	75	100	75	83	32	31	88	45	19
8	Process Alternative VIII	6	1	-1	0	0	1	75	100	75	83	2	25	88	32	1
9	Process Alternative IX	3	10	4	0	51	14	75	75	25	58	6	42	50	30	8
10	Process Alternative X	0	0	0	0	0	0	25	50	25	33	0	8	38	13	0

After completion of the Final Scorecard, there are many possibilities of presenting the scores. It could not be decided at forehand what would be the best way of calculating a trade off between the criteria. That is the reason that two calculations are done, one is called the *Average Score*, the other *Filter Score*; N is the number of scores.

$$\text{Average Score} = \frac{\sum \text{Qualitative Scores} + \sum \text{Quantitative Scores}}{N_{\text{All Scores}}} \quad \text{Equation 8.1}$$

$$\text{Filter Score} = \frac{\sum \text{Quantitative Scores}}{N_{\text{Quantitative Scores}}} \times \frac{\sum \text{Qualitative Scores}}{N_{\text{Qualitative Scores}}} \quad \text{Equation 8.2}$$

As becomes clear from the two equations, the Average Score is the non-weighted average of all scores; the Filter Score is the average of the quantitative criteria times the average of the qualitative criteria, in this sense the average of the quantitative criteria is corrected or filtered for the qualitative impact. Since it is not decided in the SRT method which would be the correct calculation method, the design team can play with the influence of the various criteria on the final result. From Table 8.3, it is concluded that different kinds of calculation gives different ranking results, so the decision making should be very careful.

8.4.3 *Concluding remarks on the SRT case study*

In the described industrial project, many proposals for improvement of the design are being studied and a screening tool to guide the final selection in terms of overall sustainability was useful. The following conclusions can be drawn: i) the Sustainability Ranking Tool delivers insight in the various alternative designs of the case study, ii) the method is fast and cheap and it is a tool to support discussion within a team after the brainstorm session.

8.5 **Concluding remarks**

The evaluation of the design results is the final stage of the decision-making sequence, here it becomes clear if the design solution really contributes to sustainable development. The design evaluation stage consists in three elements: 1) goal and scope satisfaction, 2) criteria satisfaction, 3) concept communicability. It is important that a distinction is made between the analysis of alternatives and the evaluation of the design result.

The evaluation of the design is a more value-laden topic in which the design concept is required to satisfy economic, social, and ecological criteria simultaneously. For this evaluation it is not only relevant to present a technical validation of the design solution, but also to confront the design to a group of stakeholders. The involvement of stakeholders during the evaluation of the design is crucial for the societal embedding of the design result. For that, scenario building and forum discussion with stakeholder groups are useful. Various tools can stimulate the effectiveness of the design evaluation stage. In this Chapter, the sustainability ranking tool (SRT) is presented.

- The description of the sustainability ranking tool (SRT) and the accompanying case study shows that sustainable development can be made applicable at the processing system level in the early steps of the design framework by societal evaluation. Sustainability is translated into both qualitative and quantitative assessment criteria. For the conceptual design phase, the following considerations are made: i) *economic issues*: short and long term costs have to be internalized, this can be done quantitatively, ii) *ecological issues*: avoidance of wastes or emissions and use of renewable feedstocks, those factors can be calculated; also the consideration of the life cycle of processes and products is important, this is done qualitatively, iii) *social issues*: equity and precaution are main parts of the sustainability debate, they can only be valued by qualitative factors.
- It is assumed that the SRT method also can be applied to other system levels, which requires other definitions of the criteria (economic, ecological, and societal). This can be done in a similar way as described, based on guiding principles and intensive discussions of what sustainability means in this case. In the described industrial project, proposals for improvement of the design are being studied and a screening tool to guide the final selection in terms of overall sustainability was useful. The sustainability ranking tool delivers insight in the various alternative designs of the case study and supports discussion within a team after the brainstorm session.

Chapter 9

EXTENSION OF THE PROCESS DESIGN METHODOLOGY TO SUSTAINABLE CHEMICAL PRODUCT DESIGN

Summary *In this Chapter the process design methodology is applied to the design of sustainable chemical products. The process design framework, presented in Chapter 4, is developed here to a product design framework. A specific tool for the evaluation of sustainable consumables (ESC) or chemical products is presented and applied to an industrial case. This tool improves the design problem definition of sustainable chemical product design.*

9.1 Introduction to product design

In this Chapter, the methodology is extended to the design of sustainable chemical products. A chemical product can be defined by:

a product that consists of a mixture of chemicals and/or brings about a chemical or physical reaction when used by the consumer.

The term *chemical product* shows clearly that such products will include (complicated) chemical processes; another word is *consumable*, which makes clear that the product is consumed during use. A sustainable chemical product or a sustainable *consumable* seems a paradox, because something that is consumed during use cannot be seen as long-lasting or durable. However, sustainability is very important for the design of chemical products, because in fact, since matter does not physically disappear, nothing actually gets consumed. The consumed materials or derivatives will always end up somewhere in the environment. It is thus very important that the use and discharge of these products are well designed and controlled.

Examples of chemical products are: detergents (e.g. cleaning products, soap, washing powders, etc.), creams (e.g. personal care, furniture care, etc.), odors (e.g. perfumes, refreshers, etc.), coatings (e.g. paint, varnish, etc.), adhesives (e.g. glue, tape etc.), dyes (e.g. pigments, colours etc.), food additives (e.g. preservatives, aromatics etc.), or agricultural products (e.g. pesticides, fertilizers, etc.). In the public debate, the term chemical product mainly is associated with toxicity and risk. The current developments of the chemical industry in general, but also the sustainable development of the chemical industry in particular, give some motives for the integration of product and process design: i) the increasing amount of products that are produced in large-scale continuous processes, ii) the life-cycle approach and the supply chain management ask for a concurrent design of both the products and the processes, iii) the tendency in the chemical industry to produce more and more high-value added chemicals or fine chemicals.

9.1.1 Product and process design

In practice, many differences exist between the design of chemical processing plants and the design of chemical products: i) the design of *chemical process plants* is focused more on the production of intermediates on a large scale and the design challenges are in the physical science and mechanical engineering field, mainly the chemistry development is not the main focus of the design, ii) the design of *chemical products* is more in the physical chemistry field or food processing and also more consumer focused.

Many design methodologies exist for both product and processes and the distinction between the two is very important. Graedel and Allenby (Graedel and Allenby 1995) give the following definition:

Products are what is sold by a corporation: paper clips, toothpaste, and airplanes for example. Processes are the techniques by which those products are made: the production of glass from lime, soda ash, and sand, for example.

However, these definitions are rather ambiguous, since something can be a product to one corporation while it may be (part of) a process to another. Therefore the authors add: *Processes are the ways in which feedstock material of one sort or another is transformed into intermediate materials*. Furthermore, Graedel and Allenby (Graedel and Allenby 1995) discuss some general differences between products and processes: i) processes require large capital investments, have long lifetimes, and are therefore typically partly redesigned and renewed, ii) processes typically produce a variety of products.

From a life-cycle viewpoint, it is easier to consider the unsustainability of a chemical processing plant than of a chemical product. The design of a chemical product deals with many different supply chains and the use, maintenance, and demolition phases are operated at indefinable and uncontrollable circumstances. In Figure 9.1, the product and plant life cycle are drawn, which illustrates that the product and process life span are perpendicular to each other: i) many processes are needed for the production of one product, ii) the location of the process is fixed, while the product location varies per life cycle step.

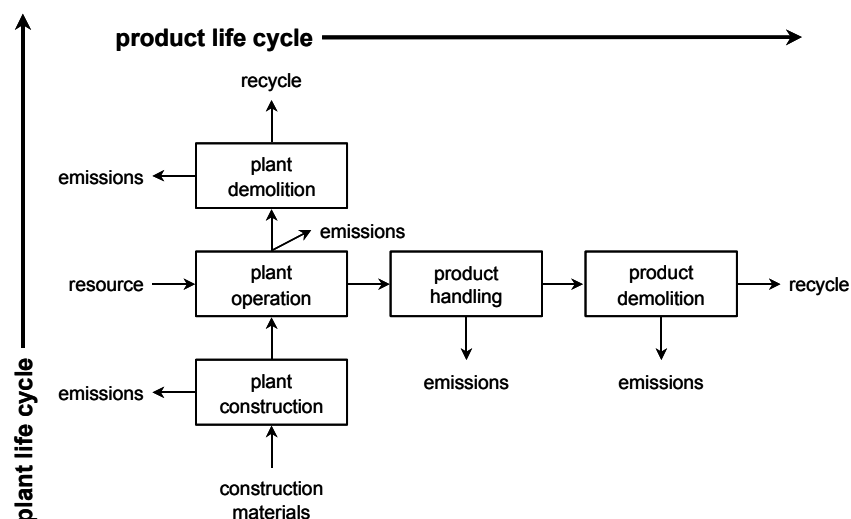


FIGURE 9.1 THE PRODUCT AND PLANT LIFE CYCLE

A life cycle approach is becoming more important in design methodologies in order to account for all effects that occur during its lifetime, from cradle to grave. The life cycle of products and processes must be distinguished.

9.1.2 Challenges in chemical product design

In Chapter 4, it is stated already that during the chemical product design qualitative and non-specific consumer requirements have to be taken into account, instead of the very precise, quantitative, target specifications usually used in process design. This means that these qualitative consumer requirements have to be translated into physical qualities, which is the greatest challenge in product design. Here a lot can

be learned from industrial and mechanical engineers, who have been involved in durable product design for a long time, and have developed many methods and procedures to improve the efficiency of product design.

A different problem is that chemical product design is not really considered as a real design activity by those who work on it. Most people have a research background, and the work is more treated like a (fundamental) research project than as a design process; mainly it is called product development, instead of product design. It is true that chemical product design sometimes is less straightforward than for other engineering design fields. The latter can for a large part be done at a drawing table, while the first will probably concern a number of chemical experiments.

However, the general framework presented in this thesis can structure the chemical product design, because the purpose of every design of consumer products is to find a creative solution for a consumer need. By using a more systematic (methodical) approach, chemical product design can be integrated more into the other design loops of for example the supply chains or the needed chemical processes. As chemical product design is a more methodical process, it will be easier to implement external factors, like design for environment, design for safety, or design for sustainability.

9.1.3 *Product design procedure*

In Figure 9.2, the general framework for the process design, as presented in Chapter 4, is modified with the terms for chemical product design. In Table 4.5, a glossary is provided. In this way it is illustrated how the *general framework* can be applied to various kinds of design, while the *decision-making sequence* stays the same.

Mainly a product design starts with some idea from an external stakeholder (defined by for example R&D or marketing). If a rather strict definition of the assignment is given, the goal and objectives will already be pretty much set. In that case still an in-depth analysis of needs will have to be performed before a final goal can be set, in order to verify the feasibility of the assignment. It is important to identify the drivers that are influential for the start of a project. The drivers that initiate the project will influence the goal and the objectives to be met in the project. It is important to check if key drivers match the chosen project goal.

Initial project ideas will come from either a pull mechanism (e.g. market pull) or a push mechanism (e.g. technology push). Many projects have both push and pull mechanisms to drive them. Examples for *pull mechanism* are: i) consumer needs, ii) societal needs, iii) environmental needs; examples for *push mechanism* are: i) new and improved technology, ii) company strategy (simplification, cost reduction, etc.), iii) regulations. In general the same steps can be followed for both cases, but the exact contents and purpose of each step may differ. Where for a market pull mechanism the first phase serves mainly to identify all needs, for a technology push project it serves to verify that the application of the new technology is useful.

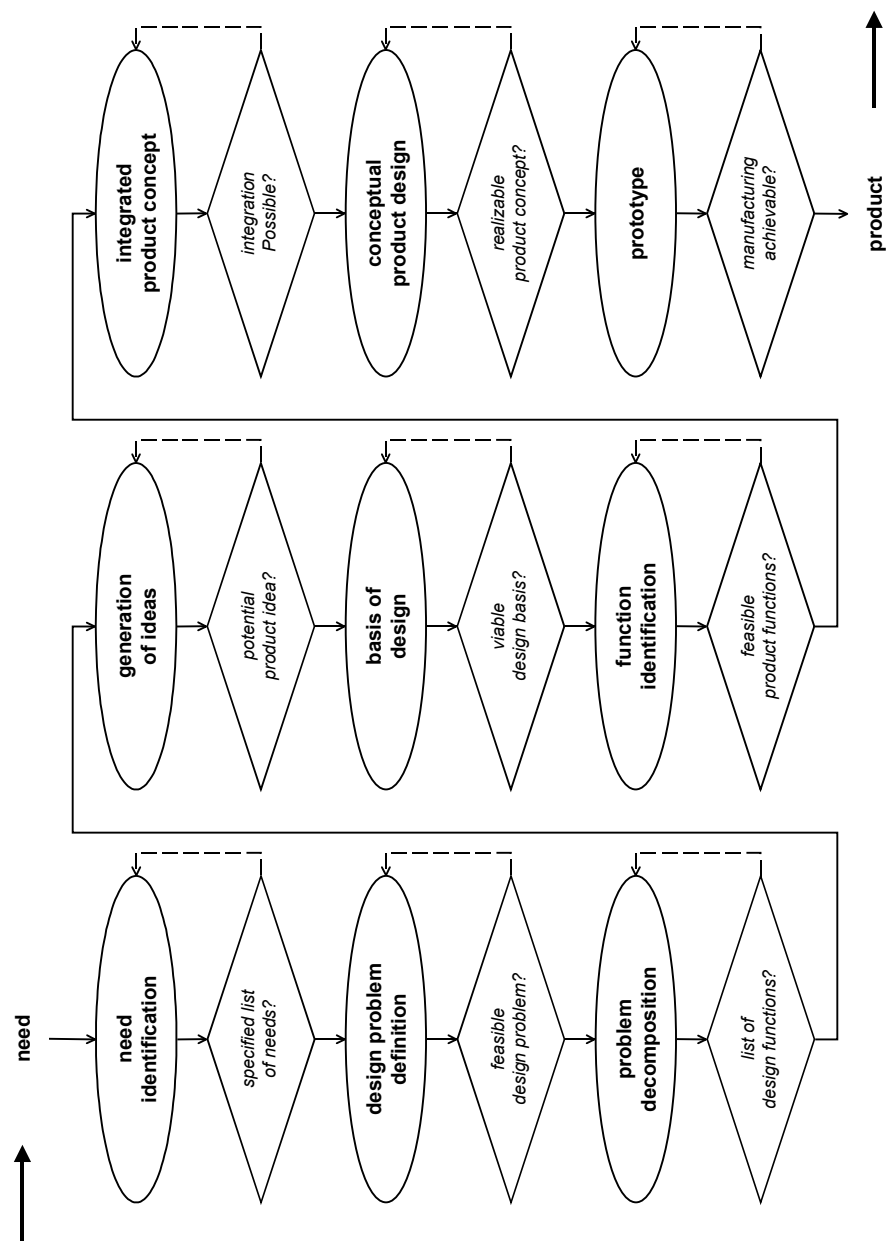


FIGURE 9.2 OVERVIEW PRODUCT DESIGN

TABLE 9.1 GLOSSARY OF THE DESIGN FRAMEWORK FOR PRODUCT DESIGN

need identification	The whole design project starts with a question for the fulfillment of a need, its character can be societal, economical, environmental, and technological. <i>specified list of needs?</i>
design problem definition	From the need a design problem is derived that can be solved within given constraints. Together with the design problem, the system boundaries and the evaluation criteria are defined. <i>feasible design problem?</i>
problem decomposition	Mainly, the identified needs and the derived design problem are abstract and can be solved in many ways. Thus, the designer decomposes the design problem into various design functions. <i>list of design functions?</i>
generation of ideas	Possible solutions are generated based on the existing knowledge, experience, and creativity. These are rough ideas of basic chemistry, plant innovation, market strategy or whatever. <i>potential product idea?</i>
basis of design	While the final result is a chemical plant, the designer or the design team have to come up with a design basis that, within the given goal and battery limits, ensures that a solution is feasible. <i>viable design basis?</i>
function identification	Within the basis of design, functions are identified that represent the original design problem and innovation is possible. <i>feasible product functions?</i>
integrated product concept	The <i>integrated product concept</i> describes the interactions of the product components and the possibility to combine them to one product. <i>integration possible?</i>
conceptual product design	The <i>conceptual product design</i> contains all specifications of the product. Evaluations on economics and safety, health, and environment issues are performed. <i>realizable product concept?</i>
prototype	The product is developed in order that it can be manufactured on large scale. The process for manufacturing is designed and a commercial plan is made. <i>manufacturing achievable?</i>

Andreasen (Andreasen and Hein 1987) describes product development activities on three levels of resolution, depending on the focus of attention. These are *general problem solving* (i.e. generic decision making), *product synthesis* (i.e. the entire product design) and *integrated product development*. *Integrated product development* describes the product development from a company's viewpoint. This level concerns the activities of a general manager of a company and falls outside of the scope of this research, which is focused on the activities of design team. This level will not be discussed in this thesis. The difference between *product synthesis*

and the *general problem solving*, can be compared with the difference between the General Design Framework and the Decision Diagram in this thesis, see Chapter 4.

9.2 Evaluation of sustainable consumables tool

The ESC tool identifies and evaluates important design issues from a sustainability viewpoint. It arranges issues over a set sustainability and life cycle criteria, and classifies a (reference) product into one of four categories, ranging from good to problematic. The tool is developed for the exploratory phase of the design process, in which the first ideas are presented. In existing tools, e.g. as developed in design for environment methodologies, the subjects are not treated extensive enough to encompass all sustainability aspects (like the triple bottom line) and all issues relevant for chemical product design.

9.2.1 Structure and purpose of the tool

The tool consists of a checklist containing a number of impact criteria for which a concept must be ranked one of four categories: A= problematic, B= moderate, C= sufficient, D= good. An extra category 'D' is added compared to the original format of the ABC analysis, because the 3 categories do not offer enough distinction to give a clear ranking of products.

A new and extensive set of impact criteria has been developed. The impact criteria are divided into two categories, general sustainability criteria (economy, environment and society) and life cycle criteria. The first treat the intrinsic properties of the product and all the materials used, the second focus on how these materials are used in the products life cycle. This means that some issues might be treated twice, but in a different context.

A set of guidance questions has been developed to help to fill in the tool. Some questions are taken from existing ecodesign checklists and industrial ecology checklists, and the remainder is newly developed. The aim of these questions is to make sure all issues are regarded, to explain the contents of the category cells and to provide guidance. A polar chart is used to visually show the results of the analysis, and to compare concept, or a concept to a base case.

The ESC tool helps to make a qualitative analysis of a product, reference product, or product concepts, on sustainability and life cycle criteria. The category table serves as a checklist, to ensure that all relevant sustainability issues are considered and to identify a product's key issues concerning sustainability (even potential 'make or break' issues) at an early stage.

Figure 9.3 shows a polar chart of the results of a ESC evaluation of project X and an appropriate benchmark (reference). This chart shows clearly what the most important issues are for both products, and how they compare. One can for instance see that where the environmental criteria are concerned these two options present a choice between a product that produces more water pollution, or one that produces more atmospheric pollution. Also project X scores very well on consumer needs analysis, but might have problems with social acceptance. The benchmark is socially accepted, but does not serve consumer needs as well. On the other hand, project X scores much better for energy use in the use phase.

The tool can identify gaps in the knowledge that is available on the product, stimulate people to think about sustainability, and creates more awareness on sustainability issues. Finally, a graphical comparison of different concepts, or a product and its reference product is possible. A quantitative comparison is possible, if values and weighting factors are assigned to each category and each impact criterion. This is however not the main purpose of the tool, and results should always be regarded with care, since the evaluation is strongly dependent on the personal values of the designers.

9.2.2 *ESC procedure*

The ESC is used as follows: i) define one or more solutions to the design problem, together with a reference product design, ii) answer the guidance questions, see Appendix F, iii) select the appropriate category (ABCD) from the category table, see also Appendix F, and iv) fill in the selected category in the worksheet by marking the appropriate column, if necessary accompanied by some comments, see Table 9.2.

If it cannot be determined which category is applicable because of lack of information a question mark should be entered in the expected category. If major uncertainties are present, it should be ranked at least category B. Impact criteria that are ranked A (problematic, action required) identify potential *make or break issues*. These issues will have to be solved before the product can be approved of. Impact criteria ranked B (moderate, to be observed and improved) identify further key issues. These issues should also be improved, but are not as problematic as issues ranked A. However, if a question mark appears in B this will have to be solved as soon as possible, for it could end up as an A ranking. Impact criteria ranked C (sufficient, no direct action required) are not yet perfect, but are sufficient for the time being. Impact criteria ranked D (good) are good, also for the (near) future. Since the categories do not take into account specific circumstances of a product, such as for instance regional circumstances, specific company policies or political viewpoints, these issues should be born in mind when evaluating the results of the tool. That can be done quantitatively by applying weighting factors, or qualitatively by evaluating the different point in for instance a discussion.

If two or more concepts, or a product and a reference product must be compared the results from the worksheets can be plotted in a chart. Suggested is the use of a radar graph. If a more quantitative result is desired a value can be given to each category (A= 1, D= 4), and results summed for the product. In this case it is recommended to assign a weighting factor to each of the criteria. This weighting factor should take into account specific circumstances for the product, company policy, and general sustainability criteria. It should be mentioned that this is not meant to be a quantitative tool, and that this quantitative analysis serves an extra illustration, but should not be seen as a definite result. Since an evaluation like this is always subjective, caution should be taken when comparing evaluations by different people.

TABLE 9.2 ESC WORKSHEET

Impact Criteria	Categories			
	A (problem)	B (moderate)	C (sufficient)	D (good)
<i>General sustainability criteria</i>				
<i>Social Criteria</i>				
Compliance with government regulation				
Consumer need analysis				
Social acceptance				
Human toxicity				
Risk of accidents				
<i>Environmental criteria</i>				
Eco-toxicity				
Atmospheric pollution				
Water pollution				
Solid waste				
<i>Economic criteria</i>				
Company				
Consumer				
Depletion of scarce resources				
<i>Life cycle criteria</i>				
<i>Pre-production</i>				
<i>Raw materials extraction</i>				
<i>Production of ingredients</i>				
Choice of ingredients				
Manufacturing and processing				
Logistics				
<i>Use phase</i>				
Substances				
Energy				
Service				
Auxiliary materials				
Packaging				
<i>End of Life</i>				
<i>Recyclability</i>				

Figure 9.3 shows a polar chart of the results of a ESC evaluation of project X and an appropriate benchmark (reference). This chart shows clearly what the most important issues are for both products, and how they compare. One can for instance see that where the environmental criteria are concerned these two options present a choice between a product that produces more water pollution, or one that produces

more atmospheric pollution. Also project X scores very well on consumer needs analysis, but might have problems with social acceptance. The benchmark is socially accepted, but does not serve consumer needs as well. On the other hand, project X scores much better for energy use in the use phase.

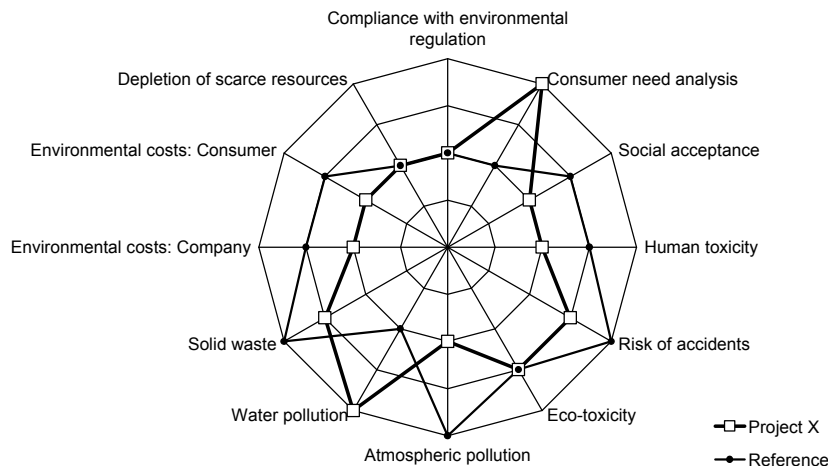


FIGURE 9.3 GRAPHIC REPRESENTATION OF ESC SUSTAINABILITY RESULTS

The tool does not give a strict answer as to which of the concepts is the better one. The area occupied by the project to be assessed and of the reference, which represents the overall sustainability, is roughly the same for both products. If a weighing system were applied it would be possible to get a more quantitative answer. The most important benefit of the tool is that it shows very clearly what the positive and negative aspects of a new concept are and which issues would require further work. Other circumstances can be taken into account during the evaluation, such as regional differences, political or business strategies, public opinion, etc.

9.2.3 Evaluation of ESC in an industrial context

The ESC tool was tested in several different ways. It was sent to a number of people within Unilever Research, Vlaardingen, in order to test the tool. They were asked to fill in the tool for the project they were currently working on. Of the respondents, most were working on the same project, project X, so that the results from different people could be compared. In this way the consistency of the results could be tested. From the people working on other projects only qualitative opinions were obtained. Finally, a meeting was held with people from Unilever in Port Sunlight working on ecodesign initiatives to exchange experiences and receive feedback. This feedback is not presented here separately, but included in the general evaluation of the tool.

TABLE 9.3 CONSISTENCY AND STANDARD DEVIATION

Impact Criterion	Respondent									s
	1	2	3	4	5	6	7	8	9	
Regulation compliance	B	C	A	C	B	D	A	B	C	1.00
Consumer need analysis	D	B	D	B	C	D	B	C	C	0.87
Social acceptance	B	B	B	B	B	B	B	B	C	0.33
Human toxicity	B	C	B	C	D	C	A	B	C	0.88
Risk of accidents	C	C	B	C	D	D	A	C	C	0.93
Eco-toxicity	C	C	C	C	B	B	B	C	C	0.50
Atmospheric pollution	B	B	B	A	B	D	A	B	A	0.93
Water pollution	D	B	C	B	D	D	A	B	C	1.09
Solid waste	C	C	B	B	C	B	B	C	B	0.53
Company	B	B	B	A	B	B	A	B	C	0.60
Consumer	B	B	B	B	C	B	B	B	B	0.33
Depletion scarce resources	B	C	B	C	C	D	B	C	C	0.67
Raw materials extraction	B	D	C	C	C	C	B	B	C	0.67
Production of ingredients	B	C	B	B	C	D	B	C	C	0.71
Choice of ingredients	D	D	B	C	C	D	A	C	B	1.05
Manufacturing	C	C	B	B	B	D	A	B	C	0.88
Logistics	B	D	C	B	B	D	B	B	C	0.87
Substances	B	C	C	C	B	D	A	B	C	0.88
Energy	D	B	C	C	C	D	B	D	C	0.78
Service	D	D	C	B	C	D	B	D	C	0.83
Auxiliary materials	C	C	C	B	C	D	B	B	D	0.76
Packaging	C	C	B	B	C	D	B	C	D	0.78
End of Life	A	C	A	C	B	B	B	B	B	0.71
Recyclability	C	C	B	B	C	D	B	D	C	0.78

Consistency

As already mentioned, to test the consistency of the tool a number of people who work with project X, ranging from project team members to environmental or regulatory specialists and management, were asked to fill in the tool for the project. Nine people completed a SusCon analysis for the project. Table 9.3 shows the distribution of the categories marked for each impact criterion. A standard deviation was also calculated for each of the impact criteria. This was done by attributing a value to each of the rankings (A=1, B=2 etc.), assuming the correlation to be linear. The standard deviation can theoretically range from 0 (no deviation) to 1.6 (maximum deviation). Most impact criteria have a standard deviation around 0.6–0.8, which is reasonable.

Although the consistency of the tool is not very good, this does not necessarily mean that the tool does not perform well. If one remembers the purposes of the tool (identifying key issues, serving as a checklist, creating awareness), one can see that the tool fulfils these purposes well, even without its results being very consistent.

Another thing one could see from these results is that results depend on who filled in the tool, since nobody is totally objective. People with an environmental or regulatory job (respondent 7 and 4) were much more negative than members of the project team itself (respondent 2 and especially 6). This is not surprising, since project team members tend to be ‘champions’ rather than critics of the project. The extreme positivism of respondent 6 however is stretching this a bit, and possibly something else is the matter here. The product might not have been rated for the concept as it was at the time, but on how it is supposed to be when it is launched. Care should be taken that people fill in the tool for the product as it is at the moment of evaluation, with all its uncertainties and problems. Respondent 7 on the other hand, who has a regulatory background, also shows a rather exaggerated criticism for the product.

This shows that it is important who fills in the tool. Therefore the tool should not be filled in solely by the project leader. Different people could fill it in separately, and then organise a meeting in which the results, especially the differences in rankings, are discussed. In that way discussion is forced, which should give good results. Another possibility is to let the project leader fill it in with the project team, possibly assisted by an environmental expert.

Applicability

From the comments given by the respondents the applicability of the tool in an industrial context could be evaluated. Generally respondents were very positive about the tool. They considered it clear, easy to work with and to fill in. It helped them to think about sustainability issues in a structured way and consider all necessary issues. If categories were not exactly clear, the guidance questions helped to make things clear. Several respondents answered that they felt the tool could be a useful addition to the Unilever project management system, and that they would like to work with it on new projects.

Critical remarks were made, like: it is difficult to include specific circumstances, such as regional differences in the analysis. This is true, but as mentioned before, these issues should be taken into account during the evaluation or just for a specific project, and are not included in the tool. Some designers complained that the discriminative capacity was not large enough. Category A is not often marked since it is almost a definite ‘no go’, and not many projects will be so good that they deserve a D. On the other hand, if there would be more categories the tool would become more difficult to handle.

9.2.4 Concluding remarks on the ESC tool

Generally the tool is thought to be more effective for projects in the ideas phase, to identify key issues. Just before the launch of a product there is already a lot of paperwork to fill in (environmental and safety clearance, etc.) and people are afraid of bureaucracy. In the first phases (usually research departments) there are less things to fill in at that moment, and guidance is appreciated, especially if it adds value.

The tool could be included easily in existing innovation management systems or the general design framework. It is important to fill in the analysis in an objective way,

but some designers complained that they did not know enough to fill in the tool completely. It should be clear that this is not a problem, since one of the purposes of the tool is to identify gaps in the knowledge available on the project. Altogether, it can be concluded that the ESC tool is suitable and useful in an industrial context. Especially for research projects that consider new product concepts such a tool is essential. One problem that remains to be solved however is how to get people to use the results of the analysis in their work, and not only treat it as another thing to fill in. For this purpose the project team should be obliged to present a plan for how all issues ranked critical in the ESC analysis will be further investigated and managed. The real implementation of the tool, is really dependent on the company structure and organization.

9.3 Concluding remarks

The process design methodology presented in Chapter 4 is also applicable to chemical products. This is validated by using the design methodology in product design environment. The three units of the design methodology, the general framework, the decision diagram, and the design methods, also hold for the development of products. In the case of product design, the structure of the general framework is kept the same, while the definition of its steps has changed slightly. The decision-making procedure for both product and process design is the same, since this is a general procedure for every kind of decision-making. In the product design, specific design tools are applied, focused on the need specification or the chemical properties.

Such a tool is the evaluation of sustainable chemical products tool (ESC), which is presented in this Chapter, together with its industrial application.

- The ESC tool is developed for projects in the idea identification design step. It provides guidance for the problem definition stage and it explicitly adds a sustainability value. The ESC is performed as a questionnaire.
- The ESC tool can be included in existing innovation management systems or the general design framework. It is important to fill in the questionnaire in a replicative way, since one of the purposes of the tool is to identify gaps in the knowledge available on the project, which must be closed by further research.
- The ESC tool is suitable and useful in an industrial context. Especially for research projects that consider new product concepts such a tool is essential. The project team should be obliged to present a plan for how all issues ranked critical in the ESC analysis will be further investigated and managed.

Chapter 10

CONCLUSIONS AND RECOMMENDATIONS

Summary *In this Chapter, it is shown that the hypotheses, given in Chapter 1, are satisfied. An integral design methodology is developed for chemical process design, consisting in three parts as described in Chapter 4. The methodology contains various types of design methods, which show that sustainability can be considered during the design of chemical processes, described in the Chapters 5 to 8. The design methodology also holds for chemical products as is shown in Chapter 9. The case studies described in this thesis are of great importance to show the validity of the design methods and to illustrate the incorporation of sustainability into chemical process design. After the final concluding remarks, some recommendations for further research are given.*

10.1 Conclusions of this thesis

Every Chapter of this thesis contains its own concluding remarks. Here the final conclusions of the thesis are drawn referring to the presented three hypotheses of Chapter 1, by mentioning the relevant Chapters and their main outcome for each hypothesis.

10.1.1 Hypothesis 1; integral design methodology

Sustainable development of chemical processes and products can best be realized by an integral design methodology that 1) clearly locates the various design tools that are available or are to be developed and that 2) forces the designer to define the problem, to propose and analyze creative solutions, and to evaluate the design in a consistent and structured way.

- In Chapter 2, an general overview of the sustainability debate is given. This overview shows that a general approach is needed to the design of chemical processes and products, if this design should contain external factors. Chapter 3 makes this more explicit.
- Chapter 3 and 4 show that such an integral methodology does not exist in the current literature on chemical process design. This hiatus required the development of a design methodology that is flexible to various sets of criteria, various kinds of knowledge levels, and possibly realizes the interchange of design results between stakeholders and designers. Such an integral methodology is proposed at the end of Chapter 4.
- In Chapters 5 to 8, tools are described that help the designer of design team to formulate design problems, to generate new design solutions, to analyze these solutions, and to evaluate the final results. The designers are confronted with the main principles of the sustainability debate and make specific criteria for their own project.

10.1.2 Hypothesis 2; novel design methods

The incorporation of sustainable development in the design of chemical products and processes requires specific skills and tools. The design methodology should contain enough tools to cover the whole area from need to plant. If tools are newly developed their location in the design methodology should be identified.

- In Chapter 4, the design methodology is presented. The structure of the methodology is open to a variety of design methods. In this thesis some of these methods are developed, but many kinds of methods can be used along with the design framework.
- The Chapters 5 till 8 give methods that are specifically focused on the integration of sustainability in chemical engineering practice. The tools are illustrated with case studies.
- It is expected that the newly developed design tools are not strictly dependent on the company structure and organization. The tools have a clearly defined place in the design framework. From this location in the

design framework, it is possible to locate the tools in another design framework.

- The decision sequence ranking tool (DSR) gives a hierarchical approach to problem definition and solving. The industrial case study shows that this method indeed can structure decision-making. The tool used the experience and knowledge of the members of the design team and it reflected their intuitions well.
- The system boundaries and closed cycles tool (SBDCC) focuses the design to the fixed input-output scheme. In this way the final design has closed system boundaries and closed cycles as defined in the design problem definition. The case study shows that all material cycles are indeed closed including the feedstock exploitation and the use of the final product.
- The chemical route selection tool (CRS) compares alternative processing routes based on exergy analysis. In this way, in a early stage of the design, routes can be compared and the route with the lowest exergy loss can be preferred. The use of the exergy theory in this stage of the design, during the generation of alternatives, is new. The case study shows that such an exergy calculation can be obtained in a reasonable time with reliable outcomes.
- The set of heuristic guidelines for process synthesis (GPS) gives the designer a tool for the use of exergy during the generation of alternatives stage. Although many authors describe the method of exergy analysis, it is not integrated in the synthesis of chemical process designs. The translation of exergetical insights in guidelines is a new way of integration of exergy and process design, which is developed during this thesis research. The case study shows that the use of guidelines improves the design in an exergetical way, but that the designer should be careful in applying the guidelines for separation design.
- The exergy analysis tool (EA) gives the possibility to compare different block schemes for the basis of design level on the degree of exergy loss. The exergy analysis tool in itself is not new. In this research however it is used specifically for the comparison of two system boundaries on which conclusions to support the incorporation of exergy insights early in the design phase.
- The sustainability ranking tool (SRT) and the accompanying case study shows that sustainable development can be made applicable at the processing system level in the early steps of the design framework by societal evaluation. Sustainability is translated into both qualitative and quantitative assessment criteria. It is assumed that the SRT method also can be applied to other system levels, which asks for other definitions of the criteria (economic, ecological, and societal). This can be done in a similar way as described, based on guiding principles and intensive discussions of what sustainability means in this case.

10.1.3 Hypothesis 3; useful for process and product design

A general design methodology, like proposed in hypothesis 1, together with the tools from hypothesis 2, is applicable for both chemical processes and chemical products.

- In Chapter 9, the validity of the methodology for product design is shown. It becomes clear that the framework, proposed in Chapter 4, holds for both the process design and product design. The general framework provides a methodology for detailing decision-making.
- The design methodology is tested in an industrial product development company and a specific design tool for the identification of needs during product development is made. This shows that the design methodology is relevant in current industrial practice. It is clear that chemical product development is focused on consumers needs and societal demands more than the process design.
- The evaluation of sustainable chemical products tool (ESC) is developed for projects in the idea identification design step. It provides guidance for the problem definition stage and it explicitly adds a sustainability value. The ESC is performed as a questionnaire. The ESC tool can be included in existing innovation management systems or the general design framework. The ESC tool is suitable and useful in an industrial context, especially for research projects that consider new product concepts.

10.1.4 The case studies

The use of case studies in this thesis is essential, for the following reasons: i) real design cases have many design variables that have to be considered, ii) a clear case focuses the design methodology, iii) illustrations pave the way towards chemical engineering practice.

The case studies show, firstly, that the design tools can improve the design of chemical plants and are able to incorporate sustainability into the design. Secondly, the case studies provide designs of chemical processes, which can be seen as examples of sustainable processes. Thirdly, the case studies validate generic design methods that can be applied to other design cases.

However, it is not the focal point of this thesis to provide totally new design tools for process development, but to provide a new design methodology that incorporates existing tools and stimulates the development of new tools.

10.2 Recommendations

Recommendations are given for further research and about the use of this thesis.

- Chapter 2 gives an overview of the societal sustainability debate. It is strongly recommended that in a similar way as described in this Chapter, companies or institutes take note of the contents of the debate and derive criteria from this knowledge.
- In Chapter 4, the framework of the design methodology is developed. During the research not all fields in this framework could be filled with new design methods. The framework of Chapter 4 provides a structured pathway for further research on sustainable development and chemical engineering

design, because the empty spaces give clear definition of the tools that have to be developed for the design of sustainable chemical processes. From Table 4.6 it becomes clear that at least for the following design steps design tools have to be developed: i) problem decomposition tools regarding to sustainable development, ii) structured problem definition tools for the more detailed process design steps, iii) evaluation tools for the more detailed process design steps.

- This thesis is a first exploration in the field of design methodology for chemical process and product design related to sustainable development. In this research the process design methodology is applied to chemical product design. In further research it is useful to consider the chemical process design and the chemical product design concurrently. For such a research, results from the fields of Design for Sustainability, Design for Environment or EcoDesign can be very useful.
- In this thesis many case studies illustrate the use of the various design tools. It would be very useful if the entire methodology could be applied to one case study. The design of a network of chemical processes for the production of synthetic sustainable fuels can be a very good choice, because a lot of expertise is available for that in the Delft University of Technology and because some of the case studies in this thesis consider already some parts and alternatives for the production of synthetic sustainable fuels.

Appendices

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Appendix A

BACKGROUND INFORMATION OF THE INDUSTRIAL PROJECT

In this appendix, some additional information is given on the industrial project, described in Chapter 5. This project was carried out in 2002 in cooperation with Shell Chemicals, Amsterdam. The detailed contents cannot be given in this thesis, because of confidentiality reasons. However, it is only important here how the various areas of the design project influence each other; they are represented in general terms.

A.1 Introduction to the industrial project

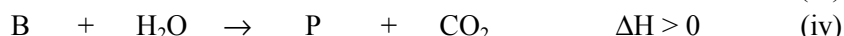
Nowadays, the chemical P is produced in a process in which the following reaction takes place:



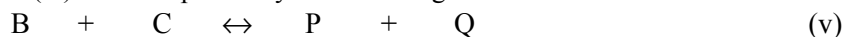
In absence of an excess of water, the following unwanted side reactions occur:



To prevent these side reactions, reaction (i) is carried out in an excess of water (~5%). Later this enormous amount of water has to be separated from the product stream. This process can be expensive, as this separation is energy consuming. However, if reaction (i) is not carried out in an excess of water, the side reactions do occur and hence the process does not only use its resources inefficiently but also loses product. It can be argued that both options of operating the process do not support the concept of sustainability. Using resources inefficiently and the use of enormous amounts of energy are highly affecting the carrying capacity of the earth and will increase costs unnecessarily. Another route to produce chemical P is defined by the following reactions:



This process uses less water and therefore less energy is needed to separate water from the product stream. Besides this, no side reactions occur; hence fewer by-products will be produced. An additional advantage of this production route is that reaction (iv) can be replaced by the following reaction:



By replacing reaction (iv) by reaction (v), the overall process can help in reducing CO₂ emissions, as CO₂ is converted to useful product.

A.2 Areas of influence and influence factors

The following areas of influence are distinguished in the project after interviews with all the team members and a group discussion about the results of those interviews (for all factors abbreviations are introduced):

Cat: Catalyst choice (homogeneous or heterogeneous)

Mat: Type of construction materials

PI: Level of process integration / energy integration

Feed: Choice of feed type (crude / pure)

CO₂: Choice of CO₂ partial pressure

pH: Level of pH

P/T: Process conditions (temperature / pressure)

Specs: Product specifications / Waste streams

Those various areas of influence can be defined into more detailed influence factors as given below.

Catalyst choice (homogeneous or heterogeneous) influence factors

- Homogeneous or heterogeneous
- Activity and selectivity
- Catalyst reduction
- Possible corrosive behavior
- Price
- Stable up to 150 °C
- Recycling issues (purge / bleed / make up)
- Possible combination of catalyst types

Type of construction materials influence factors

- up to 250 °C and $8 < \text{pH} < 12$, construction materials are available
- up to 250 °C and $\text{pH} < 7$, construction materials have to be tested
- Pressure levels in this case are no problem, regarding construction materials
- Possible formation of anionic compounds (decomposition of catalysts) and presence of H_2O have large influence on the choice of construction materials

Level of process integration / energy integration influence factors

- Energy reduction can be obtained by reduction of the waste water stream
- Minimal energy use from a sustainability point of view
- Best energy integration can be obtained at high temperature

Choice of feed type feed (crude / pure) influence factors

- Availability of the feedstock
- Prices (crude is cheap, pure is expensive)
- Composition and type of impurities in the crude feed
- pH level of the crude feed

Choice of CO_2 partial pressure influence factors

- The partial pressure of CO_2 determines largely the acidity of the flows
- The partial pressure of CO_2 influences the level of process integration

Level of pH influence factors

- $8 < \text{pH} < 12$ stable condition for construction materials
- for $\text{pH} > 12$ mechanical stress can occur
- Feed: $\text{pH} < 7$
- Partial pressure of CO_2 strongly determines pH level

Process conditions (temperature / pressure) influence factors

- Reactor size (large reactor $\Rightarrow$ low P; small reactor $\Rightarrow$ high P)
- Homogeneous catalyst reaction is exothermic; at $P \approx 50$ bar $\Rightarrow$ runaway
- Homogeneous catalyst is best operated at $T > 150$ °C
- Heterogeneous catalyst reaction is endothermic; preferred liquid phase is H_2O
- At $T < 100$ °C: HCO_3 , H_2CO_3 can be formed

Product specifications / waste streams influence factors

- Production of light ends
- Production of heavy ends < 10 %
- Waste water streams
- Production of CO₂
- Toxic levels of the waste streams
- At high temperature it is easier to remove impurities from the waste water stream

A.3 Network analysis of the industrial project

In the tables below (see from Table A.1 to Table A.8), the influence factors are discussed. In Table 5.4, the summary of the network analysis is given, and the active and passive totals are calculated together with the average.

TABLE A.1 CATALYST CHOICE (HOMOGENOUS OR HETEROGENOUS)

Catalyst choice (Cat) influences		
Mat	The type of catalyst influences the materials, as the homogeneous type of catalyst is corrosive, which affects the materials. However, it was mentioned that this only occurs in presence of water.	1
PI	The type of catalyst influences the energy / process integration. Although this influence is indirect, it is a very strong and important influence.	2
Feed	The type of catalyst has no influence on the type of feed used.	0
CO ₂	The type of catalyst could influence the partial pressure P _{CO₂} . However, nobody mentioned explicitly if this is a strong or weak influence.	1
pH	The type of catalyst could influence the pH by its composition.	1
P/T	The type of catalyst strongly influences the temperature of the first reaction.	2
Specs	The type of catalyst influences the waste; when a homogeneous catalyst is used it is quite well possible that it ends up in the waste stream.	2

TABLE A.2 TYPE OF CONSTRUCTION MATERIALS

Type of construction materials (Mat) influences		
Cat	The type of construction material influences the type of catalyst that can be used. Some construction materials cause difficulties with a homogeneous cat, but it is said that this is only in combination with water.	1
PI	The type of construction material influences the energy efficiency indirectly, as construction materials influences the temperature.	1
Feed	The type of materials weakly influences the type of feed as the crude feed contains acids. This is not a problem as pH stays in the range of $8 < \text{pH} < 12$	1
CO ₂	The type of material has no influence on the pressure	0
pH	The type of material strongly influences the choice of the pH	2
P/T	Construction materials weakly influence the temperature only in combination with acid.	1
Specs	The type of material has some influence on the waste; it determines if acids are allowed.	1

TABLE A.3 LEVEL OF PROCESS INTEGRATION / ENERGY INTEGRATION

Level of process integration / energy integration (PI) influences		
Cat	Energy integration indirectly influences the catalyst as it requires a specific T.	1
Mat	Energy integration indirectly influences the materials, because of T.	1
Feed	Process integration has no influence on the feed choice.	0
CO ₂	A low partial pressure of CO ₂ is better, regarding process integration.	1
pH	Energy integration has no influence on the pH.	0
P/T	Process integration has direct influence on the T as it requires $T > 150^{\circ}\text{C}$	2
Specs	Process integration has no influence on waste.	0

TABLE A.4 CHOICE OF FEED TYPE

Choice of feed type (Feed) influences		
Cat	The type of feed has no influence on catalyst	0
Mat	The type of feed weakly influences the materials because the crude feed contains acid. However with $8 < \text{pH} < 12$ no problems occur.	1
PI	The type of feed will not influence energy	0
CO ₂	Type of feed will not influence the P_{CO_2}	0
pH	Type of feed weakly influences pH as it contains acid. However, no specs of feed were available.	1
P/T	The type of feed has no influence on the T.	0
Specs	Type of feed strongly influences the waste.	2

TABLE A.5 CHOICE OF CO₂ PARTIAL PRESSURE

Choice of CO₂ partial pressure (CO₂) influences		
Cat	The choice for a P _{CO2} fixes more or less the choice for a catalyst type	1
Mat	P _{CO2} has no impact on materials.	0
PI	P _{CO2} strongly influences the energy integration	2
Feed	P _{CO2} has no influence on the choice of the feed composition	0
pH	P _{CO2} strongly influences the pH	2
P/T	P _{CO2} has no influence on the T	0
Specs	P _{CO2} has no influence on the waste	0

TABLE A.6 LEVEL OF PH

Level of pH (pH) influences		
Cat	pH has no influence on the catalyst	0
Mat	The pH strongly influences the construction materials (E)	2
PI	The pH has no effect on the energy	0
Feed	pH has no influence on the feed	0
CO2	pH has weakly influence on P _{CO2}	1
P/T	pH has no influence on the temperature	0
Specs	pH has weakly influence on the waste (acid in waste)	1

TABLE A.7 PROCESS CONDITIONS

Process conditions (P/T) influences		
Cat	Temperature strongly influences catalyst because of stability.	2
Mat	Temperature directly influences the construction materials.	2
PI	Temperature has a direct influence on the possibility for energy integration.	2
Feed	The temperature has no influence on the feed.	0
CO2	The temperature has no influence on the P _{CO2} .	0
pH	The temperature has no influence on the pH.	0
Specs	Temperature has a weak influence on the waste as a T > 180°C facilitates the removal of impurities.	1

TABLE A.8 PRODUCT SPECIFICATIONS / WASTE STREAMS

Product specifications / Waste streams (Specs) influences		
Cat	No homogeneous cat is allowed in waste, but it is not sure that cat will be in waste.	1
Mat	No influence on the choice of construction materials.	0
PI	The type of waste influences in some way the level of process integration.	1
Feed	If the product specifications and the composition of the waste streams are fixed, then little freedom is left for the choice of the feed type.	2
CO ₂	No influence on the CO ₂ partial pressure.	0
pH	The product specifications determine to a certain extent which pH is allowed.	1
P/T	Waste streams can be treated better at higher temperature	1

TABLE A.9 SUMMARY OF THE NETWORK ANALYSIS

	Cat	Mat	PI	Feed	CO ₂	pH	P/T	Specs	Act.
Cat		1	2	0	1	1	2	2	9
Mat	1		1	1	0	2	1	1	7
PI	1	1		0	1	0	2	0	5
Feed	0	1	0		0	1	0	2	4
CO ₂	1	0	2	0		2	0	0	5
pH	0	2	0	0	1		0	1	4
P/T	2	2	2	0	0	0		1	7
Specs	1	0	1	2	0	1	1		6
Pass.	6	7	8	3	3	7	6	7	5,9

Appendix B

BACKGROUND INFORMATION ON THE EXERGY CONCEPT

In this Appendix some background information is given on the exergy concept. The theory presented here is focused on the calculation of exergy as is needed in the tools of Chapter 6 and 7 (CRS, GPS and EA). This overview is not meant as a comprehensive introduction to exergy analysis.

B.1 Introduction to the concept of exergy

In order to quantify the quality of energy or work potential, the concept of exergy was already introduced by Rant in 1956. Szargut defines exergy as follows (Szargut, Morris, and Steward 1988):

The exergy of a material stream is the maximum obtainable amount of shaft work when this stream is brought from actual conditions (P, T) to thermo mechanical and chemical equilibrium at ambient conditions (P_0, T_0) by reversible processes with heat only being exchanged with the environment at T_0 .

The first law of thermodynamics deals with the *quantity* of energy and asserts that energy cannot be created or destroyed. The mathematical formulation of this law is known by every chemical engineer (disregarding kinetic and potential energy):

$$\Delta U = Q - W \quad \text{Equation B.1}$$

In words, this equation states that the total energy change of the system is equal to the heat added to the system minus the work done by the system. This equation applies to the changes, which occur in a constant-mass system over a period of time. Engineers use this first law as merely a bookkeeping tool. The second law of thermodynamics, however, provides insight in the *quality* of energy or *work potential* (shaft work, electricity). More specifically, it is concerned with the degradation of energy during a process. The abstract formulation of this law is less known by engineers and even less applied:

$$\Delta S_{total} = \Delta S_{system} + \Delta S_{surroundings} \geq 0 \quad \text{Equation B.2}$$

In words, this equation states that every process proceeds in such a direction that the total entropy change associated with it is positive: the more entropy is generated the lower the quality of energy becomes or the less work it can do. A process is called *reversible* in the limiting case of zero entropy production. However, this is not possible in reality and each process therefore exhibits a certain extent of *irreversibility*. The difference between the theoretical amount of work required or done in the reversible case and the actual amount of work (reality) is called *lost work*. The relation between this lost work (W_{lost}) and the entropy change is given by the Gouy-Stodola relation, in which T_0 is the temperature of the environment:

$$W_{lost} = T_0 \cdot \Delta S_{total} \quad \text{Equation B.3}$$

The equations discussed above are also known as *engineering* or *classical thermodynamics*, as they describe steady state processes from a macroscopic perspective. They are therefore very useful for engineers who typically work with this kind of processes. Unfortunately, the engineering thermodynamics do not provide insight in the origins of irreversibility, as this is the domain of *irreversible thermodynamics*. The main objective of this science is to quantitatively describe interacting transport processes from a microscopic perspective. More specifically, irreversible thermodynamics deals with non-equilibrium situations, i.e. transport of heat and material under the influence of driving forces. If sufficiently close to equilibrium, the entropy production can be described as follows:

$$\Delta S_{total} = \sum_i^n J_i \cdot X_i \quad \text{Equation B.4}$$

In which J_i is the rate at which the process proceeds, e.g. heat flow rate, reaction rate and the like, and X_i is the associated driving force. With this in mind, one can combine the engineering and irreversible thermodynamics to understand the relation between lost work and driving forces:

$$W_{lost} = T_0 \cdot \sum_i^n J_i \cdot X_i \quad \text{Equation B.5}$$

Since the rate J_i typically is proportional to the driving force (e.g. Fourier's law), this relation makes clear that large driving forces lead to fast process with large losses. Accordingly, the challenge is to minimize the driving forces while still achieving reasonable rates.

The exergy concept is little used in industry, because it is based on the second law of thermodynamics, which is rather abstract and difficult to apply. The concept, however, has two important benefits in process synthesis and analysis:

- It provides fundamental insight in the **quality of energy** whereas the first law of thermodynamics only identifies the quantity of energy, i.e. in an energy balance. For example, it is a difference if a process requires 1 MW of low-pressure steam or 1 MW of fuel.
- The exergy concept is **generally applicable** for all material and energy streams whereas other measures of energy can only be used for a specific category of materials, e.g. the Lower Heating Value (LHV) in the case of combustible materials.

The first benefit provides insight in the exergetic performance of processes, which is a basis for possible improvements. The second benefit facilitates the comparison between processes with different types of energy and material streams.

B.2 Performance of an exergy analysis

Calculation of exergy

The exergy of a certain amount of substance in an open system can be formulated as follows, disregarding the kinetic and potential exergy terms:

$$Ex = (H - H_0) - T_0 \cdot (S - S_0) \quad \text{Equation B.6}$$

In which the subscript 0 refers to the conditions of the reference environment defined by Szargut (Szargut, Morris, and Steward 1988). According to this equation, the exergy of a heat stream Q at constant temperature T is described by:

$$Ex = \left(1 - \frac{T_0}{T}\right) \cdot Q \quad \text{Equation B.7}$$

The term between parentheses is also known as the Carnot Factor. The exergy of material streams can be divided in three components, i.e. physical, chemical and mixing exergy, according to:

$$Ex_{total} = Ex_{physical} + Ex_{chemical} + \Delta_{mix} Ex \quad \text{Equation B.8}$$

In order to determine the chemical exergy of a pure component, the composition of the reference environment must be defined. Szargut (Szargut, Morris, and Steward 1988) selected a reference substance for each element that is abundantly present in the air, oceans, etc. These reference substances are given an exergy value of zero. The chemical component of the pure reference substance is equal to the maximum amount of work that can be obtained by diffusing it to reference concentration P_{ref} . Since the process is isenthalpic, the following equation follows from Equation A.1 and the ideal gas law:

$$Ex_{chem,ref}^0 = RT_0 \cdot \ln \frac{P_0}{P_{ref}} \quad \text{Equation B.9}$$

When a substance does not exist in the reference environment it must first be converted to reference substances through chemical reaction. The associated decrease in chemical exergy equals the standard Gibbs energy of reaction. Szargut (Szargut, Morris, and Steward 1988) determined the exergy values of all elements, which can be used to calculate the chemical exergy of other substances:

$$Ex_{chem}^0 = \Delta_f G^0 - \sum_j^n n_j \cdot Ex_{chem,j} \quad \text{Equation B.10}$$

In which $\Delta_f G^0$ is the standard Gibbs energy of formation and v_j is the stoichiometric coefficient of the element j in the formation reaction. The $\Delta_f G^0(l/v)$ should be used in accordance with the phase of the component at reference conditions. Appendix 0 shows the chemical exergy values of all substances that occur in this work. The chemical exergy of a mixture is then calculated as follows:

$$Ex_{chem}^0 = L^0 \sum_i^n x_i^0 \cdot Ex_{chem,i}^{0l} + V^0 \sum_i^n y_i^0 \cdot Ex_{chem,i}^{0v} \quad \text{Equation B.11}$$

In which L^0 and V^0 are the liquid and vapour fraction at reference conditions. The corresponding values of the chemical exergy should correspond with the phase of the components. The physical exergy equals the amount of work that can be obtained if the stream is brought to reference conditions. If the stream contains condensable substances, the physical exergy is calculated according to:

$$Ex_{phys} = \Delta_{actual \rightarrow 0} \left[L \left(\sum_i^n x_i \cdot H_i^L - T_0 \sum_i^n x_i \cdot S_i^L \right) + V \left(\sum_i^n y_i \cdot H_i^V - T_0 \sum_i^n y_i \cdot S_i^V \right) \right]$$

Equation B.12

In which L and V are the mole fractions of liquid and vapor at stream conditions, respectively. Finally, the exergy contribution associated with mixing of pure species is calculated according to:

$$Ex_{mix} = \Delta_{mix} H - T_0 \cdot \Delta_{mix} S \quad \text{Equation B.13}$$

The physical and mixing components are usually combined, as flow sheeting simulators provide values for the overall enthalpy and entropy.

The following procedure for calculating the exergy values of material streams was used in this work:

- Collect or estimate data. The Gibbs energy of formation should be collected first. If not available, select an appropriate estimation method for each component.
- Calculate the chemical exergy of all components.
- Calculate the chemical exergy of the streams.
- Calculate physical and mixing exergy by:

$$\begin{aligned}
 Ex_{physical+mix} &= \left(H_{actual} - \sum x_i H_i^0 \right) - T_0 \left(S_{actual} - \sum x_i S_i^0 \right) \\
 &= Avail - \sum x_i G_i^0
 \end{aligned}$$

Equation B.14

(Avail is a function in Aspen Plus that calculates $H-T_0S$)

- Calculate total exergy value by adding both terms.

In this thesis, the chemical exergy of the liquid phase was taken if the component is liquid at reference conditions. This implies that this component completely condenses when the stream is brought to reference conditions while it could be present in the vapor phase. However, the error made is then small (<1%).

Thermodynamic properties of substances

		Phase	Mw (g/mol)	Source DHF/DGF	Source Exergy	DHF (kJ/mol)	DGF (kJ/mol)	LHV (kJ/mol)	LHV (GJ/ton)	Exergy (kJ/mol)	Exergy (GJ/ton)
C	Carbon (graphite)	s	12,0	I	I	0,0	0,0	393,5	32,8	410,3	34,2
H	Hydrogen	g	1,0	I	I	0,0	0,0	-	-	117,0	116,1
O	Oxygen	g	16,0	II	II	0,0	0,0	-	-	2,0	0,1
S	Sulfur (rhombic)	s	32,1	II	II	0,0	0,0	296,8	9,3	609,6	19,0
Ca	Calcium	s	40,1	II	II	0,0	0,0	-	-	712,4	17,8
CaCO3	Calciumcarbonate	s	100,1	III	I	-1207,6	-1129,1	-	-	-0,4	0,0
CaO	Calciumoxide (lime)	s	56,1	III	I	-634,9	-603,3	-	-	111,1	2,0
CaH2O2	Calciumhydroxide	s	74,1	III	I	-985,2	-897,5	-	-	52,9	0,7
CaSO4	Calciumsulphate	s	136,2	III	I	-1434,5	-1322,0	-	-	7,9	0,1
CH4	Methane	g	16,0	III	I	-74,6	-50,5	802,5	50,0	827,9	51,6
CH4O	Methanol	g	32,0	III	I	-201,0	-162,3	676,1	21,1	718,1	22,4
	(Tb=338 K)	l	32,0	III	I	-239,2	-166,6	637,9	19,9	713,8	22,3
C2H6	Ethane	g	30,1	III	I	-84,0	-32,0	1428,4	47,5	1490,8	49,6
C3H6	Propylene	g	42,1	VI	I	20,4	60,7	1926,3	45,8	1993,8	47,4
C3H8	Propane	g	44,1	III	I	-103,8	-23,4	2043,9	46,4	2143,7	48,6
C3H6O	Propylene oxide (PO)	g	58,1	VI	I	-92,8	-25,8	1813,1	31,2	1909,3	32,9
C3H6O3	Lactic acid (LA)	g	90,1	VI	I	-621,0	-516,0	1284,9	14,3	1423,0	15,8
	(Tb=447 K, DHV(Tb)=58,2 kJ/mol)	l	90,1	VI	I	-695,2	-540,7	1210,7	13,4	1398,3	15,5
C3H6O3	Dimethylcarbonate (DMC)	g	90,1	VII	I	-570,1	-455,5	1335,8	14,8	1483,5	16,5
	(Tb=363 K, DHV(Tb)=34,4 kJ/mol)	l	90,1	VII	I	-608,1	-459,2	1297,8	14,4	1479,8	16,4
C3H8O2	Propyleneglycol (MPG)	g	76,1	VI	I	-421,5	-304,5	1726,2	22,7	1866,6	24,5
	(Tb=461 K, DHV(Tb)=54,5 kJ/mol)	l	76,1	VI	I	-488,2	-328,1	1659,5	21,8	1843,0	24,2
C4H6O3	Propylene carbonate (PC)	g	102,1	VII	I	-582,5	-455,5	1716,9	16,8	1893,9	18,6
	(Tb=515 K, DHV(Tb)=51,8 kJ/mol)	l	102,1	VII	I	-647,2	-482,8	1652,2	16,2	1866,6	18,3
C6H10O5	Cellulose	s	162,1		I			2611,0	16,1	3018,7	18,6
C6H12O6	Glucose (a-D-galactose)	s	180,2		II			2529,6	14,0	2928,8	16,3
C6H14O3	Dipropyleneglycol (DPG)	g	134,2	VI	I	-628,0	-406,0	3425,6	25,5	3700,1	27,6
	(Tb=505 K, DHV(Tb)=62,2 kJ/mol)	l	134,2	VI	I	-718,5	-443,1	3335,1	24,9	3663,0	27,3
C8H8	Styrene	g	104,1	VI	I	147,4	213,8	4262,6	40,9	4432,6	42,6
	(Tb=418 K, DHV(Tb)=46,3 kJ/mol)	l	104,1	VI	I	101,1	200,5	4216,3	40,5	4419,3	42,4
C8H10	Ethylbenzene	g	106,2	VI	I	29,8	130,6	4386,8	41,3	4583,4	43,2
	(Tb=409 K, DHV(Tb)=42,4 kJ/mol)	l	106,2	VI	I	-12,6	119,1	4344,4	40,9	4571,9	43,1
C8H10O	a-phenylethanol	g	122,2	IV	I		-2,8			4452,0	36,4
C8H10O2	Ethylbenzeneperoxide	g	138,2	IV	I		-79,4			4377,4	31,7
C12H22O11	Sugar (saccharose)	s	342,3		II			5166,2	15,1	6007,8	17,6
CO	Carbon monoxide	g	28,0	III	I	-110,5	-137,2	283,0	10,1	275,1	9,8
CO2	Carbon dioxide	g	44,0	III	II	-393,5	-394,4	-	-	19,9	0,5
H2	Hydrogen	g	2,0	III	I	0,0	0,0	241,8	119,9	234,0	116,1
H2O	Water	g	18,0	III	II	-241,8	-228,6	-	-	9,5	0,5
		l	18,0	III	II	-285,8	-237,1	-	-	0,9	0,0
H2S	Hydrogensulphide	g	34,1	III	I	-20,6	-33,4	518,0	15,2	810,2	23,8
H2SO4	Sulfuric acid	l	98,1	III	I	-814,0	-690,0	-	-	161,6	1,6
SO2	Sulfurdioxide	g	64,1	III	I	-296,8	-300,1	98,9	1,5	313,5	4,9
SO3	Sulfurtrioxide	g	80,1	III	I	-395,7	-371,1	-	-	244,5	3,1
O2	Oxygen	g	32,0	III	I	0,0	0,0	-	-	4,0	0,1
N2	Nitrogen	g	14,0	III	II	0,0	0,0	-	-	0,7	0,1
Wood	Poplar (C4.2H5.9O2.6)	s	100,0	III	V	-566,0	-473,1	1800,0	18,0	1945,8	19,5

Source:

- | | | |
|-----|---|------------------------|
| I | Calculated | |
| II | Szargut (1988) | |
| III | Handbook of Chemistry and Physics | |
| IV | Estimated by method of Van Crevelen and Chermin (1977) | |
| V | Estimated by B-value of Szargut (1988) (see Appendix E) | |
| VI | Chemical Properties Handbook | } DGF(I) estimated by: |
| VII | Aspen Plus | |
- $$\Delta_f G^{0l} \approx \Delta_f G^{0v} - \Delta_{vap} H^0 \left(1 - \frac{T_0}{T_b} \right) \quad \text{if } \Delta_{vap} H^{T_b} / \Delta_{vap} S^{T_b} \gg \Delta_{T_b \rightarrow T_0} H / \Delta_{T_b \rightarrow T_0} S$$

Appendix C

BACKGROUND INFORMATION MONOPROPELENEGLYCOL CASE

This appendix contains information about an industrial MonoPropeleneGlycol (MPG) case, used as illustration for the CRS case study in Chapter 6. All relevant information is found in literature.

C.1 Assumptions to the MPG case

CO₂ emission

CO₂ emissions formed in chemical reactions, as in the fermentation of lactic acid, are calculated through mass balances. Energy-related emissions are calculated as follows:

$$CO_2 \text{ emission} = e \cdot \Delta H \quad \text{Equation C.1}$$

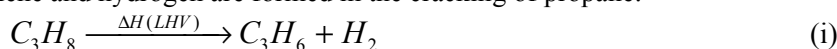
In which e is the emission factor of the fuel used, i.e. ton CO₂/GJ fuel. ΔH represents the amount of energy that is required or used (on LHV basis). The emission factors for natural gas, oil, and coal are taken as 0.055, 0.067 and 0.093, respectively.

Extraction and refining

The amount of crude oil in GJ(LHV) that is required for propane production is calculated through employing and overall efficiency of oil production and refining. The efficiency of oil products amounts to 88% from well to gate.

Thermal cracking of propane

Propylene and hydrogen are formed in the cracking of propane:



This reaction requires 124 kJ/mol (LHV), which is provided through combustion of natural gas. The thermal efficiency of the corresponding furnace is assumed to be 32%:

$$h_{furnace} = \frac{\Delta_{combustion} H^0(LHV)}{\Delta_{cracking} H^0(LHV)} \quad \text{Equation C.2}$$

The selectivity of the cracking reaction is irrelevant when applying this method; the by-products that are formed are considered useful and are allocated the corresponding propane.

Peroxide process

The co-production of styrene and PO consist of three basic steps:

- Oxidation of ethyl benzene (EB) to ethyl benzene peroxide (EBPox).
- Reaction of EBPox with propylene to PO and α -phenyl ethanol (APE).
- Dehydration of APE to styrene.

The process is modeled with the yields of step 1 and step 2, which are 90% and 95% (in propylene), respectively (Kirk and Othmer 1998). The amount of exergy that is transferred to APE is accounted to styrene production:

$$Ex_{to\ styrene} = Ex_{APE} - Ex_{EBPox} \quad \text{Equation C.3}$$

$$Ex_{lost} = (Ex_{Propylene} - Ex_{PO}) - Ex_{to\ styrene} \quad \text{Equation C.4}$$

Biomass production

The following data are used for the production of wood, sugar cane and beets, see Table C.1, Table C.2 (Ullman 2000) and Table C.3 (Kuesters and Lammel 1999).

TABLE C.1 COMPOSITION OF SUGAR CANE AND BEETS

Component	Sugar cane (%)	Sugar beet (%)
Sucrose (C ₁₁ H ₂₂ O ₁₁)	11	17
Cellulose (C ₆ H ₁₀ O ₅)	14	3
Other (water, proteins, etc.)	75	80

TABLE C.2 BIOMASS GROWTH

Type	Yield (ton/ha/yr)	CO ₂ fixation ¹ (ton/tonds)	CO ₂ fixation ¹ (ton/ton)	NR-input (GJ/ton)
Sugar beet	11	1.58	0.32	0.95
Sugar cane	14	1.62	0.40	0.09
Wood (poplar)	75	1.85	1.48	0.15

¹) Calculated from composition.

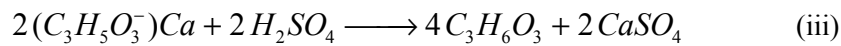
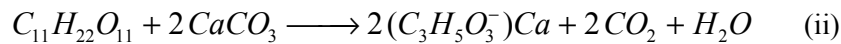
TABLE C.3 NON-RENEWABLE INPUT OF BIOMASS GROWTH

Component	Input ¹
Fuel (harvesting, preparation, etc.)	5.3 GJ/ha
Nutrients (fertilisers, pesticides)	8.0 GJ/ha
Transport (25 km)	0.017 HJ/ton

¹) CO₂ emission factor of oil.

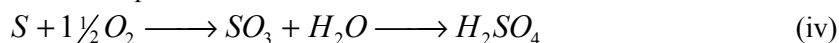
Fermentation of sugar to LA

The fermentation of sugar to lactic acid proceeds according to the following reactions with a yield of 90% in sugar (Kirk and Othmer 1998).



Sulphuric acid production

Sulphur is a waste from refineries and natural gas production (desulphurisation) and is converted to sulphuric acid as follows:



Hydrogen production

Hydrogen can be produced from natural gas, wood and fibers (cellulose) through Catalytic Partial Oxidation (CPO) and gasification, respectively. The hydrogen is produced from synthesis gas by using the water gas shift reaction (the corresponding data are shown in Table):



TABLE C.4 PRODUCTION OF HYDROGEN FROM WOOD AND NATURAL GAS

	Wood (gasification)	Cellulose (gasification)	Natural gas (CPO)
yield H_2 (ton/ton feedstock)	0.12	0.12 ¹	0.33
CO_2 emission (ton/ton H_2)	15.4	13.6	7.6
CO_2 emission (ton/ton feedstock)	1.85	1.63	2.51

¹) Same hydrogen yield as wood.

The hydrogen content of cellulose is higher than that of wood, but the gasification process is complex and not stoichiometric. Therefore the same yield as wood is assumed. The CO_2 emission, however, is calculated on the basis of the molecular formula ($C_6H_{10}O_5$).

Methanol production

Methanol is produced from natural gas via conventional steam reforming, data are taken from the synthesis case: 42.3 $GJ_{\text{exergy}}NG/\text{tonMeOH}$ and 0.86 $\text{tonCO}_2/\text{tonMeOH}$, including natural gas extraction with an efficiency of 92%.

Other assumptions

MPG is transported per ship from Brazil to Europe (chain 3) over 6000 km with an energy use of 0.3198 $MJ(\text{energy})/\text{tonkm}$. This results in 2.0 $GJ(\text{exergy})/\text{tonMPG}$ (Kuesters and Lammel 1999).

Lower Heating Values are converted to exergy by using the β -value (Szargut, Morris, and Steward 1988). Crude oil has a β -value of 1.07 and natural gas 1.05. For streams that have unknown exergy values, an β -value is used of 1.05, e.g. pesticides, energy for transport, etc. The corresponding CO_2 emission factors were assumed to be equal to that of oil (0.067 ton/GJ).

C.2 Data on supply chain 1

Extraction and refining				
	IN	OUT	IN	OUT
	Mass (ton/ton)		Exergy (GJ/ton)	
Crude oil (LHV)	38,56		41,25	
Propane		0,73		35,59
Carbon dioxide		0,31		0,00
Exergy loss				5,67
Total			41,25	41,25

Thermal cracking				
	IN	OUT	IN	OUT
	Mass (ton/ton)		Exergy (GJ/ton)	
Propane	0,73		35,59	
Fuel (LHV)	6,54		6,87	
Propylene		0,70		33,10
Carbon dioxide		0,36		0,00
Hydrogen		0,03		3,88
Exergy loss				5,47
Total			42,45	42,45
All. Factor	Propylene	0,89		
	Hydrogen	0,11		

Peroxide process				
	IN	OUT	IN	OUT
	Mass (ton/ton)		Exergy (GJ/ton)	
Propylene	0,70		33,10	
Ethylbenzeneperox.	2,18		69,07	
PO		0,84		30,11
a-phenylethanol		1,93		70,12
Waste		0,11		
Exergy loss				1,93
Total	2,88	2,88	102,16	102,16
To styrene	1,06			
All. Factor	PO	0,97		
	Styrene	0,03		

MPG production				
	IN	OUT	IN	OUT
	Mass (ton/ton)		Exergy (GJ/ton)	
PO	0,92		30,11	
Water	0,26		0,00	
DPG		0,18		4,81
MPG		1,00		24,22
Exergy loss				1,08
Total	1,18	1,18	30,11	30,11
All. Factor	MPG	0,83		
	DPG	0,17		

Exergy losses				
	Cum. AF	Overall	All. MPG	
Extraction and refining	0,72	5,67	4,09	
Thermal cracking	0,72	5,47	3,95	
Peroxide process	0,81	1,93	1,56	
MPG production	0,83	1,08	0,90	
Total		14,15	10,49	

Overall exergy balance				
	IN	OUT	Allto MPG	
	Exergy (GJ/ton)			
Crude oil	41,25		29,76	
Fuel (NG)	6,87		4,95	
MPG		24,22		
DPG		4,81		
Hydrogen		3,88		
To styrene		1,06		
Lost		14,15		
Total	48,12	48,12		
Carbon dioxide		0,67	0,48	

C.3 Data on supply chain 2

Extraction and refining				
	IN	OUT	IN	OUT
	Mass (ton/ton)		Exergy (GJ/ton)	
Crude oil	32,13		34,38	
Propane		0,61		29,65
Carbon dioxide		0,26		0,00
Exergy loss				4,72
Total			34,38	34,38

Thermal cracking				
	IN	OUT	IN	OUT
	Mass (ton/ton)		Exergy (GJ/ton)	
Propane	0,61		29,65	
Fuel	5,45		5,72	
Propylene		0,58		27,58
Carbon dioxide		0,30		0,00
Hydrogen		0,03		3,24
Exergy loss				4,56
Total			35,38	35,38
All. Factor	Propylene	0,89		
	Hydrogen	0,11		

Peroxide process				
	IN	OUT	IN	OUT
	Mass (ton/ton)		Exergy (GJ/ton)	
Propylene	0,58		27,58	
Ethylbenzeneperox.	1,82		57,56	
PO		0,70		25,09
a-phenylethanol		1,61		58,44
Waste		0,09		0,00
Exergy loss				1,61
Total	2,40	2,40	85,14	85,14
To styrene	0,88			
All. Factor	PO	0,97		
	Styrene	0,03		

MPG production				
	IN	OUT	IN	OUT
	Mass (ton/ton)		Exergy (GJ/ton)	
PO	0,76		25,09	
Water	0,24		0,00	
MPG		1,00		24,22
Exergy loss				0,87
Total	1,00	1,00	25,09	25,09
All. Factor	MPG	1,00		

Exergy losses				
		Cum. AF	Overall	All. MPG
Extraction and refining		0,86	4,72	4,08
Thermal cracking		0,86	4,56	3,94
Peroxide process		0,97	1,61	1,56
MPG production		1,00	0,87	0,87
Total			11,76	10,45

Overall exergy balance			
	IN	OUT	MPG
	Exergy (GJ/ton)		
Crude oil	34,38		29,72
Fuel (NG)	5,72		4,95
MPG		24,22	
Hydrogen		3,24	
To styrene		0,88	
Lost		11,76	
Total	40,10	40,10	
Carbon dioxide		0,56	0,48

C.4 Data on supply chain 3

The data of ‘Extraction and refining’, ‘Thermal cracking’ and ‘Peroxide process’ are the same as in supply chain 2.

MPG production				
	IN	OUT	IN	OUT
	Mass (ton/ton)		Exergy (GJ/ton)	
PO	0,76		25,09	
Carbon dioxide	0,58		0,00	
Methanol	0,84		18,76	
MPG		1,00		24,22
DMC		1,18		19,45
Exergy loss				0,18
Total			43,85	43,85

Overall exergy balance				
	IN	OUT	MPG	DMC
	Exergy (GJ/ton)		Exergy (GJ/ton)	
Crude oil	34,38		29,72	
Fuel (NG)	5,72		4,95	
Natural gas	35,58			35,58
MPG		24,22		
DMC		19,45		
Hydrogen		3,24		
To styrene		0,88		
Lost		27,90		
Total	75,69	75,69		
Carbon dioxide		0,70	0,48	0,22

Extraction and methanol production				
	IN	OUT	IN	OUT
	Mass (ton/ton)		Exergy (GJ/ton)	
Natural gas (LHV)	33,89		35,58	
Methanol		0,84		18,76
Carbon dioxide		0,72		0,00
Exergy loss				16,82
Total			35,58	35,58

Exergy losses				
	Overall	All. MPG	All. DMC	
Extraction and refining	4,72	4,08		
Thermal cracking	4,56	3,94		
Peroxide process	1,61	1,56		
MPG production	0,18	0,87		-0,69
Extraction and MECH prod.	16,82			16,82
Total	27,90	10,45	16,14	

C.5 Data on supply chain 4

Biomass growth				
	IN	OUT	IN	OUT
	Mass (ton/ton)		Exergy (GJ/ton)	
NR-input	1,08		1,13	
Sugar cane		12,62		57,27
Carbon dioxide		0,18		0,00
Allocation to fibers		0,57		
Allocation to Sugar		0,43		

Gasification				
	IN	OUT	IN	OUT
	Mass (ton/ton)		Exergy (GJ/ton)	
Fibers	1,77		32,90	
Hydrogen		0,21		24,62
Carbon dioxide		2,88		0,00
Exergy loss				8,28
Total			32,90	32,90

Fermentation				
	IN	OUT	IN	OUT
	Mass (ton/ton)		Exergy (GJ/ton)	
Sugar	1,39		24,37	
CaCO ₃	0,99		0,00	
Sulfur (H ₂ SO ₄)	0,23		4,45	
Lactic acid		1,32		20,42
Carbon dioxide		0,44		0,00
Waste (incl. CaSO ₄)		0,86		0,00
Exergy loss				8,40
Total	2,62	2,62	28,82	28,82

MPG production				
	IN	OUT	IN	OUT
	Mass (ton/ton)		Exergy (GJ/ton)	
Lactic acid	1,32		20,42	
Hydrogen	0,06		6,85	
MPG		1,00		24,22
Waste		0,37		0,00
Exergy loss				3,05
Total	1,37	1,37	27,27	27,27

Exergy losses				
	Cum. AF	Overall	All. MPG	
Biomass growth (NR)	0,59	1,13	0,66	
Gasification	0,28	8,28	2,30	
Fermentation	1,00	8,40	8,40	
MPG production	1,00	3,05	3,05	
Transport fuel	1,00	2,00	2,00	
Total		22,86	16,41	

Overall exergy balance				
	IN	OUT	MPG	H ₂
	Exergy (GJ/ton)			
NR-input	1,13		0,66	0,47
Solar (in sugar cane)	57,27		33,52	23,75
Sulfur	4,45		4,45	
Transport	2,00		2,00	
MPG		24,22		
Hydrogen		17,77		
Lost		22,86		
Total	64,85	64,85	40,63	
Carbon dioxide		3,63	1,34	2,29
Fixation		5,10	2,98	2,11
Net emission		-1,47	-1,64	0,17

C.6 Data on supply chain 5

The data of ‘Fermentation’, ‘Sulphuric acid production’ and ‘MPG production’ are the same as in supply chain 4.

Biomass growth			
	IN	OUT	
	Mass (ton/ton)		Exergy (GJ/ton)
NR-input	1,41		1,48
Sugar beets		8,41	29,54
Wood		0,21	
Carbon dioxide		0,10	0,00

Exergy losses	
	Overall
Biomass growth (NR)	1,48
Gasification	1,66
Fermentation	8,40
MPG production	3,05
Total	14,59

Gasification			
	IN	OUT	
	Mass (ton/ton)		Exergy (GJ/ton)
Fibers	0,28		5,17
Wood (moist)	0,21		3,34
Hydrogen		0,06	6,85
Carbon dioxide		0,87	0,00
Exergy loss			1,66
Total			8,51

Overall exergy balance	
	IN
	OUT
	Exergy (GJ/ton)
NR-input	1,48
Solar (in beet and wood)	32,87
Sulfur	4,45
MPG	24,22
Total	38,81
Carbon dioxide	1,41
Fixation	2,97
Net emission	-1,56

C.7 Data on supply chain 6

The data of ‘Fermentation’, ‘Sulphuric acid production’ and ‘MPG production’ are the same as in supply chain 4.

Hydrogen production (CPO)			
	IN	OUT	
	Mass (ton/ton)		Exergy (GJ/ton)
Natural gas	0,19		9,99
Hydrogen		0,03	2,98
Carbon dioxide		0,20	0,00
Exergy loss			7,01
Total			9,99

Exergy losses	
	Overall
CPO	7,01
Biomass growth (NR)	1,48
Gasification	1,30
Fermentation	8,40
MPG production	3,05
Total	14,23

Gasification			
	IN	OUT	
	Mass (ton/ton)		Exergy (GJ/ton)
Fibers	0,28		5,17
Hydrogen		0,03	3,87
Carbon dioxide		0,48	0,00
Exergy loss			1,30
Total			5,17

Overall exergy balance	
	IN
	OUT
	Exergy (GJ/ton)
NR-input	1,48
Solar (in sugar beet)	32,87
Sulfur	4,45
NG	9,99
MPG	24,22
Total	48,80
Carbon dioxide	1,65
Fixation	2,66
Net emission	-1,01

Appendix D

BACKGROUND INFORMATION METHANOL CASE

This appendix contains information about the Methanol case, used as illustration for the GPS case study in Chapter 6. All relevant information is found in literature.

D.1 Assumptions to the methanol case

The RK-Soave equation of state was used for all simulations with interaction parameters taken from the Aspen Plus databank. For steam properties, the steam tables are applied.

Modelling of the reactors:

- The reaction of the reactor feed was assumed to be 80 bars and 70 °C.
- The Lürgi tubular reactor was modelled as one equilibrium reactor with specified temperature (265 °C). The pressure drop was taken as 1.0 bar, the feed was preheated to reaction conditions.
- The ICI tube-cooled reactor was modelled as one equilibrium reactor with zero heat duty (adiabatic). The pressure drop was taken as 1.0 bar, the feed was preheated to 135 °C.
- The ICI quench reactor was modelled as four adiabatic reactors (as ICI tube-cooled) with fresh feed between each reactor. The feed distribution was calculated in Aspen by a design specification on the feed temperature to each bed. The pressure drop was taken as 0.5 bars per reactor, the feed was preheated to 200 °C.
- The Kellogg spherical reactors were modelled as four adiabatic reactors (as ICI tube-cooled) with intermediate heaters with specified temperature. The pressure drop was taken as 0.5 bars per reactor, the feed was preheated to 200 °C.

Assumptions in the entire synthesis loop:

- The syngas composition of conventional steam reforming was used
- The purge ratio was taken as 7%.
- The recycle compressor was modelled as single stage with a polytropic efficiency of 80%. Compression of fresh syngas is accomplished by a 2-stage compressor with an interstage cooling temperature of 50 °C.
- The temperature of the process condensate is set to 50 °C.
- The energy consumption of distillation of crude methanol: 2.80 GJ/ton methanol at 130 °C. Methanol and water are recovered at 100% purity. The remaining components were considered as light ends.

D.2 Balances of the Lürgi reactor

Individual reactor:

Exergy balance (/ton MeOH)		
	IN	OUT
Feed	191,84	
Cold out		190,94
Heating	1,20	
Recovery		0,61
Reactor		0,89
Loss		0,60
Total	193,04	193,04

Heat balance (/ton MeOH)		
	IN	OUT
Feed	-16,59	
Cold out		-17,49
Heating	3,84	
Recovery		2,19
Reactor		2,55
Total	-12,75	-12,75

Balances of synthesis loop:

Exergy Balance (GJ/ ton MeOH)		
	IN	OUT
Streams		
Syngas	36,03	
Purge		12,10
MeOH		22,38
H ₂ O		0,00
Exergy input		
Heating reactor feed	0,94	
Compressors	0,81	
MeOH separation	0,73	
Heat recovery		
Reactor out		0,69
Recovery		0,63
Cooling		0,69
External losses		0,69
Internal losses		2,00
Total	38,50	38,50

Mass balance (ton/ ton MeOH)		
	IN	OUT
Syngas	1,45	
Purge		0,25
MeOH		1,00
H ₂ O		0,20
Total	1,45	1,45

Energy balance (GJ/ ton MeOH)		
	IN	OUT
Syngas	-7,60	
Purge		-1,11
MeOH		-7,56
H ₂ O		-3,20
Electricity	0,81	
Heat in	6,06	
Heat recovery		4,26
Waste		6,89
Total	-0,73	-0,73

D.3 Balances of the ICI tube-cooled reactor

Individual reactor:

Exergy balance (GJ/ton MeOH)		
	IN	OUT
Feed	191,81	
Cold out		190,92
Heating	0,27	
Recovery		0,61
Reactor		0,00
Loss		0,55
Total	192,08	192,08

Heat balance (GJ/ton MeOH)		
	IN	OUT
Feed	-16,58	
Cold out		-17,48
Heating	1,29	
Recovery		2,19
Reactor		0,00
Total	-15,29	-15,29

Balances of synthesis loop:

Exergy Balance (GJ/ton MeOH)		
	IN	OUT
Streams		
Syngas	35,95	
Purge		12,03
MeOH		22,38
H ₂ O		0,00
Exergy input		
Heating reactor feed	0,27	
Compressors	0,81	
MeOH separation	0,73	
Heat recovery		
Reactor out		0,00
Recovery		0,64
Cooling		0,69
External losses		0,69
Internal losses		2,01
Total	37,76	37,76

Mass balance (ton/ton MeOH)		
	IN	OUT
Syngas	1,44	
Purge		0,24
MeOH		1,00
H ₂ O		0,20
Total	1,44	1,44

Energy balance (GJ/ton MeOH)		
	IN	OUT
Syngas	-7,58	
Purge		-1,09
MeOH		-7,56
H ₂ O		-3,21
Electricity	0,81	
Heat in	4,15	
Heat recovery		2,31
Waste		6,92
Total	-2,62	-2,62

D.4 Balances of the ICI quench reactor

Individual reactor:

Exergy balance (GJ/ton MeOH)		
	IN	OUT
Feed	191,84	
Cold out		190,94
Heating	0,34	
Recovery		0,61
Reactor		0,00
Loss		0,62
Total	192,18	192,18

Heat balance (GJ/ton MeOH)		
	IN	OUT
Feed	-16,59	
Cold out		-17,49
Heating	1,29	
Recovery		2,19
Reactor		0,00
Total	-15,29	-15,29

Balances of synthesis loop:

Exergy Balance (GJ/ ton MeOH)		
	IN	OUT
Streams		
Syngas	35,44	
Purge		11,53
MeOH		22,38
H ₂ O		0,00
Exergy input		
Heating reactor feed	0,22	
Compressors	0,79	
MeOH separation	0,73	
Heat recovery		
Reactor out		0,00
Recovery		0,52
Cooling		0,68
External losses		0,68
Internal losses		2,06
Total	37,18	37,18

Mass balance (ton/ ton MeOH)		
	IN	OUT
Syngas	1,42	
Purge		0,22
MeOH		1,00
H ₂ O		0,20
Total	1,42	1,42

Energy balance (GJ/ ton MeOH)		
	IN	OUT
Syngas	-7,47	
Purge		-0,96
MeOH		-7,56
H ₂ O		-3,23
Electricity	0,79	
Heat in	3,63	
Heat recovery		1,93
Waste		6,78
Total	-3,04	-3,04

D.5 Balances of the Kellogg reactor

Individual reactor:

Exergy balance (/ton MeOH)		
	IN	OUT
Feed	192,45	
Cold out		191,56
Heating	1,09	
Steam		0,81
Recovery		0,62
Loss		0,56
Total	193,54	193,54

Heat balance (/ton MeOH)		
	IN	OUT
Feed	-16,64	
Cold out		-17,53
Heating	3,59	
Recovery		2,21
Reactor		2,28
Total	-13,05	-13,05

Balances of synthesis loop:

Exergy Balance (GJ/ ton MeOH)		
	IN	OUT
Streams		
Syngas	34,20	
Purge		10,34
MeOH		22,38
H ₂ O		0,00
Exergy input		
Heating reactor feed	0,57	
Compressors	0,76	
MeOH separation	0,73	
Heat recovery		
Reactor out		0,81
Recovery		0,23
Cooling		0,64
External losses		
		0,64
Internal losses		
		1,86
Total	36,26	36,26

Mass balance (ton/ ton MeOH)		
	IN	OUT
Syngas	1,37	
Purge		0,17
MeOH		1,00
H ₂ O		0,21
Total	1,37	1,37

Energy balance (GJ/ ton MeOH)		
	IN	OUT
Syngas	-7,21	
Purge		-0,60
MeOH		-7,56
H ₂ O		-3,33
Electricity	0,76	
Heat in	4,96	
Heat recovery		3,45
Waste		6,55
Total	-1,49	-1,49

Appendix E

BACKGROUND INFORMATION SYNGAS CASE

This appendix contains information about the syngas case, used as illustration for the EA case study in Chapter 7. All relevant information is found in literature.

E.1 Assumptions to the syngas case

The following assumptions were taken from Hinderink (Hinderink, Kerkhof, Lie, et al. 1996b; Hinderink, Kerkhof, Lie, et al. 1996a) with minor adjustments:

- The Peng-Robinson equation of state is used with interaction parameters taken from the Aspen Plus databank. For steam properties, the steam tables are applied.
- In order to obtain the desired feed pressure, feedstock and fuel are depressurized isenthalpically, thereby destroying part of the exergetic potential of these process inputs.
- All reactors are modeled as a Gibbs reactor to calculate the equilibrium composition.
- Air is modeled as dry air containing 79% nitrogen and 21% oxygen.
- Combustion in the reformer furnace takes place ideally with an excess amount of air giving an oxygen content of 4 vol% in the exhaust gases.
- The outlet temperature of the reformer furnace is set to 1000 °C. This implies that the heat of combustion is transferred at 1000 °C to the reformer tubes.
- Air separation is modeled as black box unit operation. Oxygen recovery and purity is set to 95% and 100%, respectively. Before entering the air separation unit, the air is compressed to 600 kPa.
- The temperature of stack gases is set to 150 °C before disposal to the environment. The temperature of the process condensate is set to 50 °C.
- Except for oxygen and CO₂ compression, compressors are modeled as being single stage with a polytropic efficiency of 80%. Compression of oxygen and CO₂ is accomplished by 4-stage compressors with an interstage cooling temperature of 50 °C.
- Natural gas is available at 25 °C and 600 kPa, the composition is shown in Table E.1. The LHV of this mixture is 50 GJ/ton.

TABLE E.1 NATURAL GAS COMPOSITION

Component	Vol %
CH ₄	94.7
C ₂ H ₆	2.8
CO ₂	0.2
N ₂	2.3

- The composition of the biomass feed (poplar) is shown in Table E.2 (Roeterink and Stikkelman 2000), which corresponds with the formula C_{4.2}H_{5.9}O_{2.6} with a molar weight of 100. Its LHV is 18 GJ/ton, which corresponds with 20 GJ_{ex}/ton, as is estimated by the following relation [Szargut, 1988]:

$$\frac{\text{Exergy}_{\text{wood}}}{\text{LHV}_{\text{wood}}} = \beta = \frac{1.0412 + 0.2160 (Z_{\text{H}_2} / Z_{\text{C}}) - 0.2499 (Z_{\text{O}_2} / Z_{\text{C}}) [1 + 0.7884 (Z_{\text{H}_2} / Z_{\text{C}})] + 0.0450 (Z_{\text{N}_2} / Z_{\text{C}})}{1 - 0.3035 (Z_{\text{O}_2} / Z_{\text{C}})}$$

Equation E.1

TABLE E.2 BIOMASS COMPOSITION

Component	Mass %
C	50.8
H	5.9
O	41.0
Ash	2.3

- The combustion air is not preheated.
- The amount of power consumed is used for the compressors.
- CO₂ removal is accomplished by conventional stripping with an aqueous MEA solution (20 w%). The overall energy consumption, mainly required for regeneration of the MEA solution, is assumed to be 5 MJ/kgCO₂. This energy is applied at 120 °C in the form of low temperature level exergy, corresponding with 1.5 MJ_{exergy}/ kgCO₂. Heat is removed in the condenser of the regenerator at 90 °C, corresponding with an external loss of 1.1 MJ_{exergy}/ kgCO₂.

E.2 Modeling of the biomass gasifier

In this study, the gasifier was chosen to be an autothermal fluidised bed reactor as described by Roeterink (Roeterink and Stikkelman 2000). The bed consists of quartz sand, which makes the reactor less sensitive for changes in feed structure or composition.

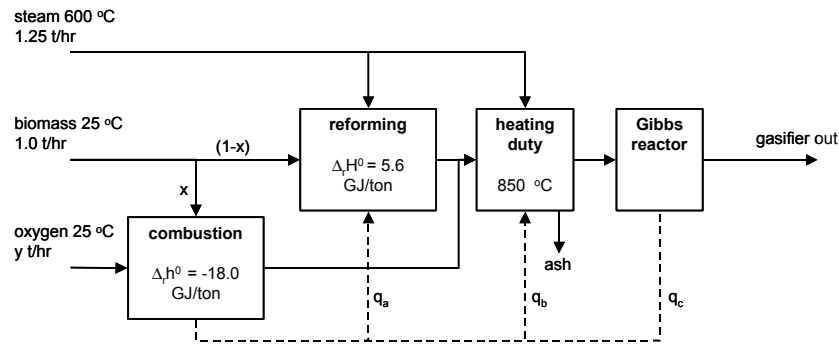


FIGURE E.1 SCHEMATIC REPRESENTATION OF GASIFIER MODEL

Figure E.1 shows how the gasifier was modeled, the final results for the mass and heat balances are given in Table E.3.

TABLE E.3 MASS AND HEAT BALANCE OF THE BIOMASS GASIFIER

Stream	Mass balance (ton/ton Biomass)		Energy Balance (GJ/ton Biomass)	
	IN	OUT	IN	OUT
Biomass	1.00		-5.66	
Oxygen	0.42		0.02	
Steam	1.25		-15.35	
Ash		0.02		0.02
Crude syngas		2.65		-11.24
Total	2.67	2.67	-20.99	-20.87

TABLE E.4 COMPOSITION OF CRUDE SYNGAS

Component	Vol %
CH ₄	0.5
H ₂ O	41.3
CO ₂	16.8
CO	12.7
H ₂	28.7
Total	100.0

E.3 Conventional steam reforming

SR balances

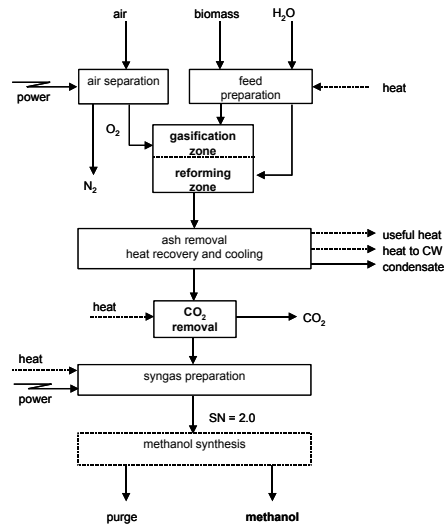
Exergy Balance (/ton MeOH)					Mass balance (/ton MeOH)		
					IN	OUT	
Material streams							
NG					39,02		
Air					0,03		
H2O					0,04		
Fluegas						0,64	
Syngas						32,75	
Condensate						0,03	
Purge					8,85		
Heat							
Feed prep	L				0,29		
	M				2,58		
Cooling						0,61	
Heat recovery							
Reformer	H					0,90	
	M					1,37	
	L					0,26	
Furnace	H					1,83	
	M					2,02	
	L					0,13	
Exergy losses							
External						1,28	
Internal						10,27	
Total					50,81	50,81	

Enthalpy balance (/ton MeOH)		
IN	OUT	
NG	-3,48	
H2O	-31,64	
AIR	0,00	
Purge	-0,37	
Condensate		-19,26
Syngas		-6,72
Fluegas		-19,81
Export heat		7,64
Waste		2,67
Total	-35,49	-35,48

Syngas Composition (/ton MeOH)									
Component	CH4	H2O	CO2	CO	H2	N2	C2H6	O2	CH3OH
kmol	2,16	0,62	8,35	16,06	80,68	0,60	0,00	0,00	0,00

E.4 Biomass gasification

BM model



BM balances

Exergy Balance (/tonMeOH)

		IN	OUT
Streams			
Biomass		31,66	
Air		0,04	
H2O		0,01	
N2			0,43
Syngas			24,88
Condensate			0,04
Char			0,13
CO2			0,70
Power			
Air sep		0,91	
Heat			
Feed prep	L	0,25	
	M	2,48	
	H	0,15	
CO2 removal	L	1,87	
Cooling			0,66
Heat recovery			
Gasifier	H		0,89
	M		1,65
	L		0,45
Purge		1,07	
	H		0,27
	M		0,11
	L		0,01
	Ex		0,08
Import exergy			
	H	6,87	1,72
	M		0,69
	L		0,07
	Ex		0,48
Exergy losses			
External			2,52
Internal			12,08
Total		45,32	45,32

Enthalpy Balance (/tonMeOH)

	IN	OUT
Air separation		
AIR	0,00	
N2		0,00
Power	0,91	
Heat loss		0,87
O2		0,04
Feed prep		
H2O	-32,41	
Heat	7,48	
Steam		-24,93
Gasifier+recovery		
Steam	-24,93	
Biomass	-9,19	
O2	0,04	
Condensate		-26,71
Crude Syngas		-18,24
Char		0,04
Recovered Heat		11,04
Syngas preparation		
Crude Syngas	-18,24	
Syngas		-4,28
CO2		-13,95
CO2 removal	7,80	7,80
Combustion		
Heat from combustion		7,38
Purge	1,03	
Additional biomass	6,34	
Total	-61,17	-60,96

Mass Balance (/tonMeOH)

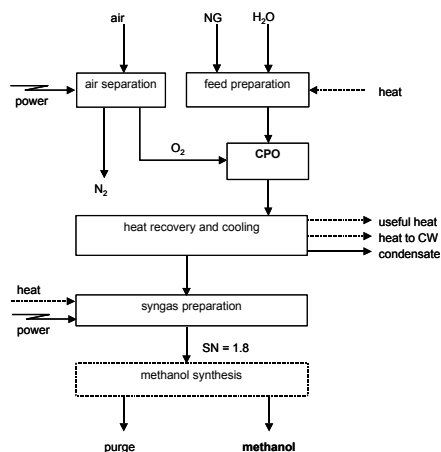
	IN	OUT
AIR	5,69	
H2O	2,03	
Biomass	1,98	
COND		1,68
CHAR/Ash		0,05
N2		2,41
Syngas		1,07
CO2		1,56
Fluegas		2,94
Total	9,70	9,70

Syngas Composition (/ton MeOH)

Component	CH4	H2O	CO2	CO	H2	N2	C2H6	O2	CH3OH
kmol	1,29	0,27	2,40	28,81	64,82	0,00	0,00	0,00	0,00

E.5 Catalytic partial oxidation

CPO model



CPO balances

Exergy Balance (/ton MeOH)

		IN	OUT
Streams			
NG		29,04	
Air		0,01	
H2O		0,02	
N2			0,38
Syngas			25,20
Condensate			0,02
Power			
Air sep		0,86	
Heat			
Feed prep	L	0,18	
	M	1,25	
	H	0,13	
Cooling			0,28
Heat recovery			
Gasifier	H		0,83
	M		0,88
	L		0,25
Purge		1,31	
	H		0,39
	M		0,13
	L		0,01
	Ex		0,04
Exergy losses			
External			0,72
Internal			4,36
Total		32,78	32,78

Enthalpy balance (/ton MeOH)

	IN	OUT
NG	-2,59	
H2O	-11,39	
AIR	0,00	
N2		0,00
Condensate		-10,32
Syngas		-6,10
Electricity	0,86	
Export heat		1,20
Useless		2,10
Total	-13,12	-13,12

Mass balance (/ton MeOH)

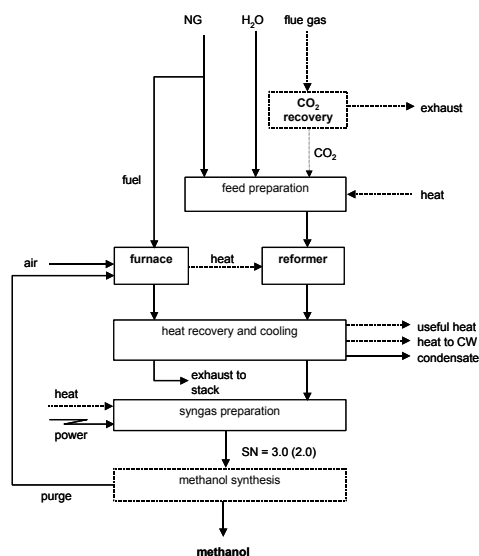
	IN	OUT
NG	0,58	
H2O	0,71	
AIR	2,76	
N2		2,15
Condensate		0,65
Syngas		1,25
Total	4,05	4,05

Syngas Composition (/ton MeOH)

Component	CH4	H2O	CO2	CO	H2	N2	C2H6	O2	CH3OH
kmol	1,54	0,37	8,10	25,14	68,49	0,80	0,00	0,00	0,00

E.6 Steam reforming with additional CO₂

SRCO₂ model



SRCO₂ balances

Exergy Balance (/ton MeOH)

		IN	OUT
Streams			
NG		36,70	
Air		0,02	
H ₂ O		0,03	
Fluegas			0,42
Syngas			24,93
Condensate			0,03
Purge		1,26	
Power			
CO ₂ compr		0,08	
Heat			
Feed prep	L	0,22	
	M	2,01	
CO ₂ removal	L	0,40	
Cooling			0,48
Heat recovery			
Gasifier	H		0,72
	M		1,10
	L		0,21
Furnace	H		1,57
	M		1,73
	L		0,11
Exergy losses			
External			0,93
Internal			9,42
Total		40,73	40,73

Enthalpy balance (/ton MeOH)

		IN	OUT
Streams			
NG		-3,27	
H ₂ O		-23,87	
AIR		0,00	
Purge		-0,13	
Condensate			-15,65
Syngas			-6,91
Fluegas			-13,72
Power			
Electricity		0,08	
Export heat			5,25
Waste			3,85
Total		-27,19	-27,18

Mass balance (/ton MeOH)

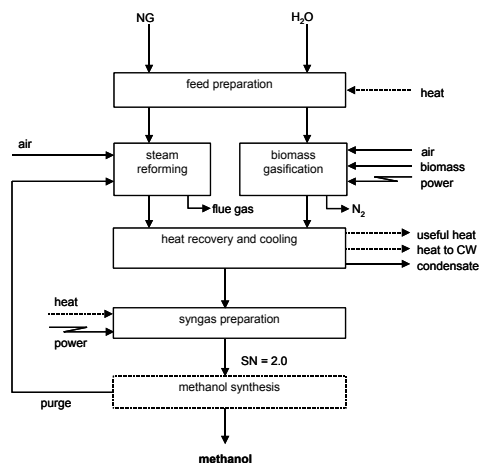
		IN	OUT
Streams			
NG		0,73	
H ₂ O		1,49	
AIR		7,00	
Purge		0,04	
Condensate			0,99
Syngas			1,26
Fluegas			7,02
Total		9,27	9,27

Syngas Composition (/ton MeOH)

Component	CH ₄	H ₂ O	CO ₂	CO	H ₂	N ₂	C ₂ H ₆	O ₂	CH ₃ OH
kmol	1,50	0,62	11,56	19,65	74,04	0,58	0,00	0,00	0,00

E.7 Steam reforming with additional biomass gasification

SRBM model



SRBM balances

Exergy balance (/ton MEOH)

		IN	OUT
Streams			
NG		29,27	
Biomass		5,57	
H2O		0,00	
Air		0,00	
Purge		1,31	
N2			0,07
Condensate			0,03
Syngas			24,95
Fluegas			0,70
Char/Ash			0,04
Heat			
Feed prep	L	0,22	
	M	2,05	
	H	0,03	
Cooling			0,50
Power			
Air sep		0,20	
Heat recovery			
	L		0,04
	M		2,44
	H		1,96
Exergy loss			
External			1,34
Internal			7,92
Total		38,66	38,66

Mass balance (/ton MEOH)

	IN	OUT
NG	0,59	
Biomass	0,23	
H2O	1,59	
Air	6,08	
Purge	0,04	
N2		0,42
Condensate		1,05
Syngas		1,29
Fluegas		5,82
Char/Ash		0,01
Total	8,53	8,59

Syngas Composition (/ton MeOH)

Component	CH4	H2O	CO2	CO	H2	N2	C2H6	O2	CH3OH
kmol	1,58	0,54	13,33	17,88	75,76	0,48	0,00	0,00	0,00

Appendix F

GUIDANCE QUESTIONS AND CATEGORY TABLE FOR THE ESC TOOL

This appendix gives the relevant background information to the ESC tool: the guidance questions and the category table. In Chapter 9, the ESC tool is introduced.

TABLE F.1 ESC GUIDANCE QUESTIONS

Impact Criteria	Guidance Questions
<i>Compliance with government regulation</i>	Do regulations exist for all components of the product? Do any non-regulatory agreements, like covenants, exist related to the product? If not, what kinds of regulations are expected? Are regulations expected to change in the future, and in what way?
<i>Consumer need analysis</i>	Has a need assessment/ analysis been performed? What (social) need does the product fulfill? How does it fulfill this need, what are the products main and auxiliary functions? Is the product the most efficient, i.e. state of the art, way to fulfill this need? (Considering performance, eco-efficiency) Will the need for the product change in the future, and if so in what way?
<i>Social acceptance</i>	Is there any -non regulatory- opposition against the use of the product or substances used? (i.e. by NGO's) Is there any (expected) trend that will influence the impact of or opposition against the product or substances used in the future?
<i>Human toxicity</i>	Is any of the components toxic to humans? Is there any combined effect of the ingredients? Do the components accumulate in the human body?
<i>Risk of accidents</i>	Has a risk analysis (i.e. HAZOP) been performed? Is the product safe to be handled by consumers? What are the flammability, explosion risk of all the ingredients? Does the combination of ingredients enhance the effects?
<i>Eco-toxicity</i>	What is the eco- toxicity of each of the components? Is there any combined effect of the ingredients? Do the components accumulate in living organisms or eco-systems?
<i>Atmospheric pollution</i>	Are any vaporous, gaseous or particulate components emitted into the atmosphere during any stage of the product life cycle? What are the effects of these components in the atmosphere? Do the products accumulate in the atmosphere? What are degradation products and what is their effect? Is there an expected contribution to one of the following: global warming, photochemical ozone creation, stratospheric ozone depletion, or acidification. Are any strongly odorous substances emitted?
<i>Water pollution</i>	Are any substances released into ground water or surface waters during any stage of the product life cycle? Is any hot cooling water released to ground or surface water? Is any liquid waste produced during use that will end up in household sewage? What are the effects of these components? (in nature/ for humans)? Is there an expected contribution to eutrophication or acidification? What degradation products may be formed and what are their effects?
<i>Solid waste</i>	Is any solid waste produced during the product life cycle? Where does this waste end up (landfills, combustion)? Do dissipative emissions to land occur during product use? What are the expected effects of these emitted components?
<i>Company costs (insurance, costs for personnel and investments, fees for waste)</i>	Do taxes, fees or similar have to be paid related to the product? Do any subsidies exist related to the product? Are any large changes (investments) at company level required to implement the production of the new product? Is the product more expensive to produce than alternatives?

Impact Criteria	Guidance Questions
<i>Consumer costs</i>	Do any taxes, fees or similar have to be paid related to the product? Do any subsidies exist related to the product? Is the product more expensive than alternatives?
<i>Depletion of scarce resources</i>	Are any of the materials used in the product scarce? At what scale is the product expected to be produced/ sold? Is the product designed to minimize the use of materials in restricted supply? Is the use of renewable resources considered?
<i>Raw material extraction</i>	Is the product designed to minimize the use of materials whose extraction is energy extensive? Does raw material extraction give rise to environmental impact through emissions? Does raw material extraction result in the damaging of eco-systems, or reduce bio-diversity?
<i>Production of ingredients</i>	Is the environmental impact of the production processes of the ingredients known? Is the product designed to minimize the use of materials whose production involves the generation of large amounts of waste, or requires large amounts of energy? Are the suppliers of ingredients screened on their environmental and social performance? (do they follow a 'code of ethics' or similar, do they violate human rights)
<i>Choice of ingredients</i>	Is the purpose and function of each of the ingredients clear? Is the product designed to utilize recycled materials wherever possible? Are all materials the least toxic and most environmentally friendly for the function to be performed? Have alternatives been investigated for all ingredients? Has material use been minimized, i.e. product made as compact as possible?
<i>Manufacturing and processing</i>	Is the use or emission of toxic or hazardous substances avoided or minimized? Is recycling or re-use of materials maximized? If auxiliary chemicals are used, is their use minimized and have alternatives been investigated? Have different, 'cleaner', or less energy consuming processes been considered? Is the current process 'state of the art'? Has the use of other ('green') energy sources been considered?
<i>Logistics</i>	Is transport most efficiently organized? Are supplier's locations selected for minimal transport? Is transport necessary? What means of transport are used? What kinds of transport packaging are used? If any take back program is in place, how is it organized?
<i>Substances</i>	Are any substances emitted to the direct use environment? What are the effects of these substances? Is there direct human (skin) contact with the product? Is the product dosing minimized?
<i>Energy</i>	Does the product require energy during its use? If so, is the amount of energy necessary minimized? Are different kinds of energy to be used investigated? Are product alternatives that require less or no energy considered?
<i>Service</i>	Is the product information clear? Does the producer provide additional information or service if required, such as a help-desk? Is any maintenance needed, and if so is it clear by whom and how it should be done?
<i>Auxiliary materials</i>	What and how much auxiliary materials are required for the use of the product? What is the environmental impact of these materials? Is the use of auxiliary materials minimized, and is the use of alternatives investigated? Is any equipment needed with the use of the product? Is the combined use of product and equipment optimized?

Impact Criteria	Guidance Questions
<i>Packaging</i>	Have efforts been made to use recyclable or biodegradable packaging materials? Is there a take-back program for elaborate packaging? Has the packaging material been minimized?
<i>End of Life</i>	Where does the product or its components end up after use? (Sewage, household garbage, ground). Are the components biodegradable? Do the components decompose in a common water/ waste treatment process? Is there a take-back program for (part of) the product? Are any (toxic) emissions produced during the disposal? Is the product compostable? Do components end up in nature that accumulate there?
<i>Recyclability</i>	Is it possible to re-use or recycle (components of) the product? Has an effort been made to make the product recyclable?

TABLE F.2 ESC CATEGORY TABLE

A = problematic, action required; B = moderate, to be observed and improved; C= sufficient, no direct action required; D = good, no action required

Impact Criteria	Categories			
	A (problematic)	B (moderate)	C (sufficient)	D (good)
<i>Compliance with government regulation</i>	No compliance with regulations.	There will be stricter regulation than the present. Compliance for the near future only (0-1 yr.). At least B if the product contains new components for which no regulation exists.	Compliance is sufficient, also for the future (1-5 yr.).	Compliance for the long term (5-10 yr.).
<i>Consumer need analysis</i>	A (societal) need is not properly fulfilled by the product.	The product does fulfill a (societal) need, but is not the best possible solution. The need could, or is expected to change in the future. At least B if no need assessment/analysis is performed.	Product is the best possible solution for a need in society. No changes expected that will effect the need for the product in the future.	Product is the best possible solution for a need in society. The need for the product is expected to increase in the future.
<i>Social acceptance</i>	Highly criticized, demands for banning the substance.	Mildly criticized, or criticism expected to increase in the future.	No criticism is known, but it might arise in the future.	No criticism is known or expected in the future.

A = problematic, action required; B = moderate, to be observed and improved; C= sufficient, no direct action required; D = good, no action required

Impact Criteria	Categories			
	A (problematic)	B (moderate)	C (sufficient)	D (good)
<i>Human toxicity</i>	One or more components highly hazardous to health; carcinogenicity, teratogenicity, genotoxicity.	One or more components hazardous to health, allergenic potential.	According to current knowledge there are no (unacceptable) health hazards.	Product is (inherently) safe.
<i>Risk of accidents</i>	High risk of accidents. Ranking according to regulation on hazardous substances with respect to: Flammability: high or medium. Danger of explosion: high or medium, danger of explosion at ambient temperatures. Risk of accidents bearing high danger to men and environment. Products of combustion toxic according to A under 'Toxicity'	Medium risk of accidents, bearing high danger to men and environment. At least B if no risk analysis has been performed.	Little or no (unacceptable) risk of accidents according to current knowledge or a risk properly managed.	No (unacceptable) risk of accidents.
<i>Eco-toxicity</i>	Highly toxic, toxic or less toxic, according to hazardous substances regulations.	Limit value existing, like TLV (occupational threshold limit value), and quite small safety margins maintained.	Limit value existing, but large safety margins maintained.	All components non-toxic according to current knowledge.

A = problematic, action required; B = moderate, to be observed and improved; C= sufficient, no direct action required; D = good, no action required

Impact Criteria	Categories			
	A (problematic)	B (moderate)	C (sufficient)	D (good)
<i>Atmospheric pollution</i>	Emission of vaporous, gaseous or particulate substances (or degradation products) that destroy atmospheric ozone, contribute to global warming, acidification, photochemical ozone creation, or are ranked A under 'toxicity'.	Emission of vaporous, gaseous or particulate substances (or degradation products) that contribute to smog and dust pollution, are strongly odorous, or are ranked B under 'toxicity'. Emission of components of which no adverse effects are known but that accumulate in the atmosphere. At least B if not enough is known but effects are expected.	Emission of vaporous, gaseous or particulate substances with no adverse effects according to current knowledge. No accumulation of products.	No emission of vaporous, gaseous or particulate substances.
<i>Water pollution</i>	Emission of components highly toxic/ toxic to humans or water flora and fauna, according to national regulation. Severe contribution to acidification or eutrophication. Accumulation of toxic components. Persistent residues after sewage treatment.	Emission of components less toxic to humans or water flora and fauna according to national regulation. Contribution to acidification or eutrophication. Emission of components of which no adverse effects are known but that accumulate in ground water. At least B if not enough is known but	Products emitted which are in general not toxic to humans, or water flora and fauna. Does not make water unfit for further use in any way.	No products emitted to ground or surface waters.

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Impact Criteria	Categories			
	A (problematic)	B (moderate)	C (sufficient)	D (good)
<i>Solid waste</i>	Emission of solids (or degradation products) into the environment that accumulate or have toxic effects as ranked A under 'toxicity'.	Emission of solids (or degradation products) into the environment that accumulate or have toxic effects as ranked B under 'toxicity'. At least B if not enough is known but effects are expected.	Only emission of harmless substances according to current knowledge, no accumulation.	No emission of solids.
<i>Company (insurance, costs for personnel and investments, fees for wastes)</i>	High (fees to be paid), expected to increase.	Higher than average, or average but expected to increase	Average, no change expected. Or high but expected to decrease.	Lower than average (through subsidies and similar), or expected to decrease.
<i>Consumer</i>	High, expected to increase.	Higher than average, or average but expected to increase	Average, no change expected. Or high but expected to decrease.	Lower than average (through subsidies and similar), or expected to decrease.

A = problematic, action required; B = moderate, to be observed and improved; C= sufficient, no direct action required; D = good, no action required

Impact Criteria	Categories			
	A (problematic)	B (moderate)	C (sufficient)	D (good)
<i>Depletion of scarce resources</i>	Large quantities of scarce resources are used, or any extremely scarce resource.	Scarce resources are used, but only small quantities, or not very scarce materials.	Relatively scarce resources used, but only in small quantities, or large quantities of not very scarce resources.	Only renewable or abundant resources used.
<i>Raw materials extraction</i>	Raw materials extraction is associated with high environmental impact by emissions, waste production or energy use. Raw materials extraction gives rise to severe disturbance of ecosystems (e.g. deforestation of rain forests).	Raw materials extraction is associated with environmental impact by emissions, waste production or energy use. Raw materials extraction gives rise to disturbance of ecosystems.	Raw materials extraction is not associated with environmental impact by emissions, waste production or energy use.	Sustainable/ renewable resources are used, taking care of sustainable production methods.

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Impact Criteria	Categories			
	A (problematic)	B (moderate)	C (sufficient)	D (good)
<i>Production of ingredients</i>	During production of ingredients substances ranked A under 'raw materials extraction' are used as raw materials, auxiliary materials or fuels, or substances are emitted which have a high environmental impact, or the production process is highly energy intensive. Suppliers have unethical working methods.	During production of ingredients substances ranked B under 'raw materials extraction' are used as raw materials, auxiliary materials or fuels, or substances are emitted that give rise to environmental impacts, or that the production process is unnecessarily energy intensive. At least B if nothing is known about the supplier and its production processes.	The production of ingredients does not lead to any mayor environmental impacts, or the production process is state of the art.	The production of ingredients does not lead to any environmental impacts.
<i>Choice of ingredients</i>	Ingredient function, concentrations and material are not analyzed. Alternatives have not been considered. Hazardous, toxic or high environmental impact ingredients are used.	Ingredients fulfill their function well enough, but alternatives have not been thoroughly screened.	Alternatives have been considered.	All ingredients are the best possible option (function, material, concentration). All possible alternatives have been investigated. Recycled materials are used where possible

A = problematic, action required; B = moderate, to be observed and improved; C= sufficient, no direct action required; D = good, no action required

Impact Criteria	Categories			
	A (problematic)	B (moderate)	C (sufficient)	D (good)
<i>Manufacturing and processing</i>	During manufacturing and processing, substances are used or emitted, which are ranked A under 'Toxicity' No recycling of substances takes place. Process is highly energy intensive.	During manufacturing and processing, substances are used or emitted, which are ranked B under 'Toxicity' Only limited re-use of materials. Process is fairly energy intensive.	Production of waste with no environmental impacts. Hazardous substances are used in the process, but do not leave the process, and are well managed. Process energy use is fair.	The process is a 'closed system', all wastes are recycled. Process energy use is little, or fully optimized. During manufacturing and processing no substances are used or emitted, which give rise to environmental impacts.
<i>Logistics</i>	Transport is excessive and not efficiently organized in order to reduce environmental emissions and energy use.	Much transport, but attempts are made for efficiently organization in order to reduce environmental emissions and energy use.	A fair amount of transport, but efficiently organized in order to reduce environmental emissions and energy use.	Minimal transport, organized in a way that minimizes environmental emissions and energy use.
<i>Substances</i>	Substances are emitted in the direct use environment ranked A under 'toxicity'.	Substances are emitted in the direct use environment ranked B under 'toxicity'.	Only harmless substances emitted during the use.	No emissions take place during the use.

A = problematic, action required; B = moderate, to be observed and improved; C= sufficient, no direct action required; D = good, no action required

Impact Criteria	Categories			
	A (problematic)	B (moderate)	C (sufficient)	D (good)
<i>Energy</i>	Product is very energy consuming. Alternatives are not seriously considered.	Energy use during product use is reasonable, but can be further minimized.	The use process is energy efficient according to current standards.	Energy use during product use is none or minimal.
<i>Service</i>	Product information is missing, incorrect or unclear. No additional service by the producer.	Product information on basic level only. No additional service by the producer (if required)	Product information is clear. Moderate additional service (if required) by the producer.	Additional service (if required) is provided by the producer.
<i>Auxiliary materials</i>	Many auxiliary materials and/ or equipment needed, that have a negative environmental impact. Materials ranked A under 'toxicity' or 'raw materials extraction' are used. No consideration of the entire product-equipment-auxiliary materials system.	Materials ranked B under 'toxicity' or 'raw materials extraction' are used, or large values of materials in restricted supply (including water). The product-equipment-auxiliary material system is partly considered.	The whole product-equipment-auxiliary material system is considered. Many auxiliary materials required, but they have no adverse environmental impacts.	The whole product-equipment-auxiliary material system is considered. Auxiliary material use is minimal. Materials used have no adverse environmental impacts.

A = problematic, action required; B = moderate, to be observed and improved; C= sufficient, no direct action required; D = good, no action required

Impact Criteria	Categories			
	A (problematic)	B (moderate)	C (sufficient)	D (good)
<i>Packaging</i>	Packaging is elaborate and non-recyclable or biodegradable.	Packaging non-recyclable or biodegradable or recycling of the material through complex process.	Packaging amount is minimized and consists of recyclable or biodegradable materials.	Packaging amount is minimized and consists of recyclable or biodegradable materials. If possible, packaging is made of recycled materials. A take-back program exists for elaborate packaging.
<i>End of Life</i>	Waste treatment leads to severe environmental impacts. Accumulating substances present in waste.	Waste treatment leads to environmental impacts. Some accumulating substances present in waste.	Deposition as municipal waste. No accumulation or persistent residues after treatment.	No waste deposition, instead reuse, recycle or composting.
<i>Recyclability</i>	Durables: Product is not recyclable or there is no recycling facility. Consumables: Recycling is not even considered.	Durables: Product is partly recyclable, or has an extremely complex or energy consuming recycling procedure. Recycling procedure is not state of the art. Consumables: Recycling considered impractical but not	Durables: Product is recyclable. Consumables: Recycling is considered but not sensible.	Highly recyclable, according to the state of the art.

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SUMMARY

SUSTAINABLE CHEMICAL PROCESSES AND PRODUCTS: NEW DESIGN METHODOLOGY AND DESIGN TOOLS

This thesis deals with the question: *how can a trained chemical engineer develop a conceptual design of a chemical process plant in such a way that the final result clearly contributes to sustainable development?* Reading this question brings two issues in mind: a) what is a conceptual design of a chemical process plant and what is the task of the chemical engineer in this kind of design, and b) what is sustainable development and how can a contribution to sustainable development in a chemical engineering context be validated.

Three hypotheses are described, as the framework for this research:

Hypothesis 1; Sustainable development of chemical processes and products can best be realized by an integral design methodology that 1) clearly locates the various design tools that are available or are to be developed and that 2) forces the designer to define the problem, to propose and analyze creative solutions, and to evaluate the design in a consistent and structured way.

Hypothesis 2; The incorporation of sustainable development in the design of chemical products and processes require specific skills and tools. The design methodology should contain enough tools to cover the whole area from need to plant. If tools are newly developed their location in the design methodology should be identified.

Hypothesis 3; A general design methodology, like proposed in hypothesis 1, together with the tools from hypothesis 2, is applicable for both chemical processes and chemical products.

As validation to the hypotheses the results are presented mainly in two parts: the *general methodology* and its *design tools*.

The main goal of this thesis is the development of a *new general design methodology* that enables the incorporation of issues from the sustainability debate into the design practice of the chemical engineering field. An elaborated design methodology for the chemical engineering field does not exist as such, so the development of such a design methodology is a clear contribution to the chemical engineering discipline.

The proposed *new design tools* in this thesis resulted from the experience gathered during this research combined with scientific insight. These tools and their case studies function as illustrations of how the general design methodology is applied. Besides that the tools show partially how the contents of the sustainability debate can be incorporated in the early stages of chemical process design. The tools are in still in a conceptual stage, but it is already clear that they fill empty spaces in the current chemical engineering practice.

Chapter 4 gives the description of the general design methodology and also presents the framework for the remaining part of the thesis. In Chapters 5-8 the various steps of the process design methodology are elaborated and illustrated by case studies. Chapter 9 illustrates the application of the proposed design methodology to the development of chemical products. Finally, conclusions and recommendations are given in Chapter 10.

After the introduction in Chapter 1, Chapter 2 gives an overview of the sustainability debate, the history of the debate is sketched and the most influential visions on sustainable development are discussed. In many descriptions of sustainable development, a division is made in social, ecological, and economic sustainable development. This thesis also uses this division and applies it to the chemical process and product development.

It is quite possible to derive society and ecology focused engineering principles from the societal sustainable development debate. These principles have the following main characteristics: i) closing the cycles, ii) improving the energetical and material efficiency, iii) defining the system levels, iv) improving the decision-making, v) involving society.

From the discussion in Chapter 2, it becomes clear that the chemical industry is of essential importance to the sustainable development of modern society, but also environmental problems originate from the chemical industry. The chemical industry has a lot of knowledge to solve such environmental problems. Existing environmental-focused technologies, like green engineering, pollution prevention, waste minimization, or process intensification etc. do contribute to sustainable development of the chemical industry. However, for the traditional chemical engineer it is hard to incorporate or locate these tools in the current practice. Therefore it is necessary to have a general design framework in which these tools are located and their interrelations become clear. In Chapter 3, the field of conceptual process design is investigated. First, the relevance of conceptual process design research is identified. Then conceptual design is placed in a societal context. After a brief discussion of generic design principles, the currently standard approaches of conceptual process design are discussed. This description of conceptual process design can be used to put all developments made in the remainder of the thesis into general conceptual process design perspective.

Chapter 4 starts with an overview of the status quo of design methodologies, with respect to engineering in general and the chemical engineering discipline in particular. Based on this overview, demands to a new design methodology for the sustainable conceptual design of chemical processes and products are derived. From own experience and based on literature sources a design methodology is developed and presented in Chapter 4.

The methodology consists in three parts: 1) decision-making sequence, 2) design framework, and 3) design tools. The decision-making sequence is the repeating part of the design methodology, consisting of a problem definition stage, a generation of alternatives stage, an analysis of alternatives stage and a design evaluation stage. The design framework is based on current chemical engineering practice and presents the relevant levels of detail. The design tools fill the design framework in relation to the decision-making sequence. It is presented that existing green engineering tools fit in the methodology. Besides that some stages of the methodology are filled in with specific design tools for sustainable chemical processes, developed during this research.

Chapter 5 deals with the problem definition and the definition of system boundaries. The problem definition consists in three elements: 1) the goal and scope definition, 2) the criteria determination, 3) the knowledge mapping. These three elements are elaborated in this Chapter. The identification of stakeholders is discussed. Then two tools, developed during this research, are described extensively and illustrated with case studies: the *decision sequence ranking tool* (DSR) and the *system boundaries and closed cycles tool* (SBDCC).

Chapter 6 deals with the generation of design alternatives, which can be considered as the creative heart of every design where integrative and innovative solutions are developed. The generation of alternatives is more explored by dividing it in three

elements: 1) creativity stimulation, 2) function identification, 3) concept integration. After that tools are discussed to improve the generation of alternatives by creativity. Then a *chemical route selection tool* (CRS) is described together with a design case. Design guidelines are becoming increasingly important as the complexity of the design methods increases, this lead to the *guidelines for process synthesis tool* (GPS).

Chapter 7 deals with the analysis of alternatives, that consists in three elements: 1) concept simulation, 2) concept reliability analysis, and 3) concept feasibility analysis. These elements are explored in this Chapter. Sets of checklists and metrics are described that help the designer to focus on sustainability during the analysis of the design. Furthermore a design method is discussed relating to the analysis of design alternatives. The *exergy analysis* (EA) tool compares the exergy loss within a given set of design block schemes. The exergy loss is a measure for the primary energy required and the efficiency of mass use.

Chapter 8 deals with the design evaluation of the proposed solution that consists in three elements: 1) goal and scope satisfaction, 2) criteria satisfaction, 3) concept communicability. After the exploration of those issues, various tools are presented that can stimulate the carrying out of the evaluation phase. Primarily the stakeholders, aided by the designer, do the evaluation. The *sustainability ranking tool* (SRT) is a method that enables the evaluation of a set of rough ideas based on sustainability criteria. This method is developed and illustrated with an industrial case study.

In Chapter 9 the newly developed process design methodology is applied to the design of sustainable chemical products. The process design framework, presented in Chapter 4, is developed here to a product design framework. A specific tool for the *evaluation of sustainable consumables* (ESC) or chemical products is presented and applied to an industrial case. This tool improves the design problem definition of sustainable chemical product design.

Chapter 10 summarizes the conclusions of this thesis. The hypotheses given in Chapter 1 are satisfied. Further, this Chapter gives some recommendations for further research.

Delft, April 2004, Gijsbert Korevaar

SAMENVATTING

DUURZAME CHEMISCHE PROCESSEN EN PRODUCTEN: NIEUWE ONTWERPMETHODOLOGIE EN ONTWERP-TOOLS

Dit proefschrift behandelt de vraag: *hoe kan een ervaren chemisch ingenieur een conceptueel ontwerp van een chemisch proces maken, zodanig dat het eindresultaat duidelijk bijdraagt aan duurzame ontwikkeling?* Het lezen van deze vraag brengt twee zaken naar voren: a) wat is een conceptueel ontwerp van een chemisch proces en wat is de taak van een chemisch ingenieur bij zo'n ontwerp en b) wat is duurzame ontwikkeling en hoe kan een bijdrage aan duurzame ontwikkeling binnen een chemisch-technologische context worden omschreven.

Drie hypothesen worden gegeven, die het raamwerk vormen voor dit onderzoek:

Hypothese 1; Duurzame ontwikkeling van chemische processen en producten kan het beste worden gerealiseerd door middel van een integrerende ontwerpmethodologie, die 1) helder de plaats bepaalt van reeds beschikbare en nog nieuw te ontwikkelen ontwerp-tools en die 2) de ontwerper dwingt om het ontwerpprobleem duidelijk te formuleren, om met creative oplossingen te komen en die te analyseren en om het ontwerp op een consistente en gestructureerde manier te evalueren.

Hypothese 2; De invloed van duurzame ontwikkeling op het ontwerp van chemische producten en processen vraagt om specifieke vaardigheden en tools. Daarom zal de ontwerpmethodologie genoeg tools moeten bevatten om het gehele traject te bestrijken van ontwerp-vraag tot uiteindelijk fabrieksontwerp.

Hypothese 3; Een algemene ontwerpmethodologie zoals die is voorgesteld in hypothese 1, samen met de tools van hypothese 2, zijn van toepassing op zowel het ontwerpen van chemische processen als van chemische producten.

De wetenschappelijk bijdragen van dit onderzoek zijn samen te vatten in twee delen: de *algemene ontwerpmethodologie* en de *ontwerp-tools*.

Het belangrijkste doel van dit proefschrift is de ontwikkeling van een nieuwe *algemene ontwerpmethodologie* die het mogelijk maakt om rekening te houden met het duurzaamheidsdebat tijdens het ontwerpen van chemisch technologische toepassingen. Zo'n uitgewerkte ontwerpmethodologie bestaat niet binnen de chemische technologie, daarom is de ontwikkeling van een dergelijke methodologie een duidelijke bijdrage aan dit vakgebied.

De voorgestelde *nieuwe ontwerp-tools* in dit proefschrift zijn het resultaat van de ervaring die opgedaan is tijdens het onderzoek in combinatie met wetenschappelijke inzichten. Deze ontwerp-tools, samen met hun case studies functioneren als illustratie van het werken met de algemene ontwerpmethodologie. Daarnaast laten de ontwerp-tools gedeeltelijk zien hoe de inhoud van het duurzaamheidsdebat kan worden meegenomen in de vroegste stadia van het conceptueel procesontwerp. De voorgestelde tools zijn nog slechts in een ontwikkelingsfase, maar het wordt duidelijk aangetoond dat ze lege ruimten invullen binnen de huidige ontwerp-praxis.

In Hoofdstuk 4 wordt de beschrijving gegeven van de ontwerpmethodologie, wat ook meteen het raamwerk is voor het vervolg van het proefschrift. In de hoofdstukken 5-8 worden de verschillende stappen van de ontwerpmethodologie uitgewerkt en geïllustreerd met case studies. Hoofdstuk 9 laat zien dat de ontwerpmethodologie ook van toepassing is op de ontwikkeling van chemische producten. Tenslotte worden conclusies en aanbevelingen gegeven in hoofdstuk 10.

Na de inleiding in Hoofdstuk 1, wordt er in hoofdstuk 2 een overzicht gegeven van het duurzaamheidsdebat; de geschiedenis van dit debat wordt geschetst en de meest invloedrijke visies op duurzame ontwikkeling worden besproken. In veel beschrijvingen van duurzame ontwikkeling wordt er een onderscheid gemaakt tussen sociale, economische en ecologische duurzame ontwikkeling. Dit proefschrift gebruikt ook dit onderscheid en past het toe op de ontwikkeling van duurzame chemische processen en producten.

Het blijkt goed mogelijk om maatschappij-gerichte en milieu-gerichte technologische principes af te leiden uit het duurzaamheidsdebat. Deze principes zijn: i) het sluiten van kringlopen, ii) het verbeteren van energetische en materiele efficiëntie, iii) de definitie van systemniveaus, iv) het verbeteren van het nemen van beslissingen, v) het betrekken van de maatschappij.

Uit de discussie van Hoofdstuk 2 wordt duidelijk dat de chemische industrie van wezenlijk belang is voor de duurzame ontwikkeling van de moderne samenleving, maar ook dat milieuproblemen juist ontstaan door de chemische industrie. De chemische industrie heeft veel kennis om milieuproblemen op te lossen. Bestaande milieu-gerichte technologieën, zoals 'green engineering', 'pollution prevention', 'waste minimization', of 'process intensification', etc. hebben een bijdrage in de duurzame ontwikkeling van de chemische industrie. Het is daarentegen voor de traditionele chemische ingenieur vaak moeilijk en onduidelijk om deze tools een plaats te geven in de huidige praktijk. Daarom is het noodzakelijk dat er een algemene ontwerpmethodologie beschikbaar is, waarin de benodigde ontwerp-tools een plaats hebben en waarin hun onderlinge samenhang duidelijk is.

In Hoofdstuk 3 wordt het vakgebied van het conceptueel procesontwerpen beschreven. In de eerste plaats wordt de relevantie van onderzoek binnen dit vakgebied verduidelijkt. Daarna wordt het conceptuele procesontwerp in een maatschappelijke context geplaatst. Na een korte discussie over algemene ontwerp-principes worden de huidige benaderingen voor het procesontwerpen besproken. Deze beschrijving van het conceptuele procesontwerp kan worden gebruikt om alle ontwikkelingen in de rest van het proefschrift te plaatsen in een algemeen conceptueel ontwerp-perspectief.

Hoofdstuk 4 begint met een overzicht van de status quo van ontwerpmethodologie, in relatie tot technologie in het algemeen en chemische technologie in het bijzonder. Gebaseerd op dit overzicht worden eisen afgeleid, waaraan een nieuwe ontwerpmethodologie voor duurzame conceptuele ontwerpen van chemische processen en producten moet voldoen. Uit eigen ervaring en op basis van literatuuronderzoek is een ontwerpmethodologie ontwikkeld en beschreven in hoofdstuk 4.

Deze methodologie bestaat in drie delen: 1) de volgorde van het nemen van beslissingen, 2) het ontwerpraamwerk en 3) ontwerp-tools. De volgorde voor het nemen van beslissingen is een zichzelf herhalend onderdeel van de ontwerpmethodologie, bestaande uit een probleem definitie, het genereren van alternatieven, het analyseren van alternatieven en de ontwerpevaluatie. Het ontwerpraamwerk is gebaseerd op de huidige chemisch-technologische praxis en geeft de relevante detailleringniveaus aan. De ontwerp-tools vullen het ontwerp-raamwerk volgens de volgorde van het nemen van beslissingen. Het wordt duidelijk gemaakt dat bestaande milieu-gerichte ontwerp-tools passen in de nieuwe methodologie. Daarnaast wordt de ontwerpmethodologie gevuld

met specifieke ontwerp-tools voor chemische processen en producten, zoals ontwikkeld tijdens dit onderzoek.

Hoofdstuk 5 behandelt de probleem definitie, die bestaat uit drie elementen: 1) de definitie van doelstelling en afbakening, 2) de bepaling van criteria, 3) het in kaart brengen van kennis. Deze drie elementen worden uitgewerkt in dit hoofdstuk. De bepaling van de betrokken actoren wordt besproken. Daarna worden twee ontwerp-tools, ontwikkeld tijdens dit onderzoek, uitgebreid beschreven en geïllustreerd met case studies: namelijk de 'decision sequence ranking tool' (DSR) en de 'system boundaries and closed cycles tool' (SBDCC).

Hoofdstuk 6 behandelt het genereren van ontwerp-alternatieven, wat gezien kan worden als het creatieve hart van elk ontwerp, waarin integrerende en innovatieve oplossingen worden ontwikkeld. Het genereren van alternatieven wordt verder uitgewerkt in drie elementen: 1) het stimuleren van creativiteit, 2) het identificeren van functies, 3) het integreren van het concept. Hierna worden tools besproken voor de verbetering van het genereren van alternatieven door creativiteit. Dan wordt de 'chemical route selection tool' (CRS) beschreven samen met een case study. Ontwerp richtlijnen zijn bijzonder belangrijk naarmate de complexiteit van het ontwerp toeneemt, dit leidt tot de ontwikkeling van de 'guidelines for process synthesis tool' (GPS).

Hoofdstuk 7 behandelt de analyse van alternatieven, die bestaat uit drie elementen: 1) het simuleren van concepten, 2) de analyse van de betrouwbaarheid van concepten, 3) de haalbaarheid van concepten. Deze elementen worden uitgewerkt in dit hoofdstuk. Overzichten van checklists en metrics worden beschreven, die de ontwerper helpen om zich te richten op duurzaamheid tijdens het ontwerp. Verder wordt er een ontwerpmethode besproken die betrekking heeft op de analyse van ontwerpalternatieven. Deze 'exergy analysis tool' (EA) vergelijkt het exergieverlies van verschillende blokschema's. Het exergieverlies is een maat voor de primaire energie die nodig is en voor de efficiëntie van het massagebruik.

Hoofdstuk 8 behandelt de ontwerpevaluatie van een voorgestelde oplossing die bestaat uit drie elementen: 1) de mate waarin doelstelling en afbakening zijn gehaald, 2) het voldoen aan de criteria, 3) de communiceerbaarheid van het concept. Na de uitwerking van deze punten, worden verschillende tools gepresenteerd die het uitvoeren van evaluaties kunnen bevorderen. In de eerste plaats zijn de betrokken actoren het aanspreekpunt voor de evaluatie, daarbij geholpen door de ontwerper. De 'sustainability ranking tool' (SRT) is een methode die het mogelijk maakt om conceptuele ideeën te evalueren op basis van duurzaamheidscriteria. Deze methode is ontwikkeld en wordt geïllustreerd aan de hand van een industriële case study.

In Hoofdstuk 9 wordt de nieuwe procesontwerpmethodologie toegepast op het ontwerpen van duurzame chemische producten. Het raamwerk voor het procesontwerpen, zoals gepresenteerd in hoofdstuk 4, is hier verder ontwikkeld tot een raamwerk voor productontwerpen. Een specifieke *evaluation of sustainable consumables* tool (ESC) wordt beschreven en toegepast op een industriële case study. Deze tool verbetert de probleem definitie van een duurzaam productontwerp.

Hoofdstuk 10 vat de conclusies samen van dit proefschrift. De hypothesen zoals die zijn opgesteld in hoofdstuk 1 blijken te voldoen. Verder geeft dit hoofdstuk aanbevelingen voor verder onderzoek.

Delft, April 2004, Gijsbert Korevaar

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- G. Korevaar, G. J. Harmsen, S.M. Lemkowitz, *Sustainability in Process Design Methodology*, published in: Mergers and Acquisitions; the truths, the tactics, the trends, proceedings of the 21st Annual European AIChE (NI/B section) Colloquium, The Hague, April 20, 2000
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SOLI DEO GLORIA

CURRICULUM VITAE

Gijsbert Korevaar is geboren op 11 april 1974 te Dordrecht, maar opgegroeid in Sliedrecht. Hij is getrouwd, heeft twee kinderen en woont in Den Haag.

Vanaf 1986 bezocht hij het Gymnasium Camphusianum in Gorinchem en behaalde daar in 1992 zijn diploma. Daarna studeerde hij Scheikundige Technologie aan de Technische Universiteit Delft en behaalde tevens een aantal vakken binnen de studie Wijsbegeerte aan de Universiteit Leiden.

In april 1998 studeerde hij af als scheikundig ingenieur binnen de vakgroep Anorganische Chemie op een onderzoek getiteld '*De synthese van siliciumcarbonitride dunne lagen met laser CVD en in situ analyse met massaspectrometrie*'. Dit onderzoek werd uitgevoerd onder begeleiding van dr.ir. W.F.A. Besling en prof. dr. J. Schoonman. Van mei 1998 tot juli 1999 was hij toegevoegd onderzoeker bij het laboratorium voor Anorganische Chemie, Technische Universiteit Delft. Hij werkte hier, in het kader van een door Novem gesubsidieerd onderzoek, aan de grootschalige toepassing van CO₂-laser geïnitieerde Si-depositie voor dunne-laags zonnecellen. Dit onderzoek resulteerde in twee artikelen (Korevaar et al., Journal de Physique IV **9**, 757-762 en Korevaar et al., Journal de Physique IV **9**, 763-768).

Van 1 juli 1999 tot 11 september 2003, was hij verbonden als promovendus aan de vakgroep Process Systems Engineering, waar binnen de Hoogewerff leerstoel voor '*Duurzame Chemische Technologie*' het onderzoek ten behoeve van dit proefschrift werd uitgevoerd. Tijdens dit onderzoek werden tevens 6 afstudeerprojecten begeleid. Gedurende deze periode was hij ook nauw betrokken bij de vormgeving en ontwikkeling van de keuzevakken '*Sustainable Technology I*' en '*Sustainable Technology II*' en '*Industrial Ecology*'. Verder coördineerde hij de ontwikkeling van het inleidende vak '*Introduction to Sustainability and Grand Cycles*' voor de propedeuse van de nieuwe Bachelor of Science studie '*Sustainable Molecular Science and Technology*'.

Vanaf 1 oktober 2003 is hij de projectcoördinator voor de ontwikkeling van een nieuw Master of Science curriculum '*Industrial Ecology*', het resultaat van samenwerking tussen de Technische Universiteit Delft, de Universiteit Leiden en de Erasmus Universiteit Rotterdam.