Sustainable Technological Development in Chemistry

Improving the quality of life through chemistry and agriculture

Report of the
Netherlands' Foundation for Development of Sustainable Chemistry

Wageningen
The Netherlands
1999

Sustainable Technological Development in Chemistry

Improving the quality of life through chemistry and agriculture

Report of the

**Netherlands' Foundation
for the
Development of Sustainable Chemistry**

Wageningen
The Netherlands
1999

Represented in the board of the Foundation for the Development of Sustainable Chemistry:

Akzo Nobel
DSM
Rabobank Nederland
Shell International bv

Ministry for EZ, Economic Affairs
Ministry for VROM, Housing, Spatial Planning and Environment

ATO-DLO
TNO
Twente University of Technology
University of Nijmegen
Wageningen University and Research Centre

The publication of this report was made possible by the Netherlands' Ministry for VROM and Rabobank Nederland.

Ministry of Housing,
Spatial Planning and the Environment

Rabobank

Colophon

The original version of this report appeared in November 1997 under the title: 'Duurzame technologische Ontwikkeling Chemie, vijf technologie ontwikkelingsvelden, onderzoek op maat'. It was written by Willems & van den Wildenberg (Marion H. J. Braks), The Hague, at the behest of the multidisciplinary and interministerial research programme DTO Chemistry.
In 1998 the chapters were updated by the Foundation for the Development of Sustainable Chemistry (DCO). Several members from the DCO forums contributed to the changes in the text with suggestions and information on new developments.
This publication was provided by an editing committee consisting of A.Herman de Rooij, (Editor-in-chief), Jan J.M. Mulderink and Wim F.W.M. van Heugten

Translated from the Dutch by Patricia A. Gosling of Epsilon Communications (Amsterdam).

Acknowledgements

The Foundation wishes to thank all who contributed to the accomplishment and the production of this report.
Special thanks to Willems & van den Wildenberg, (The Hague) for making the publication of the English version possible.

ISBN 90 – 804863 – 1 – 0

Contents

Introduction

A truly sustainable society will use only recyclable materials and energy sources. The reduction in consumption of fossil fuels such as oil, natural gas and coal is important — even critical — in the coming decades. In the long term, however, this prediction points to a doom scenario with the continuing exhaustion of resources and a decrease in the quality of society. In addition, excessive use of fossil reserves, now and in the near future, entails an increased dependence on countries in which political and economic problems can arise.

The challenge of renewability is immense. In the next fifty years the world's population will grow to approximately 10 billion people, all of whom will want a better life than their predecessors. This situation will manifest itself in an explosive need for more energy, urban growth, and a growing desire for private automobile ownership. The Dutch government, which is conscious of these social developments at home and abroad, took the initiative in the early 90s to establish a multi-disciplinary and interministerial group that poses the question: "What can we do technologically to reach the middle of the 21st century with a minimum of crisis and upheaval?"

In "Opportunities for tomorrow" from: DTO Vision 2040 - 1998, Technology, key to sustainable prosperity [1] , (see p. 9), approaches and possible solutions are treated in detail.

In addition to discussing topics such as transport, construction, food supply and water, the group quickly became aware that chemistry should play a special role in achieving a sustainable society. Chemistry is the driving force in all life processes and its technology is used in a vast number of products that determine the quality of modern life. Some examples are soap, pharmaceuticals, gasoline, textiles, leather, glue, dyes, modern building materials and plastics.

Chemistry is concerned with changes in materials. These materials should, eventually, derive their raw materials from bionatural sources rather than geonatural sources (fossils and minerals). In the long term, inorganic products should, if we want to continue to use them, be recycled. Organic raw materials must come from agriculture as a source of energy as well as for chemicals. This means that in addition to energy use aimed at the direct conversion of radiant sunlight, agriculture will be an increasingly important factor in sustainability strategies aimed at renewability.

Agricultural products are formed indirectly by the reduction of water and CO_2 with the help of solar energy and are renewable as long as the sun shines. Water is needed to support agriculture, and in order to obtain it at the right location, energy is often required. Even though there is more than enough fresh water on earth for an ambitious agricultural policy, combining its use with energy demands a great deal of expertise and training. Also, possibilities for saline agriculture are not to be under estimated. The task for the 21st century and beyond is to forge new links between water for the biomass and energy availability, on the one hand, and an appropriate education level on the other.

The question of whether or not there is sufficient available land for food stuffs and energy sources on this planet, and enough radiant energy from the sun, can be answered without any hesitation: "It is there in abundance." See the essay: renewable starting materials for the chemical industry" by C. Okkerse and H. van Bekkum [2].

In this report, great emphasis is given to the importance of agricultural products, their potential conversion to energy sources and their applications for fibre-reinforced construction materials.
Another potentially important technology is the conversion of sunlight into electricity such as occurs in the leaves of plants. Parallels with nature exist, even though conversions with inorganic materials have, until now, shown the most promise. The ability to control chemical reactions runs like a thread through the following chapters. The goal is to achieve high reaction efficiencies and to use fewer starting materials, both of which will lead to a reduction in environmental stress.

The five areas of development described in this report are the result of discussion in the discipline Chemistry of Sustainability. It is important to state here that the areas of development were established in collaboration with industry, government and the scientific community — the parties that hold the key to a sustainable society in the future. The choice was strongly influenced by the realisation that the developmental areas must have a large quantitative result on the production of goods and energy in order to provide earth's growing population with a better quality of life.

Operating for just two years, this programme has led to a number of current projects as well as to various projects that are still in the early phase of subsidy consideration.
An important additional point is that in the platforms, extensive exchange between the various parties may result in the emergence of surprising new developments.

Jan J.M. Mulderink

Chairman of the Netherlands' Foundation for the Development of Sustainable Chemistry

References:

[1] "Opportunities for tomorrow" from: DTO Vision 2040 – 1998, Technology, key to sustainable prosperity, Multi-disciplinary Research Programme for Sustainable Technological Development (Publisher: Ten Hagen & Stam, The Hague, December 1997)

[2] "Renewable starting materials for the chemical industry", from the work Duurzaamheid en Chemie (Sustainability and Chemistry) (Publisher: Programmabureau DTO, Delft, 1996, ISBN 90-5697-003-8). (in Dutch)

Opportunities for Tomorrow

A SUSTAINABLE SCENARIO takes into account a growing world population and increasing prosperity. More prosperity for more people. It might appear impossible, but it is a must if social justice and global stability are to be maintained. At the same time, ecological equality is needed to safeguard the quality of life of present and future generations. In a sustainable scenario ecology and economy need no longer be regarded as opposites. They can overlap and actually strengthen one another.

A SUSTAINABLE FUTURE HAS EVERY CHANCE OF SUCCESS. The environmental quality of a product is an increasingly important selling point. More and more people are opting for agricultural products which have been grown without the use of pesticides or fertilisers. More and more people are prepared to pay a little extra for electricity generated from sustainable energy sources. These are significant trends, because they open up new opportunities. Slowly but surely the whole concept of 'value' is changing. Economic value now tends to lie in services rather than in material products, making it possible to economise on energy and materials. Whereas now ownership of a car tends to be regarded as an indication of status and wealth, in the near future status will be measure by a person's ability to travel from A to B in comfort. Which particular mode of transport will prove the most appropriate remains to be seen.

AND A SUSTAINABLE FUTURE IS ACHIEVABLE. There are very few technological obstacles. Many of the steps towards sustainable development can be achieved simply by improving co-ordination between the various parties concerned. For example, efficient consultation between water boards, local authorities and drinking water businesses can lead to town and country planning being better structured to meet the demand for clean water. Other steps can be achieved by breathing new life into existing technologies or making more efficient use of them. Examples are the use of raw materials of vegetable origin for the production of basic chemicals and the construction of underground pipe networks for the transportation of goods. There are also a number of promising new technologies still in the early stages of development, for example in the fields of informatics, telecommunications, biotechnology and nanotechnology. Their application requires a minimum of raw materials and energy. They are therefore in a position to contribute to rapid economic and sustainable growth into the next century.

IT IS POSSIBLE TO BECOME TWENTY TIMES AS EFFICIENT in meeting demand for food, water, transport, housing and chemical substances used for materials and products. This means that demands can be met without damaging natural ecosystems, without causing a build-up of waste products and without exhausting supplies of raw materials. The STD programme has brought to light ways in which this can be achieved within two generations. In a process of 'learning by doing', the future of a number of crucial technologies and organisational innovations has taken shape. This will lead to a factor twenty improvement in efficiency within fifty years. No corners will be cut. Things will not be done less well, but they will be done very differently. No lessons in frugality, but the breaking of new ground in the name of progress.

Taking the future as your starting point

THE ACHIEVEMENT OF SUSTAINABILITY requires fundamental changes in almost every aspect of society. Not only the step-by-step improvement of existing technologies and systems, but also completely new ideas: new resources and materials, different production techniques and fresh organisation structures. Innovation opens up new opportunities, but also involves an element of risk. It is a question of trying to respond as well as we can to developments we can only guess at. To this end we sketch an overall outline of what we expect the world of tomorrow to look like. This can be used by decision makers as a teamwork on which to base innovation.

TAKE A JUMP IN TIME, and sketch the world as you think it will be around fifty years from now. Not a science fiction novel, but a realistic picture of a sustainable future. Not a blueprint, but a charcoal drawing of the world of the millennium generation: of those children born after the turn of the century. They will grow up surrounded by new technologies, familiar with the formation of networks, teleworking and teleshopping. It could be that fifty years form now the daily journey to school or to the office will have become a thing of the past, in the same way that nowadays we no longer pay a daily visit to the coal merchant to fetch briquettes. Maybe by then the use of coal, oil and gas will be on the wane, just as we no longer use turf. Other modes of transport may have taken over, and significant shifts in diet my well have occurred.

A LONG-TERM VISION ACTS AS A CHALLENGE, and stifles the natural tendency to extrapolate. Thinking fifty years ahead broadens our outlook and gives creativity and inspiration a chance. It provide a point of reference for sustainable technological development. The exercise of reasoning backwards from an image of the future – a method known as backcasting – brings to light ways in which sustainable development can be speeded up. Backcasting entails interaction between the future and the present, and generates ideas for both long-term and short-term innovation.

Technology in the context of culture and structure

TECHNOLOGY IS NOT AN END IN ITSELF, but a means of meeting needs. The usefulness and necessity of technology are determined by cultural and structural factors. Cultural factors determine which products and services a society demands, and which technological solutions for the meeting of those demands the consumer of the future will regard as acceptable. Structural factors, such as the way in which a society is built up, determine the relationship between supply and demand. Sustainable development is not often restricted by technological limitations. For example, in technological terms it is not difficult to switch from fossil fuels to biomass. It is far more of a challenge to make the necessary adjustments to the energy supply structure and the chemical sector. Similarly, the transition from meat to novel protein foods poses no real technological challenge. Of far more significance is the success or otherwise of the required socio-economic transition, and the consumer's willingness to change his or her dietary habits.

AN INTEGRAL APPROACH to cultural, structural and technological factors must be taken in order to bring about sustainable innovation. The STD programme points out, for example, that a system for sustainable water management requires not only better purification techniques but also improved co-operation between water management authorities, water companies and local authorities. A sustainable passenger transport system demands both the development of new modes of transport and a way of distribution the vehicles available to meet precise transport demands. Sustainable production is of little use unless we also address the whole life cycle of products, from the extraction of raw materials to the processing of waste products.

A BROAD SUPPORT BASE IS A KEY TO SUCCESS, and a foundation on which to build. The support base will be stronger when innovations do not originate exclusively from the drawing board but are developed in consultation with those who are ultimately going to be using them. We refer not just to the shareholders, but, more importantly, to the stakeholders: involved parties from other disciplines, other companies suppliers, consumer organisations, centres of excellence, social organisations and government bodies. The contribution made by third parties to the whole innovation process is crucial to its success. The extra time involved at this stage will be more than recompensed in the future.

THE STD PROGRAMME was carried out in consultation with a large number of target groups. They were actively involved in the development of scenarios and in the setting up of demonstration projects. For example, a system for distributing transport demand in the area of passenger transport was developed together with representatives from passenger organisation and transport companies. A programme for meat-substitute products was carried out together with producers and consumer representatives. A trial project for sustainable water management was initiated in consultation with administrator in Overijssel, the Netherlands. Interim results were continuously discussed with involved parties via workshops, round-table conferences and symposia. This increased the impact of the programme, and maximised the likelihood that the plans developed will indeed ultimately lead to a sustainable reality.

A future in the making

The development of sustainable technology in the long term requires a completely new working method – one which will encourage and stimulate a break with current trends. We cannot explore promising innovations and virgin territory without radically adjusting our thinking. We need to sketch a long-term scenario as a guide for short-term measures. A method for this was developed during the STD programme. It can be summarised in the form of five golden rules.

1. Develop your views on sustainability

Growth is possible, but growth without sustainability will eventually become untenable. Innovations are not likely to succeed unless they are expected to lead to sustainability in the long term. Consider, therefore, how production and consumption can be maintained without causing the depletion of resources, without damaging the ecosystem and without the build up of waste products.

2. Take the future as your starting point
Long-term thinking works as a challenge, generating creativity and presenting an opportunity to break free from the restrictions placed upon us by present day know-how. An ambitious idea of the future can form a framework for promising innovations and for niches which in the long term have the potential to develop into dominant technologies and products.

3. Co-operation is essential
Technological development is the fruit of intensive co-operation between a number of parties at a pre-competitive stage. The STD programme stimulated this form of co-operation giving rise to the formation of new, sometimes unexpected alliances. The involved parties work out the results of the programme further in this context.

4. Develop a strong support base
Technology without a strong support base is like a fish out of water. Technology can only produce results if there is a demand for it, if the users for whom it is intended accept it and if the society structure makes room for it.

5. Good results depend on inspiring project leadership
Sustainable development is both innovative and ambitious. It is not a question of following well-trodden paths. It demands idealism, creativity and expertise. An inspiring project lead can mobilise these factors and at the same time ensure that the project stays on course.

Source: "Opportunities for tomorrow" published in: DTO Vision 2040 – 1998, Technology, key to sustainable prosperity, Multi-disciplinary Research Programme for Sustainable Technological Development (Publisher: Ten Hagen & Stam, The Hague, December 1997)

Chapter 1: Background

Description of the organisational structure of DCO (Foundation for the Development of Sustainable Chemistry)

1.1 Status of this report

This report "Sustainable Technological Developments in Chemistry: Five Areas of Technological Development" serves as a primary document for sustainable technological developments in chemistry. It is a compilation of suggested topics of discussion and policy ideas with regard to starting points, general stipulations, and structure, for those interested in initiatives in the field of sustainable chemistry.

This report is aimed at policy makers in government, industry and research. It is meant to be a challenge to researchers to embrace the theme of sustainability in their research agendas.

The project that forms the basis of this report was carried out under the auspices of the multi-disciplinary and interministerial programme Sustainable Technological Development (DTO). Financial support for the DTO Chemistry project was provided by the Ministries of Economic Affairs (EZ), of Agriculture, Nature Management and Fisheries (LNV), of Transportation and Water Management (VW) and of Housing, Spatial Planning and the Environment (VROM), and the Dutch companies Akzo Nobel, DSM, SEP and Shell.

For some of the topics discussed here, there is still an insufficient network for accessing existing information; in particular, efforts were made to provide a structural framework and support to those with accessible information. The "ball" structure, with a number of starting points, is the central focus of this report. It refers to the need to define and initiate projects of a different character: R&D projects, fundamental research, competitive technology analysis, studies, evaluations, tests, brainstorming sessions, etc.

For a number of topics, an outline has already been formulated with members of industry, research institutes and the government, for a few relevant projects.
On the basis of this report, discussions will arise, subjects already chosen can be pushed ahead and furnished with additional detail, and new topics can be added and expanded upon.

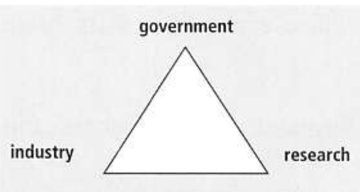
1.2 The DTO Chemistry Concept

The only way humans are going to survive in the long term is through sustainable development, i.e., the development of renewable materials. This will lead to a decrease in the use of scarce raw materials such as fossil fuel sources and reduce negative impacts on the environment. Achieving these aims requires a strong understanding of technological and cultural processes. Industry will have to change from its current, often short term strategies, to long term strategies and adopt a broader vision.

Why are long term developments necessary? If a considerable reduction is to be made on environmental stresses in the face of a doubling of the world's population in the next 50 years (coupled with a quadrupling of affluent society), then it will be necessary to increase energy efficiency by a factor of 10 to 20. With the help of incremental improvements and new designs, a significant advance can be made in the area of sustainability. To obtain the necessary reductions in energy use, however, a great leap forward, must occur. This leap can only be achieved with trend-breaking technology; for this to happen, long term technological development is critical.

New products and processes are launched onto the market by industry. Industry decides how products are created and produced; as a result, it determines the sustainability effect. To achieve a sustainable society, the role of industry must be central. Industry cannot, however, go it alone.

It is clear that co-operation with other participants — from an international perspective — is necessary for harmonious development. The government's role is to stimulate sustainable developments, establish clear goals, and define society's needs. Financial support is critical, particularly, in the planning stage.
The research institutes and universities must define the problems, generate expertise and develop technology.
The co-operation of industry, government, and research is the core of sustainable development. The activities of the three participants are played out in a different time frame, as depicted in figure 1.1:



	long term	short term
government	++	++
research	+++	+
industry	+	+++

Fig. 1.1: Cooperation of industry, government and research

Even though long term research is essential, the chemical industry is forced by competition to gear itself to short term profits. In this regard, the government can play an important role in guiding technological developments through regulations, contracts, financial support, strong educational opportunities, etc. In co-operation with the chemical industry and the research sector, appropriate projects can be defined.

Choices for long term technological developments can mean business opportunities for the short term. Making the right choices is difficult, however, as is finding the right path to short term opportunities that will lead to long term goals.

Figure 1.2 summarises the scheme described above: based on a vision of creating a sustainable future in fifty years (back-casting), the direction can be determined for an R&D agenda. The time frame for the development of a technological idea to a large-scale use of the technology is often very long. Only after the technology has made a large-scale impact can the desired sustainability effects be felt:

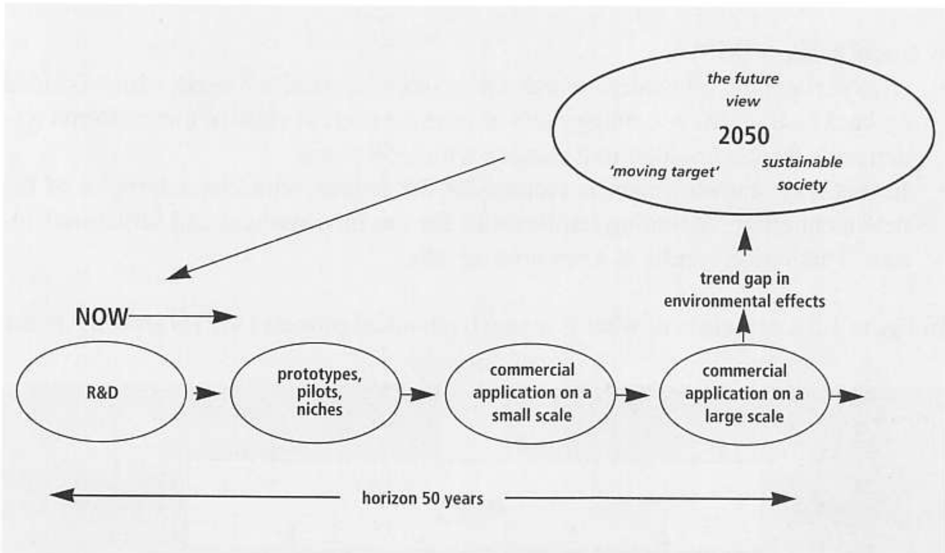


Fig. 1.2: Long term technological developments

It is important to recognise that sustainable development is not at cross purposes to the current developments in the chemical industry. The trends in the chemical industry are characterised by scaled-up operations, globalisation of business units and holdings. This trend will continue for several decades. In addition, this report identifies the trend of niche formation and small-scale decentralised production systems.

Although this appears to be contradictory, in the next 50 years — the period in which this report is concerned — these two developments will occur simultaneously.
This phenomenon has to do with the on-going individualisation in society. In spite of the strong tendencies towards globalisation — with greater product units as a result — most people want to retain control over a number of elements in their lives, even if it involves higher costs. In addition, reduced transport costs on a small scale promote sustainability. In order to achieve real changes in the next 50 years, a start must have already been made. Technological and infrastructural breakthroughs require a great deal of time. During the course of developments, a number of adjustments will naturally have to occur.

1.3 DTO Model Process

Within DTO, model processes are often referred to. Because it lacks a general definition, the term is used sparingly in this report.

A model process (MP) is :

- an experimental, innovative search for a concrete, specified need, which is aided by backcasting: the reasoning derived from a coherent view of the performance-demands that technology must satisfy within 50 years.
- In this way, a clear vision is created for the public: with characteristics of the new technology, including implications for the Environment and Structure/Culture. This vision results in a research agenda.

In figure 1.3 a depiction of what is meant by a model process (MP) is shown. On the

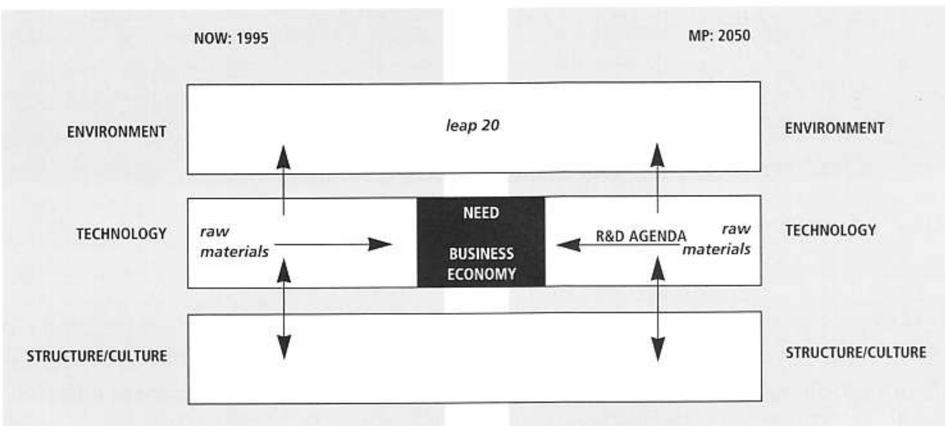


Fig. 1.3: DTO Model Process

left is a schematic diagram of the situation in 2000: how will available raw materials be converted to meet a certain need?
By "need" the corporate-economic foundation (the market) plays a crucial role. Current products and production processes have an impact on the environment as well as having an effect on economic structure and culture. On the right is a view of the future. The intended technology for the future must be, in DTO terms, a factor of 10-20 more (environmentally) efficient while satisfying minimal needs. New technology will have consequences for the economy and culture. An R&D agenda must be established concurrently to indicate the necessary steps for achieving the desired technology on a large scale.

1.4 Steps / Construction DTO Chemistry

Within DTO chemistry, parallel work has been carried out on the following steps to determine how needs and solutions mutually influence each other. In the following outline, these steps will be individually treated with emphasis placed on co-operative R&D endeavours. These steps are:

1. Outline future vision DTO Chemistry (backcasting)
2. Select model processes
3. Define technology-development fields
4. Start R&D collaborations

Step 1: Future vision DTO Chemistry through backcasting

Backcasting is the creation of a vision derived from the following questions:

- What will the (material) needs of society be in 2050?
- What does sustainability mean? In particular in terms of chemistry
- How can the chemical industry contribute to sustainability?

This vision was created in collaboration with a number of prominent representatives from political, government, scientific, and industrial sectors in the Netherlands. The latter includes members of both the industrial and financial spheres. It was agreed that the world population would double in the next 50 years and that urbanisation and individualisation would increase. Convincing also was the notion that energy consumption would grow considerably, with an increased need for electricity, in particular. Agriculture and chemistry will have a greater impact in meeting the needs for raw materials and energy sources.

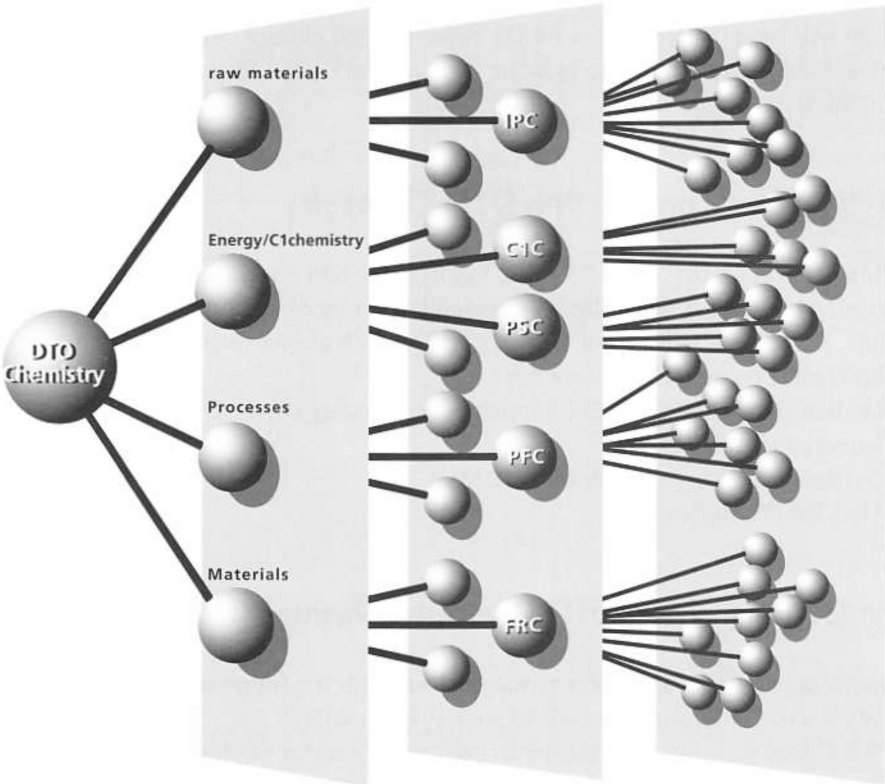
STEP 2: Selections of model process

Sustainable developments in chemistry can be described by two approaches:

1 Improvements in society, with challenges for chemistry

2 Improvement in the chemical sector itself

Both approaches are treated in this report.



Five areas for development have been chosen in the discussions for DTO-Chemie:

- *Integrated plant conversion (IPC)*

Valorisation of plant parts for raw materials and energy

- *Biomass conversion (C1 Chemistry)*

Technologies for (among others) C1-based chemicals and energy carriers

- *Photovoltaic cells (PSC)*

Technologies for the conversion of solar light into electricity

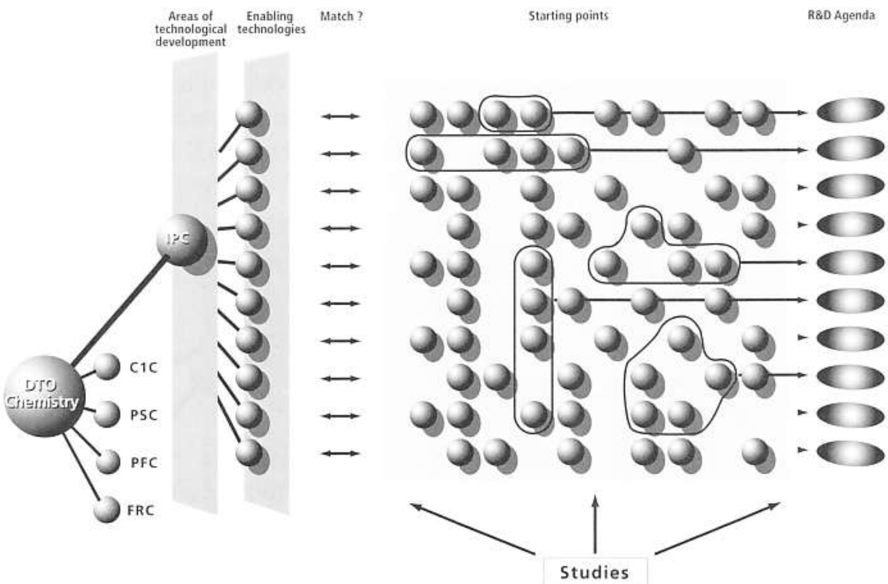
- *Process Technology in Fine chemistry (PFC)*

Methodology of manufacturing processes for Fine chemicals

- *Sustainable Construction Materials (FRC)*
Techniques for using fibre-reinforced composites in construction applications
These areas can be viewed as clusters of technologies, with a strong chemistry and agricultural component, which are necessary for achieving a sustainable future. Furthermore, it is important to recognise that technology requires a progressive development (technology lifecycle).

The five areas of technology development are tested against a number of criteria:
1 Sustainability / leap / volume
2 Horizon 2050
3 Commitment from industry
4 Recognisability / example of function
5 Step-wise approach
6 Technical feasibility / risks
7 Innovation
8 Ability to be anchored in the expertise infrastructure

Step 3: Development of the areas of technology development

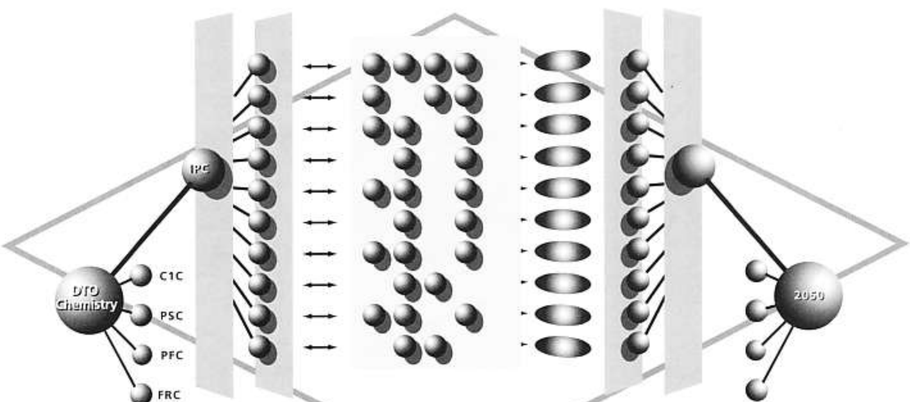


The five areas of technology development were defined according to a standard format. Relevant questions are:

- *justification:* why can this particular technology contribute to a sustainable society? What are the impulses for its development? Drawbacks are also considered.
- *description:* how do we define this technology? What are the starting points (technology suppliers and users, intermediaries)? What is the current state of the technology? What is its economic position?
- *long term vision:* What is the vision for the future; more importantly, which paths must we take to get there? What are the ten most important technologies for achieving this vision (enabling technologies)? To what extent are these technologies already available? (match with starting points). What barriers need to be overcome?
- *R&D agenda:* What research must be done now to make the long term vision and the path towards it, possible? It is crucial to initiate selected R&D options and to keep generating new options. The emphasis of the R&D agenda will be on the near future, in which the long term will also be investigated. Initially, studies will primarily be necessary for obtaining a clearer vision of the technology, future, and the R&D that is necessary to achieve them.

Step 4: R&D collaborative network

The identification of topics for sustainable technological development begins with a divergent process: 'which topics are interesting? What are their technological possibilities? How can a need be translated into technological action?' It is important, at



some point, for convergence to occur and that a start is made on drafting a clear and acceptable plan of action. Because the aim is towards a 'moving target' (the future is not predictable: what will the needs be, how many people, calamities, what is technically possible, etc?) this action plan must be continually adjusted in the direction of the goal. This report should be seen as the first step; the analysis has been partially carried out and the R&D projects mark the beginning of the achievement of this goal.

In the meantime, all five areas of development are being managed by forums consisting of representatives from the government, business sector, and academia. This will lead to an increasing stream of initiatives and precompetitive projects. Government subsidies will have an important role to play in this regard.

Chapter 2: Sustainable Chemistry

Identification of Technology Development Directions

2.1 Introduction

Designed not only for those who work in chemistry on a day to day basis, this report is also aimed at policy makers and others who work in the area of sustainable developments. An overview of chemistry and the chemical industry is given in this chapter. The overlap between sustainable development and sustainable chemistry is much greater than at first appears: chemistry is the field of material change and therefore has a direct connection with material sustainable development.

2.2 What is chemistry?

The figure below gives an idea of chemistry's relevance to sustainable development: Chemistry as intermediary between raw materials and secondary materials. Chemistry is both an economic factor and a scientific discipline, although it encompasses even more than this simple definition.

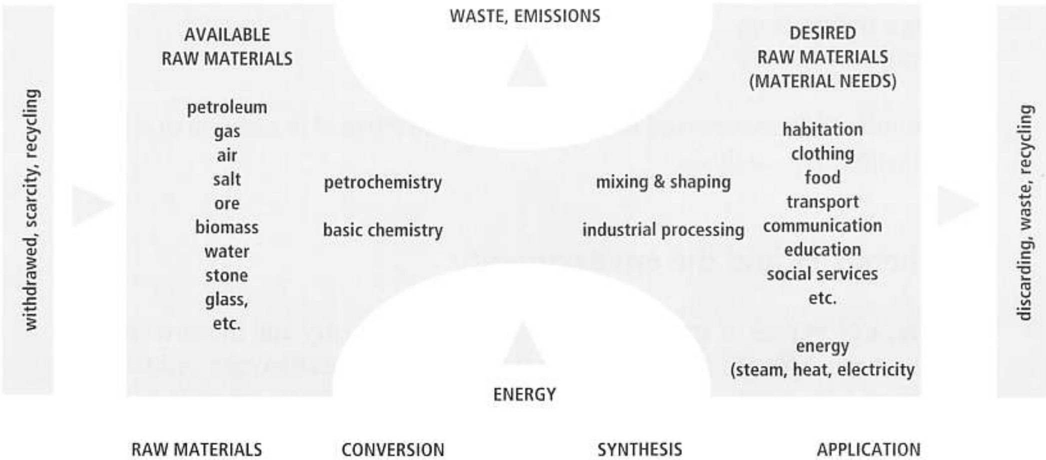


Fig. 2.1: Chemistry

2.3 Chemical research

The research carried out by the Chemistry departments in Dutch universities and institutes such as TNO and DLO will not be discussed in detail here. The Survey Consulting Committee (OCV) offers in its report 'Chemistry in Perspective, A perspective of the supply and demand in chemistry research' a description of the scientific and academic status of the field of chemistry. One of the observations the report makes is that striving for sustainability and minimising impacts on the environment have become important prerequisites for all new scientific and industrial activities. Chemical processes must become cleaner, use less energy, and deliver purer products. In addition, the chemical industry must ensure that products and materials can be recycled into the production chain in order to decrease stresses to the environment.

The areas of emphasis as defined by the commission "Future Chemical Research" (TCO) of the Royal Netherlands' Chemical Society (KNCV) and the Association of the Netherlands Chemical Industry (VNCI) provide a good indication of the important areas in which industrial and university research in the Netherlands will be directed in the future:

- catalysis
- biotechnology
- material technology
- process technology
- interfaces and thin layers
- separation technologies
- molecular modelling
- design and rheology
- pharmacochemistry

Top institutes for polymers and metals have been established in addition to a Top research institute for catalysis

2.4 Chemistry and the environment

Recently, a great deal of attention has been paid to chemistry and the environment. Much has been achieved in the chemical sector through so-called care-, end- of pipe and process-integrated emission reduction: waste and emissions have been drastically reduced by several tens of percentages. This has all been achieved with existing technology. In order to reach a reduction by a factor of 10-20, however, new technologies must be developed. The following is a short summing up of a number of recent developments in the Netherlands. for abbreviations see the Glossary.

- Responsible Care - VNCI
- Covenant chemistry with Economic Affairs
- DTO Chemistry and DCO
- Sustainable Chemistry: Association Nature and the Environment, Organisation Environmental Defence
- Conferences
  Nature as a source for chemistry, KNCV 1995 annual conference
  Chemistry as a source for energy, KNCV 1998 conference

2.5 Chemical sector

Chemical industry
The chemical industry is concerned with transforming the structure of raw materials (primarily minerals, metals and hydrocarbons) into manufactured goods and products in response to the needs of other industries and consumers. The chemical industry is often divided into a number of principal sectors:

- petrochemicals
- specialty chemicals
- fine chemicals
- pharmaceuticals
- agro-chemicals
- synthetic textiles
- inorganic chemicals
- salt / chlorine chemistry

The trade between these sectors is just as large as that with end users. These sectors (except for inorganic chemicals and salt/chlorine chemistry) are based on fossil materials.

According to the VNCI, almost 15% of the entire Dutch industrial turnover is the result of chemical activity. The Netherlands is second in the world in terms of chemistry-intensive countries, Belgium is first.

Consumers
Chemistry plays a role in practically all other industrial sectors including agriculture, the electro-technical, pharmaceutical, packing, energy service, and automobile industries.

There are numerous connections between chemistry and businesses, establishments, and other members of Dutch society that at first glance have little to do with chemistry. The following paragraphs provide some brief examples.

First, there is society, which continues to put pressure on the chemical industry to act in an environmentally responsible way. At the same time, society is one of the primary consumers of chemical products.

The energy and chemistry sectors are profoundly linked. The chemical industry is a vast consumer of energy and the energy sector makes use of chemical processes. Furthermore, both sectors use the same fossil-based raw materials.

The connection to the metal industry is clear. Raw materials are obtained from ores using chemical processes. Blast furnaces are just one example.

There are many links to the agricultural sector. Chemical products such as artificial fertilisers and pesticides are used on a large scale, but the chemical industry is also a consumer of agricultural products. Oils and fats are extracted from crops and converted into margarine and other types of shortening. Many raw materials are obtained from plants and converted into useable medicines. And of course fibres can be converted to (bio)composites. There are many more examples, too numerous to list here.

Suppliers
Suppliers to the chemical industry include equipment manufacturers, engineering firms and the chemistry from semi-factories.

The future
In the future it is likely that the boundaries between the chemical and other sectors will continue to be blurred. An electricity plant will not only produce electricity and heat, but liquid and gaseous fuels and raw materials for the chemical industry as well. The reverse is also likely: a chemical company, in addition to producing liquid energy sources or plastics, will also provide electricity.

2.6 Raw materials in global perspective

The retrieval and consumption of fossil and mineral raw materials leads not only to a depletion of these materials, but also to changes in the ecosystem. Unrestricted policies regarding current raw material use, coupled to growing population and consumption, will have far-reaching negative implications for the environment.

Energy requirements, including transport fuel, are the greatest consumers of fossil raw materials. Approximately 85% of the current commercial energy needs are provided by these non-renewable petrochemical materials (ca.40% oil, ca.25% coal, ±20% natural gas). Transport fuels make up a major portion of petroleum oil consumption (>50%).

Inorganic materials are often used for construction or specific applications (for example: catalysts, conducting materials, and artificial fertilisers).

In addition to these fossil and mineral raw materials, biomass is also an important source of starting material, not only for food, but also as chemical and construction material. In the figure below, this is referred to as traditional biomass, due to its traditional applications.

In the future, the emphasis will be on renewable raw materials and sustainable technologies. The shift from fossil fuels to biomass raw materials is shown schematically in figure 2.2. Even though fossil materials will undoubtedly be used in 2050, this is not explicitly shown in the figure.

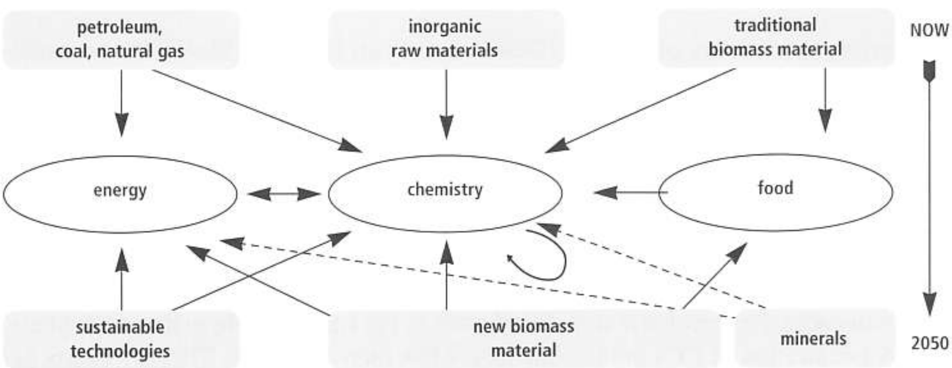


Fig. 2.2: Raw materials, now and in the future

The outline sketched below is applicable to the 'first world' (Western Europe, the United States, Japan, etc.), and the 'second world' (former eastern block countries, China, India, etc.). The 'third world' (developing countries; large parts of Africa and South America) has made few strides in industrial development, even though initiatives have begun in a number of these countries.
Important aspects of sustainability in view of current use of raw materials / chemistry are:

1. Inefficient use
Very often raw materials are used for one purpose, resulting in a vast amount of waste, partly due to the impurity of these materials. An integral approach such as cascading, for example, is a desirable development. In addition, the cost of transporting the raw materials from their source to the user, processing and consumption, requires too much energy. Much can be gained by processing materials closer to the user and by introducing energy-conscious regulations.

It is clear that current methods of utilising raw materials by the chemical industry cannot be called sustainable. It is not only undesirable to continue in this way, in the long term, it will be impossible.

2. Depletion as a consequence of using non-renewable sources
Opinions concerning the problem of resource depletion are strongly divided. In the report published by the Club of Rome, there was little optimism concerning the retrievable amounts of fossil and inorganic raw materials. Petroleum oil would be gone by the year 2000 and many metals such as gold, silver, tin and mercury would be depleted even sooner. Even though the supply of these materials appears to be much greater than previously assumed, it is clear that scarcities will occur.

According to a variety of sources (Okkerse and van Bekkum, Shell), the economically retrievable amount of fossil fuels, extrapolating from the current level of use, will be depleted within 100 years (petroleum oil 40-50 years, natural gas 60-75 years, coal >200 years). If yearly consumption increases, then this time frame will be even shorter.

3. Non-closed cycles (primarily involving carbon)
The enormous consumption of fossil fuels, along with large-scale deforestation in recent decades, has created a vast disturbance in the carbon cycle in the atmosphere. The concentration of CO_2 in the atmosphere has increased from 270 ppm (parts per million) in the pre-industrial age to 350 ppm currently. (Source: Shell publication). It is still a matter of discussion whether or not this will lead to a global increase in temperature.
The schematic concept of the Carbon-cycle is given in figure 2.3:

In several other processes and technologies, namely in the bulk chemical industry, emissions of CO_2 are unavoidable. In order not to further disturb the equilibrium, as well as to avoid the depletion of fossil resources, technology must be created that is in balance with the consumption and production of CO_2 (CO_2 neutral). Photosynthesis by plants is an example of such a process: CO_2 is consumed by the plant and converted to energy or chemical products. The net result is an equilibrium. With the

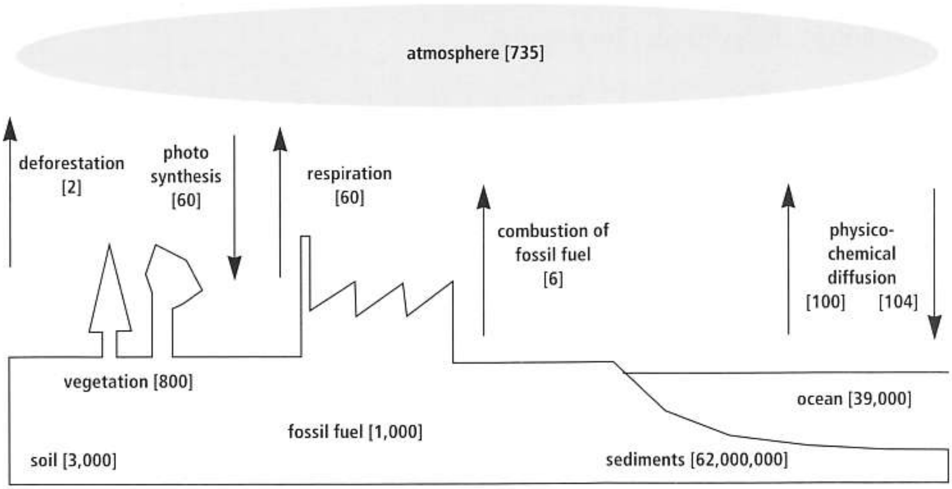


Fig. 2.3: Carbon cycle, in Gtons of Carbon (Source:Shell)

complete replacement of fossil raw materials by agricultural products, a balance will emerge in the carbon cycle in the atmosphere, in which the same amount of CO_2 is taken up as is emitted by combustion.

4. Pollution during fossil fuel production

The retrieval of petrochemical and other raw materials is often polluting as a result of leaking oil storage areas and disturbances to the natural environment. Unpredictable occurrences such as oil spills with oil tankers, drilling platforms, or terrorism or wars, can have an extremely damaging impact on the environment. Certainly at the local level, the consequences for the environment can be extreme (Exxon Valdez, Gulf War).

5. Dispersion

All materials that are retrieved from the earth are returned to the environment, either during processing or after use. These materials are released in dispersed forms. Metals such as copper and chromium, some compounds and gases such as CFCs, CO_2, SO_2, NO_x, etc. create ecological disturbances through an accumulative effect, resulting in loss of biodiversity, depletion of the ozone layer, acid rain, smog, etc.

6. Biomass availability

The question often arises if there is enough room to grow a sufficient amount of food (1st priority), for organic raw materials (2nd priority), and to provide for a large portion of energy needs (3rd priortiy).

In an essay by Okkerse and van Bekkum, a detailed start has already been made in a study of the biomass availablity. From their calculations it appears that there is sufficient room to provide for the needs listed above.
The opinions on this subject are widely divergent and the numbers need additional corroboration. It is also worthwhile to continue to investigate whether or not there is sufficient biomass to achieve the necessary goals. The possibilities of marine and saltwater biomass should be included. In addition to looking at technical feasibility, the following must be considered:

- scale size (regional, national, global)
- infrastructure (political / social)
- long term multi-disciplinary approach
- efficiency (optimise through genetic manipulation, etc.)

2.7 Topics for Sustainable Chemistry

In figure 2.4 the field of chemistry has been divided into four segments: raw materials, conversion, synthesis, and applications. By looking at the vision of the future through the lens of chemistry, one goal per segment is achieved. This can be translated into model topics, or model processes, in DTO terminology.

In the following paragraphs technologies are described that are critical for the vision of the future. The areas of technology development, which will be expanded on later, are presented on the following page:

1. Renewable raw materials: sufficient and clean starting materials (IPC)
It is expected that the need for raw materials shall strongly increase — in spite of the depletion of resources. Moreover, requirements in terms of recyclability will be even greater. Biomass as a new and important source of raw materials will coincide well with these new demands: it is, for the most part, available, suitable for all possible applications, and renewable. In addition to biomass material as an alternative for a number of applications is 'the inorganic group'. In this regard, it is necessary to take iron occurrence into account. There are, however, metal ores that are being de-

---

Explanation (fig 2.4, page 31)

The arced areas are R&D options for sustainable development. The oval surfaces indicate the area of technological development. It is clear that there is an overlap: for example, catalysis and seperation technologies are technologies that are important for several model processes.

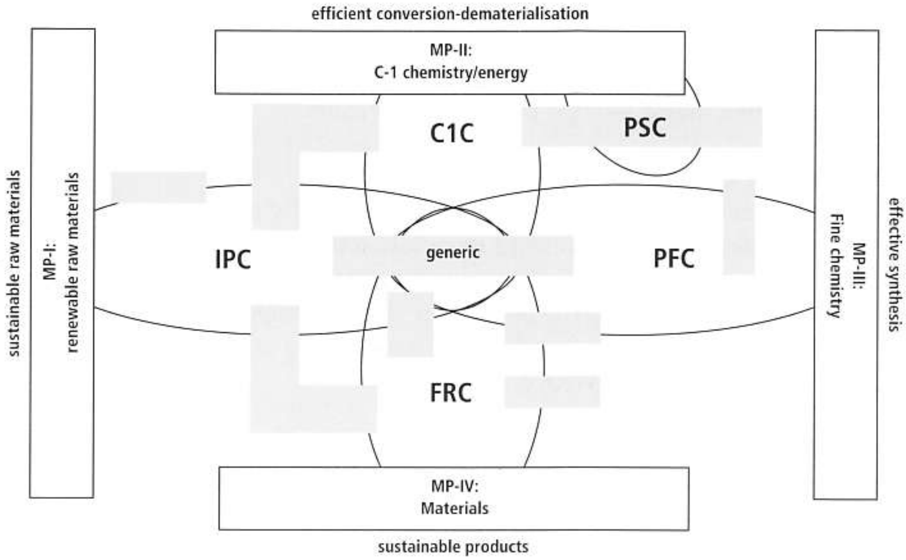


Fig. 2.4: Sustainable chemistry

pleted such as aluminium, copper, zinc and tin. Timely recycling is the solution for this problem.
Biomass material appears to have one of the greatest potentials as an important new raw material in the future

2. Energy / C1 chemistry: efficient conversion / depletion, PV cells (C1C, PSC)
Two partially coupled influences play a role in the current energy and bulk chemical industry: scarcity and non-closed cycles. It is necessary to approach and commercialise energy and materials in a new way, based on a frame of mind that embraces recycling. On the one hand, this can be achieved by using natural cycles, by using biomass as a source of hydrocarbon material. On the other hand, hydrocarbons need to be viewed as both storage and transport media for energy and as starting materials for products. Depletion and energy services will also play a role by ensuring efficient transport of heat and electricity during production.
Furthermore, PV cells and wind energy need to be developed in conjunction with storage and transport technology (this can take the form of a battery, but also be an energy source such as methanol or Fisher-Tropsch gasoline synthesised from biomass material).

C1 chemistry and PV cells have been defined as areas of technology development in order to provide for the future needs of energy and C1 chemicals. C1 chemistry is targeted as a new approach for hydrocarbon conversion. The new chemistry in PV cells and the usability of specific PV energy in chemical processes have led to the decision to further investigate the potential of PV cells.

3. Fine chemistry: effective synthesis (PFC)
The fine chemical industry generates an unproportionally large amount of waste in relation to the desired products. Until now, investments have been geared towards the development of applications. Process technology has fallen behind as a result. The optimisation level that can be obtained is still very high. A thorough analysis of this complex discipline and the establishment of existing and new technologies will provide a more detailed perspective.

In view of the relatively small process streams associated with the fine chemical industry, this sector can serve as a model area of technology development for other chemical and process technology sectors.

4. Materials: sustainable applications (FRC)
A distinction must be made between functional materials (such as photon-conversion materials for PV cells, for example) and construction materials. An important bulk use for materials is in construction. The current development of bulk materials is driven by costs and performance improvement in conjunction with sustainability: less material, increased performance, longer lifetime, recyclability, less energy throughout the entire cycle, advantages in the consumption phase, and lower costs are all areas that can be optimised. Materials are becoming more high-tech. New materials are necessary, furthermore, to satisfy the expected growth in material needs. Moreover, attention must be paid to the establishment of biomass raw materials in high-tech applications.

Fibre-reinforced composite materials form an area of technology development in which these goals are linked.

2.8 Generic Technologies

In the areas of technology development described in this report (part 3) three generic technologies are constantly mentioned as being key to sustainable development. Attention is justifiably focused on these topics (in some cases not enough) in a number of research programmes. These Generic Technologies for Sustainability are:

- Genetic manipulation
- Catalysis (including biocatalysis)
- Separation technology (primarily membrane technology)

Chemical as well as bio-technology is included in this sense; these fields are increasingly growing together.

1. Genetic manipulation

Plants need to be optimised to improve crop yields per square meter and to reduce the use of undesirable insecticides and herbicides. Optimisation can occur by natural selection (a slow process), or at a considerably faster pace through genetic manipulation. Modifying the genetic structure can influence biological processes. Examples are the insertion of the endotoxin gene from Bacillius thuringiensis for insect resistance and built- in herbicide tolerance, so that a more selective use of these chemical agents is possible. (source: TCO report, 1994).

2. Catalysis

Catalysis is already a focal point of research in the Netherlands, supported by the IOP Catalysis Programme and the Catalysis Research Institute. The role of catalysis in future processes will continue to increase. Bio- and chemical catalysis will continue to overlap.

A catalyst gets a reaction going; it increases the reaction rate and lowers the energy barrier, without being consumed during the reaction. In nature, the many proteins that function as catalysts are called enzymes. In recent years catalyst systems for regulating the exhaust from combustion engines have been increasingly improved. The same applies to the development of shape-specific catalysts, based on zeolites. Furthermore, important advances have been made with catalysts for oil refining. Currently, there is a great deal of interest in metallocenes, spatially specific 'single-site' catalysts, in which spatially regulated molecules can be made. Furthermore, chiral catalysts (for the preparation of medicines and pesticides, for example) and catalytic antibodies are of importance. The latter can be used for chemical conversions for which there are no enzymes available and which can support the high cost. (source: TCO report, 1994).

3. Separation technology

Improved techniques are needed, for example, for separating the usable parts of plants (without causing the rest to be unsuitable for use), as well as for other materials. Bio-molecular separation techniques, in particular, belongs to an area in which there is room for development.

A distinction can be made between traditional separation methods and new developments. Increasing concern about the environment has created a stimulus for separation technology. The majority of environmental problems can be traced to problems of separation.

Traditional separation methods include distillation, extraction, absorption, evaporation, crystallisation and centrifugation. Research and development in this area are primarily concerned with optimisation; the basic technology that underlies these methods has remained unchanged in the last ten to twenty years.
New developments in separation technology include membrane filtration, reverse osmosis, electrodialysis, paramagnetic separation, ion exchange and chromatography.

In the future, much is expected from membrane separation techniques, in particular. Membranes are actually a type of filter. The holes in the filter can be adjusted to separate specific molecules. Separation is also dependent on charge, temperature, pressure, and concentration differences. An interesting example of an application of membranes is in kidney dialysis, in which harmful waste products are removed from the blood.

(Source: TCO report, 1994).

Current state of the chemical industry

Of the three economic blocks, Western Europe is the most strongly oriented towards chemistry. Of the top ten corporations in Europe, eight are chemical companies. The international market has developed strongly in Europe, more than half of the OECD export occurs within Europe.
The US is an equally strong player in the chemical industry. Companies such as DuPont and DOW are in the top ten largest chemical companies in the world.
The export share of the US fell sharply between 1980 and 1990, an occurrence that can be explained by the strong pull of the domestic market. In 1992, the market share increased again. The level of investment in the US is rather low.
Even though market share is increasing, the impact of the Japanese chemical industry is limited to local areas.

Chapter 3: Integrated Plant Conversion

Valorisation of Plant Parts for Raw Material and Energy

3.1 Introduction

To preserve the quality of life enjoyed by modern society, an increase in the use of natural and renewable raw materials will have to be made. This chapter will define the characteristics of integrated plant conversion (referred to in this report as IPC) and the contributions IPC can make to the development of sustainable technologies and raw materials. IPC anticipates the future scarcity of raw materials and energy sources, which are now still available in sufficient quantities. Integral use of the plant and valorisation of the various components (cascading) play a central role in this approach.

Extensive research has already been done in the area of 'agrification'. Further technological developments will have to be based on this knowledge, i.e., the use of renewable raw materials for the production of non-food crops. This chapter will also present the initial results of agrification.

Compared to petroleum and natural gas, biomass materials are relatively expensive in western countries. One possible way to lessen this price difference is to make better use of the whole plant. Just as the various fractions of oil are used for various purposes, plants can also be used in their entirety. This is called integrated plant conversion. IPC is a general term that encompasses various techniques for making useful products from biomass materials that have a high added value.

3.1.1 Justification

The motivation for promoting IPC as an important technology for a sustainable future can be summarised by the following points.

Sustainable supply of raw materials
Renewable raw materials are an alternative not only to petrochemical raw materials, but to every kind of raw material. Imagine, for example, a car chassis made entirely of composite materials: rather than using metal for automobiles, composite parts could replace steel parts, etc. The point is to find an alternative to a whole range of raw materials used in construction, chemical compounds and as energy sources, etc.

Chapter 2 highlighted the worldwide sustainability aspects of raw materials.

Added advantage of energy retrieval
After the cascaded retrieval of high- and medium-grade substances from a plant, the low-grade waste substances can be transformed through gasification or other conversion procedures (HTU) into gaseous or liquid energy carriers.

New possibilities brought about by biotechnology
Genetic techniques can be used to alter plants in such a way that they produce more of a desired substance or less of an undesired one. The functionality of desired substances can also be altered to meet the market demand. Many products can be produced more easily from biomass material, with the help of enzymes and microorganisms, than from fossil fuels through various chemical steps. Moreover, this production will often result in a considerable reduction in energy consumption and waste.

New products based on specific properties
By making use of specific chemical, biological and physical characteristics of plants, new products can be developed.
Certain substances that commonly occur in nature are difficult or impossible to chemically synthesise (cellulose, fibers, proteins). There are many possible applications for these substances, but such applications often require extensive research and sometimes the development of very complex compounds.
An important perspective is offered by the chiral characteristics of vegetable substances. Unlike in nature, it is not always possible to chemically produce the desired stereo-isomer of a particular substance. This is particularly relevant for medicines or foodstuffs, because often only one of the many possible isomers has the desired effect. The other isomers can even cause undesirable side effects. By allowing these medicines (or foodstuffs) to be produced by plants or micro-organisms, the desired stereo-specific molecules can be produced. In this way the required dosage of natural products can be half that of chemically produced substances. Although plant waste can be problematic, some of its production can be prevented or the waste products can be used as energy sources.

Environmental impact of plant production processes
An vast number of products are based on plant-derived materials. The environmental impact of large-scale crop production and processing is often substantial. The most well-known example is the cultivation of cotton, which relies heavily on the use of pesticides. The production of viscose from cellulose is another environmentally harmful process. A new improved technology has been recently developed for this process by Akzo Nobel.

Agricultural interests
Experience gained so far with agrification has shown that agricultural interests are not the most important motivation for IPC. The increasing agricultural overproduction in western European countries is one of the reasons to develop the cultivation of crops for non-food applications. This transition was promoted in the past by the agricultural sector, but it has not yet led to the desired effects due to the low price of petrochemical raw materials. If a shift to the large-scale use of biomass material did occur, the capacity of the Dutch agricultural sector would be insufficient. Importation of crops, whether in raw or processed form, would then be necessary.

Biodegradability
One of the characteristics of biomass is biodegradability. Biodegradability as a primary characteristic is only important if it has a functional advantage either after or during use of the product. For many applications good material stability is a primary requirement. A roof drainage pipe, for example, should not develop holes after 10 years of use due to biodegradability. Efficient collection of refuse will always be important. Controlled decomposition of biomass is necessary to monitor the formation of methane. Burning or gassing in the new generation of electrical power stations is a good alternative. The advantage of biodegradability is largely compensated for if the recycling of materials is optimised. Examples of products for which biodegradability has a functional advantage are disposable nappies and certain types of plastic.

3.2 Description

3.2.1 Biomass

Biomass materials are defined here as all agricultural raw materials, including organic waste. This means that the term biomass encompasses a large diversity of trees, plants, grasses, roots, seeds, etc. Non-plant-derived biomass can also serve as a raw material (such as silk from silkworms and chitin from shrimp), but the (mass produced) plant is the most relevant source. Each one of these sources has a different composition built up from many components. The result is a very complex structure of raw materials and derivatives. Starch can be extracted from potatoes, corn and wheat, among others, and it can be used for the production of glucose or intermediate products such as coatings and foams. However, wheat can also be used as a source of cellulose, for the production of paper, textiles and various types of plastics.

Plants can be used in two ways for IPC:
- as a (mini-)factory of chemical products (often for the fine chemicals industry)

- as a raw material for the chemical and energy industries (often for the bulk chemicals industry)
In the first example, the plant produces substances called (secondary) metabolites. After being separated from the plants, these substances can be used almost directly as end products. Biotechnology and classical breeding techniques will play an important role in this area in the future, as has already been demonstrated by the efforts of a number of companies in this sector (Monsanto). Competition will always exist, however, between the various production techniques: chemical synthesis, and complete or partial biosynthesis with the help of micro-organisms or plants.

Plants are obviously a valuable raw material for chemical and production industries. Parts of plants are already used as industrial raw materials (fibres, oils, glucose, etc.). The determining factor in deciding whether or not to use plants as a raw material will always be their chemical structure in combination with availability and price.

An advantage of using plants for the synthesis of products can be the relatively low production costs (assuming that the concentration of the desired substance is high enough). A disadvantage is the seasonal character of crop cultivation and processing. In some cases it can be better to produce the desired substance in the plant's seeds, because they are easier to store. In this way the direct link between raw material production and processing can be severed, which is particularly important for the potential role of the Netherlands (see 3.2.3 and 3.2.4).

Some obvious possibilities for using biomass as the supplier of raw materials are various bulk applications such as the use of straw, hemp and flax fibres in composites and using oil from rape seed.

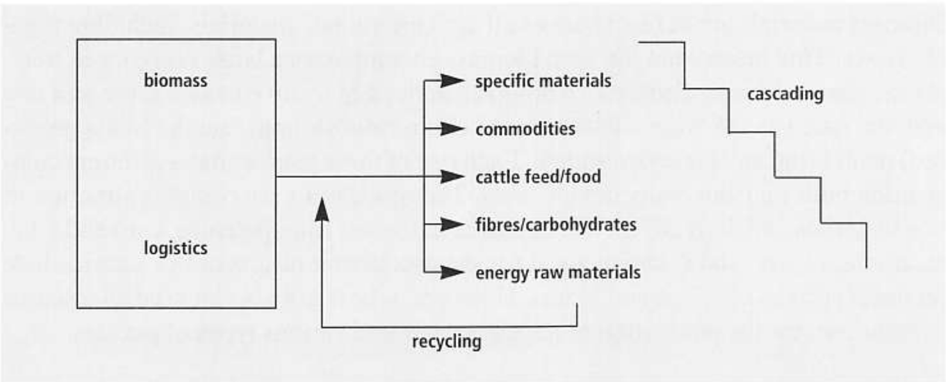


Fig. 3.1: Integrated plant conversion (IPC)

3.2.2 Integrated plant conversion

There are five possible approaches to using biomass as a raw material, in which the goal is always to achieve added value. These are presented graphically in figure 3.1.

Integral yield

By looking at the plant as a whole and splitting it up into its useful parts, the whole plant can serve as a raw material for various applications. One part of the plant could be used as a foodstuff, one part as cattle feed, one part as a raw material for the chemical industry, and the rest for gasification or fermentation. In this way, the entire plant becomes more valuable, which makes its use more economically attractive. Sugar beets, for example, can be processed into sugar, ethanol and cattle feed. Transforming the by-products into energy through incineration or gasification is almost always an option, but it does not always yield enough profit.

Certain secondary metabolites could serves as raw materials for the fine chemical industry. This is a risky undertaking, however, if the plant is not economically profitable without this retail market. Valorisation of the plant as a whole for the fine chemical industry, and especially for the pharmaceutical industry, is less attractive for two reasons:

First, the production volumes are too small to give a substantial added value to biomass material. In the fine chemical industry products are produced with a maximum volume of 1,000 tons per year. Second, the danger of alternatives is large, for example through fermentation or through the valorisation of waste streams with the help of micro-organisms. The danger of alternatives makes the risk high if a plant is cultivated for only one specific purpose.

Figure 3.2 illustrates the division of the hemp plant into separate useful parts.

Direct routes

One example of this approach is the use of unprocessed seeds, pits, or fibres as a shock resistant substitute for polystyrene foam. This area is not widely developed because quality has not been consistent.

Cascading

If the product stream can no longer be used in its present application, processing will be modified to achieve another high-grade or different lower-grade application. Eventually it can serve as a raw material for energy retrieval. Every resource in an agricultural product will have to be utilised. In effect this makes use of the 'ladder of Lansink' (a method for weighing the advantages and disadvantages of possible applications) formulated by a member of the Dutch parliament, A. Lansink. In this way the highest possible yield can be obtained from a raw material.

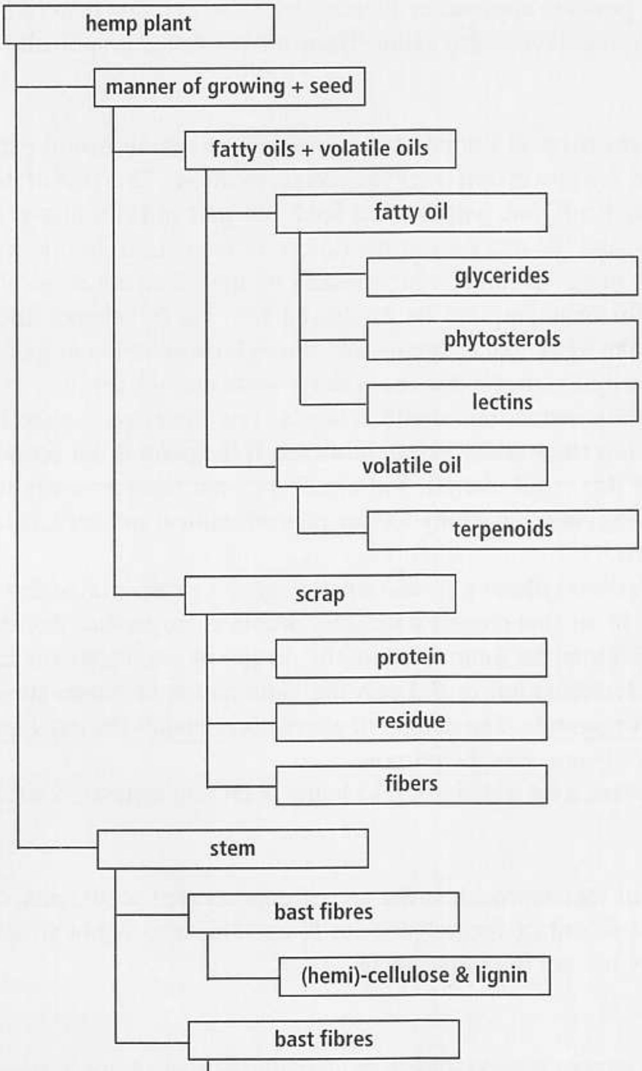


Fig. 3.2: Hemp fractions
(courtesey dr. H.J. Huizing, ATO-DLO)

New competitive properties

IPC can also be promoted by looking for new applications in which the plant-derived form of a product performs better than the 'traditional' form. One example of such an application is a new (improved) type of glue that can be produced from lignin.

Efficiency of conversion

The steps required to convert biomass into raw materials for further processing can in some cases pollute the environment. This negative impact can be lessened substantially by improving these technologies. One good example of this problem is the extraction of ethanol from sugar cane in Brazil.

N.B. Biomass crops can also have a useful application in the cultivation stage (recreation, natural sound barrier, etc.)

3.2.3 Economic significance

A number of products currently produced by the chemical industry are based on integrated plant conversion.

For many reasons (cost of raw materials, small-scale businesses, etc.) the Netherlands is not a suitable location for the large scale production of inexpensive agricultural raw materials intended for the chemical industry. The Netherlands will always be at a disadvantage, therefore, in cultivating agricultural products on a large scale for bulk chemicals and energy use. This is not the case, however, with respect to chemicals that have limited production volumes and high costs (fine chemicals, pharmaceutical products...). The Netherlands can build on its strengths in this area, namely an agricultural sector that includes agro-processing and chemical engineering. The Netherlands has a particularly strong position with respect to seed improvement and biotechnology. This position should be strengthened further through development projects on a pilot-plant scale. Unfortunately, the chemical industry has traditionally not had very much contact with the agricultural sector, which is governed by a different set of rules (e.g. EU agricultural regulations). Moreover, the availability and composition of the raw materials are less consistent than those from fossil sources.

Cooperation between these two sectors would be very useful. The agricultural firm would then perform the functions of collection, transportation and storage, and possibly pre-processing. It must be noted, however, that this type of industry is being promoted in other countries as well, and that Dutch firms do not necessarily have a head start in this field.

The fact that the Netherlands cannot become a cheap supplier of raw materials can mean that the processing of these materials will be split into a primary process carried out in the producer country and further processing carried out in the Netherlands. This occurs already with grains and soy beans, for example.

Some current small and medium scale biomass applications are the oleochemical market, consisting of cosmetics, surfactants and esters for lubricants. Large scale use of agricultural products is already underway in this area. Bio-plastics can be made from agricultural products, such as starch, sugar, and cellulose. Biopol is an example of a commercial product used for the production of shampoo bottles (Wella) and nappies (Procter and Gamble), among other applications. Avebe, which specializes in starch products, has brought a number of bio-plastic products onto the market in addition to coatings for the paper industry and various types of glue.

Unichema produces many products from triglycerides (oils), such as detergents and cosmetics. One example is an anti-adhesive used in the refuse bags that Unichema produces from eruca acid (derived from rape seed or crambe). Purac-CSM produces, among other things, cosmetics and medical products with the help of polylactic acid based on sugars from sugar beets. Purac also produces, together with Cargill, coatings and plastics from polylactic acid. These have many applications, including serving as surgical aids and as soluble coverings for medicines. A joint venture of Dow Chemicals and Cargill is actively involved in this area. Benuline, a subsidiary company of the Suiker Unie, uses inuline from sugar beets to produce phosphate substitutes for detergents. Both the costs and the techniques involved have been satisfactory.

3.2.4 Current technology

Thanks to many research programmes on integrated plant conversion (e.g. the FAIR programme of the European Union, and the PBTS, BTS and EET programmes of the Dutch Ministry of Economic Affairs), more is now known about its possibilities and the chances for its success in various possible applications. As part of a policy to promote ecologically sound agrification, the Dutch Ministry of Agriculture, Nature Management and Fisheries has devoted one hundred million guilders for research in this area, one quarter of which was subsidised.

In the past, such research was carried out mostly by agricultural interests. However, this proved to be the wrong approach. Too much attention was paid to the potential products of agricultural crops, rather than to the actual needs of the application-oriented industries. Although the agricultural products developed could not compete successfully with existing products, this research did lead to increased knowledge and a greater faith in the technical possibilities of agricultural products.
Current efforts and developments are increasingly based on sustainability considerations. Short term initiatives are often taken by the industry, while more structural

long term programmes are initiated by the government.

In 1991 (Brouwer) the possibilities for the production of engine fuels and bulk chemicals appeared to be very limited. The chances looked somewhat better for fine chemicals and 'performance' products, thanks to the specific characteristics and structures of plant-derived raw materials. However, it must be noted that this usually involved only a very small part of the plant. The chances of success for agrification with respect to energy generation, bulk chemicals and engine fuels seem to have improved in the meantime. An increasing amount of research is being carried out, both by research institutes and commercial firms, on this form of agrification.

In addition to a positive economic base (see previous paragraph), the Netherlands has a very good technological base for IPC. Research institutes have already integrated IPC into their research, such as Leiden University in the area of biotechnology, University of Twente on biopolymers and, of course, Wageningen Agricultural University. ATO-DLO also plays a central role in this area. It must be noted again that these developments are occurring rapidly in other countries as well.

An evaluation carried out by Okkerse and van Bekkum showed that currently available technology is already capable of producing the ten most important synthetics (PE, PP, PVC, etc.) from biomass material.

The following section presents the 'state of the art' technology for significant plant-derived components. The discussion focuses on what is, and what is not (yet), technically and economically possible in each area, and on products that are already being produced on a commercial scale through integrated plant conversion. The intention is not to be comprehensive, but to give an idea of the possibilities of this sustainable technology. The individual areas are (ligno) cellulose, starch, sugars, oils and fats, proteins and fibres.

Glucose is the most important building block of the polymers formed in plants. It can be seen as a building block for many plant-derived products, just as ethene and methanol are building blocks for products made from petrochemical raw materials.

Cellulose and starch, the most important carbohydrates, are polymers that are composed of the monosaccharide D-glucose. In other poly- and oligosaccharides, different monosaccharides are present, such as fructose, xylose or galactose. In forming polymers, the monomers can be linked in various ways. Thus, out of the same monomers, various di- or polymers with completely different characteristics can be formed (e.g. an unbranched cellulose polymer or a strong (amylopectin) or weak (amylose) branched starch polymer).

Current technology involving the most important plant-derived components

(Ligno)cellulose

Lignocelloses (cellulose, hemicellulose and lignine) are the most important components of trees and plants, of which cellulose makes up the majority and has the most applications. Hemicellulose and lignin are by-products that, due to their useful application, can make the production of cellulose efficient. Lignocelluloses (from wood, straw, plants GFT waste, etc.) are the cheapest and largest source of biomass material and are, therefore, of primary use compared to most other biomass raw materials.

Cellulose belongs to the group of carbohydrates that are built up from mono-saccharides. Cellulose consists of a matrix of long chains of glucose monomers. Mannose, xylose and fructose are less frequently occurring saccharides that occur in hemicellulose. The structure of cellulose is extremely strong and is insoluble in water. For these reasons, lignocelluloses are almost always hydrolysed to give solid lignin and dissolved sugars (except in their application as fibres, see chapter 7). For glucose extracted from cellulose (cheaper than from sugar or starch), many applications are already possible such as conversion into ethanol, polyesters, acetic acid and nylon-6 (see 'sugars'). Lignin and hemicellulose also hold great potential, even though development of these applications is less advanced than it is for cellulose products. Traditional agricultural crops appear to be less suitable as suppliers of cellulose. There is greater potential in other high efficiency and fast-growing annual crops such as hemp and flax, and perennials such as poplars and elephant grass.

Starch

Starch is also made up of glucose chains. They are, however, much weaker than cellulose fibres and are soluble in water. The two principal components are the polysaccharides amylose and amylopectine. These act not as construction material in plants, but as storage material. Starch is primarily found in seeds (corn, wheat, rice, peas) and bulbs and roots (potatoes, tapioca). Approximately half of this carbohydrate produced is using in the food sector. In addition, it is used in the paper industry, glues, the textiel industry, biodegradable plastics, lubricants and coatings. For a large scale application in competition with the petrochemical industry, starch is not, however, useable, partly because the moisture content in the raw material (potatoes) is high and the concentration of useable material is low. The advantage of using starch in the non-food sector is that there is already a good starch infrastructure, due to the applications in the food sector. Starch is primarily used in specific products (paper coatings, bio-plastics, adhesives), in which a number of commercial products are being produced.

Other sugars

In nature, mono-, di-, and polymer sugars occur. Table sugar, saccharose or sucrose, is a dimer of glucose and fructose. Sugars are primarily extracted from sugar cane, sugar beets, chicory, grains and grasses. A byproduct of sugar that is of lower quality, but cheaper, is molasses. Like cellulose and starch, sugar is mostly processed by first converting it into soluble simple sugars, of which several applications are possible, including ethanol, polylactic acid, biodegradable plastics and foam. Although the demand for biodegradables is not increasing as quickly as was predicted in the 1980s, the number of commercial applications is growing steadily. A major bottleneck is the high cost. There is no shortage of commercial initiatives, however (laundry soaps Suikerunie, bioethanol in Brazil and buses in Groningen).

Fats and oils

Fats and oils are esters of gylcerol and fatty acids that have different lengths and degrees of unsaturation. Only 20% are used in the non-food sector, of which tallow is an important source. A few other sources are soy bean oil, rape seed oil, palm oil and castor oil. The four important industrial application areas are lubricants, paint, soap and oleo-chemistry. The latter two are the most important. In addition to fatty acids for cosmetics, lubricants, plastics and cleaning products, the oleo-chemical industry produces glycerol for the pharmaceutical industry, cosmetics, tobacco and resins. In addition to glycerol, the soap industry produces fatty alcohols that are primarily used for laundry and cleaning products. The most commonly used lubricant is ester oil. This plant-derived ester oil is, however, four to five times more expensive than petrochemical lubricant. This is an important reason that only 1% of the lubricants is derived from natural materials. For paints and lacquers the portion of (non-natural) fats and oils is traditionally high, but is now increasing due to the increasing demand for water-based paint. This portion may increase by using better and cheaper natural oils. Linseed oil appears to be a good alternative. Different oils can potentially be used as fuels in diesel motors such as soy bean, sunflower, rape seed and palm oil. The most familiar of these is rape seed methyl ester (KME), that results from the de-esterification of rape seed oil. Diesel motors can use this material without problems as a fuel. Again, the greatest disadvantage is the high cost. Due to their chemical versatility, fats and oils are currently found mostly in specific applications such as lubricants for airplane motors or as ink derived from soy bean oil (U.S.A.).

Proteins
Proteins are polymers of amino acids. In an organism they have several functions including enzymatic catalysis, transport, structural support and hormonal influence of the metabolism. Many of the proteins processed in the Netherlands have as their source, potatoes, grain, peas, hides, bones, muscle tissue or milk. One of the major problems in the processing of proteins is the loss of function. This can happen due to a chemical reaction or by heating. The possibilities for using proteins are enormous.
Currently, proteins are mostly still produced as a by-product and processed into cattle feed or thrown away. By using better separation techniques and by actively seeking applications, these proteins can contribute to the cascading of biomass material and in this way contribute to sustainability and the valorisation of the total crop. Protein applications can be divided into food and non-food applications. Examples of food applications are: coating of food, texture improvers, protein sources in food stuffs and fat replacements. Examples of non-food applications are: biomedical applications, crop protection, cosmetics, biopolymers and photographic applications.

Fibres
Natural plant-derived fibres are built up of cellulose. Due to increasing research, the properties for construction applications are continually being improved. A number of important sources of natural fibres are cotton (textiel), hemp (textile and paper), flax (many applications) and sisal (paper, rope). The climate in the Netherlands is only suitable for the cultivation of reeds, flax and hemp. In order to be able to use the fibres from the plant, these must be unlocked, so that the cellulose fiber is released. For wood and most other plants, this is a complex and environmentally polluting process. Currently, the most important application of plant-derive fibres is rope, paper and textiles. In building and construction materials, the use of these fibres is increasing. New applications are geotextiles and as asbestos replacements (triplex and fiber board). In particular in places where biodegradability is important,

plant-derived fibres can be used.
In the Netherlands, much research into the application of different types of natural fibres, primarily at DLO (ATO). Tests are being made with flax for cardboard, non-wovens and tissues, with hemp for the production of paper and cardboard and with cotton for the production of bank notes (see also chapter 7).

[References: Brouwer, articles, annual reports]

3.3 Long term view

3.3.1 A look at the future

Based on the starting point of sustainability, the long term goal for IPC is to replace all of the raw materials humans use with sustainable raw materials, based on natural recycling. Most likely, however, a combination of technologies will be used in the future, and fossil fuels will continue to play a significant role. It is actually even preferable that we develop and use many technologies, so that we do not become dependent on only one option.

3.3.2 Enabling technologies

A number of technological developments that are relatively important for optimising IPC are summarised below.

Integral technology
A chemical description of a crop (also figure 3.2) should provide better insight into its possible (commercially feasible) applications. Pilot projects can be set up based on these insights.

Agricultural sciences
Increasing agricultural yield per hectare, extending cultivation areas and improving harvest methods all translate into specific technologies that are needed to produce agricultural raw materials at less cost and with less environmental impact. This subject is receiving much attention in relation to agricultural production for consumption.

Genetic techniques
Genetic techniques appear to play a crucial role in the economic feasibility of IPC. With the help of genetic techniques, the supply of specific components can be better attuned to the demand for them. Topics in this area include increasing or decreasing the yield of a selected substance in a crop, and improving the quality of a desired substance.

Crop separation techniques
Improved industrial crop separation techniques are needed to optimally split the component parts. One possible method is the preparation of raw materials at the farm.

Logistics and storage technology
As an increasing number of agricultural raw materials are used, a different logistics system will be needed ('contribution logistics'). Storage technology will also play an important role because of the seasonal supply and perishable nature of the crops.

Biomolecular separation techniques
Extraction of desired substances from a plant requires separation techniques at the molecular level. This technology is also needed to improve the processing steps and the valorisation of specific (waste) streams. This is a very new subject area.

Application development
The success of IPC depends largely on the development of applications. This should be the first step in the IPC process.

Fermentation technology
The conversion of bio-substances into desired products and partially manufacture goods is still a relatively small scale technology. Greater knowledge of these biological processes is needed for optimisation and extension.

Furan chemistry
Controlling the chemistry of a raw material based on C5 molecules (furan chemistry produces paints, surfactants, etc.) offers a base upon which to develop other types of chemistry.

Closure of the nutrient cycle
Supplying a recyclable solution for minerals and nutrients (K,P,N...) present in biomass materials is a desirable parallel development. As yet, very little attention has been focused on this area.

3.3.3 The road ahead

It is generally assumed that for the next 50 years no major shift will occur in the focus of fundamental chemistry from fossil fuels to agricultural raw materials. According to Shell, fossil fuels will continue to be our main energy source, especially with respect to engine fuel. Nevertheless, the desire in developed countries to achieve a sustainable future makes it seem increasingly likely that fossil fuels will be replaced with substitutes that are not as harmful to the environment, even before it becomes economically imperative to do so. Governments will play an important role by stimulating sustainable technologies. This is already the case in Sweden, where the ecotax, a tax on fossil fuels, has been initiated with the goal of limiting carbon dioxide emissions.

Integrated plant conversion will have the greatest chance of succeeding in the coming decades in areas for which the petrochemical industry does not have an automatic advantage. Some examples are
-products that are safer for humans, animals and the environment,
-specific, high-quality products that have a complex structure,
-products and energy from organic waste streams and organic waste with a low or even negative value (GFT, wood waste, straw, corn stalks, manure…).

Dutch firms will primarily supply products that have a high added value. Only a small part of biomass materials will originate in the Netherlands; the majority will be imported. There is great potential for Dutch seed improvement firms to play a leading role, because this sector can record software (knowledge) in reproducible and sellable hardware (seeds for the agriculture industry).

IPC will be most attainable in the coming decades if applied to existing (waste) streams of previously scaled-up crops. The highest added value can be obtained for streams that already have some value. A continuing effort should be made to utilise the whole plant for various applications, so that an ever-decreasing portion of the plant will be left over.

3.3.4 Requirements for technology

Despite the advantages of IPC as described above and the generally accepted need for environment-friendly industries, biomass material does have a few important disadvantages and obstacles, which will prevent a large breakthrough from occurring within the next decade. These barriers are summarised as prerequisites for success. The most important question is whether it will be possible to produce sufficient biomass at the right time and place (see chapter 2).

An important point to consider is the improvement of photosynthesis efficiency. Another is the social acceptance of biomass products that may have been modified by means of genetic techniques. There are also a number of economic and technical barriers that must be addressed. A great deal can be accomplished with existing technology, but not enough to achieve a real breakthrough. To move beyond the remaining barriers, new technologies will have to be developed.

Sufficient biomass that is available at the right time and place
Chapter 2 focused some attention on the availability of biomass. Although this does not appear to be a problem, it should be studied and discussed more thoroughly.

Social acceptance of genetic technology
Although genetic modification of crops has existed for centuries in the form of crossbreeding and natural selection, genetic technology is a subject that has sensitive ethical aspects.

A competitive price
Regardless of the application, the cost of raw materials must be as low as possible. This is especially true for the production of bulk products. At the moment there is still enough petroleum, natural gas, coal and inorganic raw materials available, so the basic chemistry industry, in particular, is not likely to switch over to new and relatively expensive raw materials and unproven technologies. Calculations vary, but it is generally agreed that the price of petroleum would have to be $25-45 per barrel (the current price is $10-14) before it would become economically feasible to substitute it with agricultural raw materials. When comparing agricultural raw materials and fossil fuels, it must be noted that cost and market prices are often used interchangeably. The comparison can never be complete anyway, because the CO^2 effect of petroleum raw materials is not (yet) taken into account.

Quality guarantee and reproducibility
Climatic changes have a great impact on the supply and quality of raw materials and therefore also on their price stability. Different and varying growing conditions (type of soil, weather, retrieval methods, etc.) can alter the composition of agricultural products, which can have serious negative effects on the product and consequently complicate the production process. If a product becomes more perishable, its quality suffers as well.
The biodegradability of biomass material can be either an advantage or a disadvantage, depending on the application. Many biological products are not resistant to micro-organisms, moisture and changes in temperature and acidity.

Improvement of the production characteristics
Despite the fact that they have superior characteristics for some applications, natural products are less suited than synthetic or artificial products for a great number of other applications. Cellulose fibres, for example, are naturally very hygroscopic and they adhere poorly to other materials.
The high moisture content of biomass material and the difficulties that can be encountered in separating its component parts, make it a very complicated material to work with (separation of cellulose, hemicellulose and lignin in pure components).

Integral use of crops
The various aspects of an integral approach have already been mentioned. It will almost always be impossible to use the whole plant for one particular application. The

by-products will, therefore, also have to have a useful application to make cultivation of a crop profitable and to prevent an increasing volume of waste. Energy retrieval is a good option for biomass materials, if the potential profit is not too low.

Supportive political climate
Current regulations make it impossible for agricultural non-food products to compete with existing raw materials, especially because cheaper import products from third world countries are not allowed to compete on a free market basis.

Smooth transfer from petroleum raw materials to agricultural raw materials
The entire industry and infrastructure is based on the use of fossil fuels. The transition to agricultural products is a very costly process. Moreover, the petrochemical industry starts with a relatively homogeneous raw material that has a limited number of retrieval locations, while biomass production starts with heterogeneous materials that have complex cultivation logistics.

Pathway in the development of IPC

In order to characterise the pathway of IPC, it is necessary to look back at the past. A distinction is made between the following phases:

Phase 1: Traditional biomass material
When the petrochemical industry was still undeveloped, biomass material was the most important raw material.

Phase 2: Petrochemistry
The current situation is dominated by the petrochemical industry. The consumption of biomass materials is still high, for example in developing countries and for particular applications such as in wood for construction.

Phase 3: Niches
There is already a large number of examples of niches in which biomass material has an added value (clay pigeons, french fry containers, etc.). This will increase. At the same time, agricultural as a complete concept will have to be developed (including the optimisation of agricultural practices). The niches must make use of agriculture crops that have already been scaled up. The scaling-up of a new crop is a long process. New crops should be judged on their potential usefulness. Scaling-up needs to be initiated, so that new biomass applications will later be possible.

Phase 4: Large-scale biomass, 2 possibilities
1 Active: large-scale IPC in 2050 is established as a goal
2 Passive: Use of minerals is no longer economically attractive; around 2050 it appears that this will be more of a reality, although that is difficult to predict due to:
-recycling, increasing dematerialization of energy, new sources and efficiency
-population growth and increased well-being is propelled in the other direction

Special considerations with respect to IPC
petrochemical raw materials used exclusively for the chemical industry

Some people support the idea that the earth's limited supply of petrochemical raw materials should be exclusively reserved for specific chemical applications, and that it should not be exhausted through continued use as an energy source. If dematerialisation in the energy sector and of large scale applications continues (see chapters 4 and 5), the threat of exhausting all petrochemical raw materials will be dramatically reduced. The ratio of energy to chemistry, which is now 90:10, will become 10:90 in the future.

The necessity of working on IPC due to a physical scarcity of fossil fuels would then no longer exist. It must be noted, however, that an economic scarcity of petrochemicals could occur because prices may increase due to the reduction in scale. It is not possible to make accurate predictions at this point.

Rational choice

The choice to use biomass as a raw material and/or energy source must always be made after a rational consideration of all possible options. Biodegradability can be important for a detergent, for example, if waste water is discharged at surface level, but the biological source of a PET bottle's raw materials can be less relevant if a recycling system is created and energy reuse is achieved. A Life Cycle Analysis (LCA) can help in making such choices.

Plastic pencils

A good illustration of a step made in the opposite direction is provided by a pencil manufacturer who decided to stop using biomass material for environmental reasons. Wood and glue were replaced by synthetic resin that is pressed directly around the graphite rod. The air-tight fit prevents the rod from fracturing and thereby greatly increases the pencil's durability. An article written about this pencil concluded: "An added advantage is that the production of these pencils is good for the environment because no more wood is used".

SALINE AGRICULTURE: THE POTENTIAL OF SUSTAINABLE AGRONOMY AND TECHNOLOGY

Saline agriculture uses seawater for the irrigation of coastal deserts. Salt tolerant crops are sown, cultivated and harvested using modern agricultural equipment, including conventional combines.

In the Middle East saline farming is practiced using pivots with a length of 400 meters. Seawater is pumped in and used to irrigate circular plots with an area of 50 hectares (50.0000 m^2). Currently, practical and relatively large-scale experience has been acquired with the saline agricultural cultivation of a Salicornia crop. In coastal desert systems with sandy soils, irrigation water is returned to the sea after having passed the root system of the Salicornia crops. There is no problem of salinisation of the soil nor of salinisation of fresh water aquifers. Fertiliser may be used, but so far no pesticides have been applied

At the end of the growing season, the aerial parts of the Salicornia crop, reaching a height of up to 1.00 meter, are harvested. Tips of shoots and branches of Salicornia are harvested separately and sold as a vegetable crop for human consumption.

The total yield of aerial biomass of saline pivot farming in the Middle East is 15 tons per hectare. The yield of tips is 2-4 tons per hectare. In addition, 0.8 tons of Salicornia oil is obtained from the harvested seeds (1.6 tons of oil per hectare is obtained with the conventional non-saline cultivation of Rape (Brassica napus).

In a US-Dutch co-operative programme various saline agricultural options are being tested on a saline farm along the west coast of northern Mexico.

Saline agriculture is being practiced nowadays in Saudi Arabia, Australia, India and Pakistan. New saline farms are being developed in South Africa and South America.

Currently, annual saline crops are being cultivated on salt farms. Research has been started to determine the agricultural potential of perennial salt tolerant crops, including salt bushes and mangroves.

The potential of saline agriculture is high. Fresh water is a scarce resource and will be primarily used for human drinking water. World-wide the use of fresh water for irrigation in conventional (fresh) water agriculture will decline, alongside a rapidly growing world population. In addition, with the current rates of economical and industrial development, the availability of other natural resources such as natural gas, coal and petroleum, is rapidly decreasing.

With extensive areas of the earth being appropriated for saline agriculture, the harvesting of bulk amounts of saline crops will provide biomass for biofuel and fodder. Fibre obtained from the Salicornia straw, in combination with a resin, is being processed into a patented, high quality "MDF-like" eco-hardboard. In this way, building material will become available in areas with saline agriculture.

In a saline biocascade approach, linking various industrial interests, it may be feasible to exploit the various resources of halophyte biomass in new agro- and chemo-technologies. Thus, the exploitation of renewable resources, supplied by saline agriculture, will form the basis of new, sustainable agro- and chemotechnologies.

3.4 R&D Agenda

The previous section promoted the development of large-scale technologies for IPC based on various niches. How this transition should actually proceed is still unclear, and requires further research. Uncertainty still exists in non-technological areas and there is a great need for:

- studies to support decision-making and priority setting, etc.
- information transfer: demonstrations of what is technically possible and what is needed for particular applications
- 'just start'

An actual R&D agenda is not suggested here, but elements are presented that should play a role in such an agenda.

3.4.1 R&D Agenda

Crop analysis

Comparative research will have to be done to determine which crops are potentially suitable for IPC. The Biocascade project, which was financed as a pilot project by the Dutch EET programme, is an example of such a study. Further progress must be achieved in the short term based on crops that have already been scaled up, taking advantage of the learning curve of crop scaling up. Moreover, improvement knowledge for these crops (including genetic modification) is already present, machines for cultivation and harvesting are available and a useful application has already been established for a part or all of the plant. Progress could thus be made with respect to:

- an oil/protein crop (e.g. rape seed)
- a fibre crop (e.g. hemp)
- a carbohydrate crop (e.g. potato, beet)

These crops can already be cultivated and processed, they are genetically accessible for fine-tuning the supply of raw material streams, they can be combined with other agricultural products (i.e. rotation schedules), they are annuals and they complement each other with respect to product streams.

The aspects of these crops that should be compared are:

- costs
- biomass yield (per hectare)
- characteristics (fibre source, cellulose…)
- agricultural advantages and disadvantages
- workability
- climatic conditions (can it be produced in the Netherlands?)

The most suitable crops for the Netherlands appear to be hemp, as a source of fibre, high-grade cellulose and oil; and potato, as a source of C6 and C5 raw materials.

This is currently being researched in the biocascade project. Eventually, the knowledge gained with hemp and potato will be used for further analysis of other crops.
Potato is a carbohydrate crop that can be valuable in the short term as a raw material for IPC. Potatoes supply starch, which has been an important raw material for industry for a long time. In modified form it can be used as a surfactant or as a phosphate substitute (a better zeolite and acrylate substitute) in detergent or as a super-absorber in babies' nappies. Through improvement, potatoes could be taught to produce C5 rings. The potato's production of biomass is high: up to 50 tons per hectare (wet weight)
Hemp can also become a IPC crop in the long term. Hemp provides fibre, oil and high-grade cellulose with a high alfa cellulose content. The oil is unsaturated and lends itself well to technical applications in coatings and thermosets.

Application project (information transfer)
Integrated plant conversion is at the outset dependent on application oriented development that focuses on product/market combinations and a valuable product in a lucrative market. This will ensure that the prospects for a project will be attractive enough. First, uses (fibres for composites, biopolymers etc.) have to be developed further and made (commercially) suitable for application. Expectations are good for this stage. Next, a specific crop must be chosen, and the appropriate technologies must be developed for production and processing. Cooperation between industry and research is essential for the achievement of market-oriented agrification research. In the end, application development will amount to strictly following the steps outlined in the schedule below. A clear description will have to be given of the physical-chemistry of the crops and their agricultural and cultural aspects, and of the genetic technology and molecular separation techniques that will be required. This will make comparative research on the suitability of the crops possible, so that the right choice of crops can be made. Eventually it will have to be demonstrated whether potato and hemp are the right choices. In choosing crops for non-food applications, preference will have to be given, if possible, to:

- accumulation of desired products in seed (for ease of storage)
- existing scaled-up agricultural crops

Availability of biomass materials
In chapter 2 the availability of biomass materials has briefly been mentioned. A positive picture was presented in an essay written under the auspices of DTO Chemistry (Okkerse & van Bekkum) on this subject. However, further discussion and details are still needed.

Plan for transition to a society based on biological raw materials
This chapter has not presented a clear plan for the transition to a society based on

biological raw materials. Clearly, a number of niches must be developed in the short term. However, further discussion is needed to determine how a large-scale change can be initiated. The political sector can stimulate this research through a target-oriented programme (e.g. the EET programme of the Netherlands' Ministry of Economic Affairs).

Effects of IPC

The economic, cultural and environmental-technical effects of IPC must be determined.

Effects of genetic engineering

A list of demands for genetic engineering must be established. Aspects to be considered include consistent quality, resistance, etc. A study should also be done on the social acceptability of genetic modification. If it was found to be unacceptable, then the possible repercussions should be investigated, as well as the possibility of influencing public opinion through the dissemination of information.

CROP \ APPLICATION	pharma	phyto-sterow	surfaetants	fatty acids	resins	oils	cellulose	fibres	(cattle) feed	energy	...
hemp											
rapeseed											
potato											
sugar beet											
wheat, grain											
GFT waste											
wood											
....											

key technologies

- molecular separation techniques
- genetic technology

Fig. 3.3: Crop-application matrix

Hemp as a test case
As previously discussed, hemp appears to be a suitable crop for providing fibres and cellulose. A study in which hemp is separated into various parts would help establish the possibilities for its integral use.

3.4.2 R&D options

Optimisation of agricultural technologies
To make IPC possible, the following technological areas must receive special attention:
- Improvement and genetic techniques
- Agronomy (including yield improvement, cultivation of brackish soil, etc.)
- Harvesting methods
- Logistics and storage technology
- Separation techniques
- Conversion technology including fermentation
- Preservation without the use of harmful pollutants

N.B. This is not a prioritised list.

One way of producing products for the chemical industry out of a varied supply of biomass raw materials is to use a biomass refinery with an integrated circuit of processes in the whole progression from raw materials to various products. How profitable such a biomass refinery would be, on what scale and for which raw materials and applications it would be suitable must still be determined. These processes must be developed further before additional biomass conversion processes can be integrated in a factory.

R&D of cluster valorisation of (existing) organic waste streams
Another important area is the development of separation technology to increase the value of waste streams. For example, in the production of oils (triglycerides) from biomass materials, many unsaturated fatty acids and anti-oxidants are still not valorised because they are not separated. New separation techniques create new valuable substance streams out of the waste stream. In addition, the waste can be processed much more easily after removal of problematic components. Separating components is easy to do on a small scale in a laboratory. However, it is not yet possible to do this on a large, economically profitable scale.

In the long term, it will be possible to increase the value of a plant by ensuring that it produces the desired substances through genetic manipulation. Genetic improvement of waste streams is definitely justified because of the large amount of material and the fact that the streams already exist. The added value gained by genetic modification is greatest for existing streams. Aside from molecular separation technologies, better crop separation technologies will also have to be developed that will make it possible to split plants into the desired main streams (e.g. the retrieval of fibres) in a way that is economically profitable.

Development of furan chemistry based on C5

As mentioned above the development of niches is important. C5 chemistry is one of the critical areas for the further development of IPC.

Unsaturated fatty acids

The use of unsaturated fatty acids in coatings is a good example of a development area directed towards the creation of bulk products based on IPC.

Carbohydrates / starch / cellulose

Our basic knowledge of vegetable substances requires more research with respect to both organic chemistry and material technology. Some research is already underway to optimise the possibilities such as for the use of polysaccharides as environmentally safe surfactants or cellulose as a raw material for fibres and biodegradable plastics and foils.

3.5 Conclusion

3.5.1 Conclusions and recommendations

IPC will definitely play a role in the future. However, there is still some reasonable doubt about the likelihood of large scale application of IPC. If alternative energy sources are tapped (such as wind, sun, etc.), enough fossil material would remain to satisfy the needs of the chemical industry for a long time. However, wind and solar energy could never completely satisfy all of our needs, so many possibilities exist for biomass materials.

Although much can already be accomplished with existing technology, more development is needed to achieve reproducible, quality products. The price of biomass materials may be more competitive with that of petrochemical raw materials if the technology becomes more commonplace. Unfortunately, competition with petrochemical raw materials will remain difficult, because the costs of the two sources are not measured equally (e.g. discounting the CO_2 effect).

The large and growing interest of the industrial sector in IPC projects is strongly directed at commercial niches and possibilities (flax in bumpers, bio-nappies, etc.).

This development is consistent with the view outlined in this chapter of a sustainable future. It is especially important that we build on experience already gained with specific scaled-up products.
Whether IPC becomes a large-scale technology or not, it can still be competitive in certain niches. A competitive edge is possible through initiatives from abroad (USA, UK, France, Germany, Sweden, Indonesia, India) and governmental support. Developments in these areas should be followed closely.

3.5.2 References

Many written sources were consulted for the compilation of this chapter. A meeting of experts was also held, which focused on the role of secondary metabolites in IPC and sustainable development. This chapter reflects the general consensus formed during this meeting concerning the approach to IPC.

Reports:

- Agteren M.H., Theoretisch en experimenteel onderzoek naar de mogelijkheid om uit organisch afval een biodegradabel biopolymeer te produceren, IVEM, Jan.1995.
- Brouwer W.G.J. (Ed.), Plantaardige grondstoffen voor de industrie, STT publicatie 51, 1991.
- Darwinkel A. and W.C.A. van Geel and H.M.G. van der Werf, Miscanthus, een meerjarig energie- en vezelgewas, 1994
- Okkerse C. and H. Van Bekkum, Renewable Raw Materials for the Chemical Industry, in 'Sustainability and Chemistry' from DTO, 1996.

Various articles:

- Agrificatie; akkerbouw voor industrie en energieproductie, samenvatting van het Ontwikkelingsplan 1991-1995 van het Duitse Ministerie van Onderzoek en Technologie, Technieuws Bonn B-92-03, 30-13, Aug. 1991.
- Kunststoffen op basis van hernieuwbare grondstoffen, Kunststof en Rubber 4, p. 21-23, April 1996.
- The Shell HydroThermal Upgrading Process, a Shell/Comprimo publication, Jan. 1995.
- Dennison M., Plastics: a reusable resource, Shell selected papers, Sept. 1990.
- Elliot P. And R. Booth, Sustainable biomass energy, Shell selected papers, Dec. 1990.
- Vlieger I. de and B. Kinoo, Bio-ethanol en biodiesel als motorbrandstof haalbaar, Duurzame energie 2, 1996.

Chapter 4: Biomass Conversion (C1 Chemistry)

TECHNOLOGIES FOR (AMONG OTHERS) C1-BASED CHEMICALS AND ENERGY CARRIERS

4.1 Introduction

In this chapter, attention is focused on energy sources and chemical raw materials based on hydrocarbons. How can hydrocarbons — from both plant-derived and fossil origin — best be utilised? The energy sector is the largest consumer of these raw materials. The chemical industry uses less than 10% of fossil materials and will therefore go along in the wake of the changes that occur in the energy sector. In this chapter, techniques concerned with C1 chemistry are described. C1 chemistry is based on molecules with 1 C-atom (CO, CO_2, CH_4, etc.). An important example is Green Synthesis Heat Power Coupling (GSHPC). Simply put, this is an electricity plant that is capable of delivering methanol or other C-containing compounds in addition to heat and power. In this regard, the gasification of biomass materials plays a significant role.

4.1.1 Justification

Importance of closed hydrocarbon conversion:

Sustainable aspects of (fossil) raw materials
In spite of the fact that stores of petrochemicals are still extremely large, an end to this supply will eventually occur. As previously mentioned, the economically retrievable amount of fossil fuel, extrapolated from current use, will be consumed within 100 years (petroleum 40-50 years, natural gas 60-75 years, coal >200 years). It is expected, however, that energy consumption will continue to grow. Okkerse and van Bekkum estimate that energy needs in 2040 will be 2.5 times greater than current needs.
In scenarios described by Shell (see figure 4.1) an increase in energy needs has been taken into account. The scarcity of fossil raw material needs to be examined with subtlety, however, because new oil fields are continually being discovered, albeit with stores and retrievability below expectations. In addition, regulations concerning energy reduction play a role.

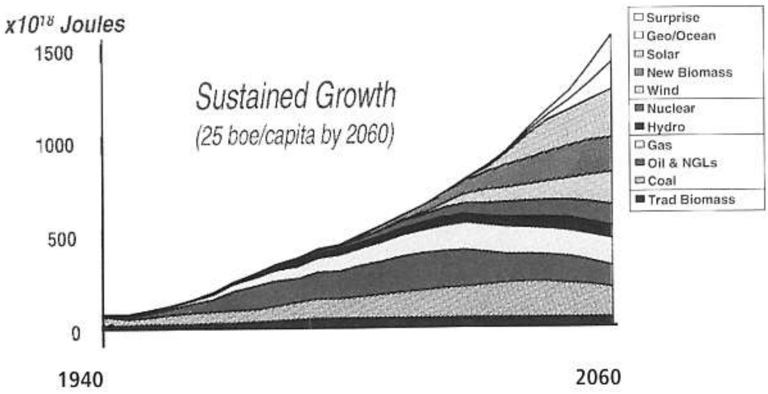


Fig. 4.1: Possible energyscenario, courtesy of Shell

Optimisation of raw material and energy stores

Energy and raw material supplies need to be estimated in a more optimal manner. A raw material consists of both a material and an energy component (oil is both an energy source and a supply of material). Currently, raw materials are often viewed as being one or the other, depending on their application.

For example: In power stations, hydrocarbons are gasified for energy generation. By-products are CO_2 and H_2O. If these compounds were to be oxidised to CO and H_2 (partial oxidation to give Synthesis gas), then the situation would be completely different. In addition to the energy released, this gas mixture can be used as a raw material for the chemical industry.

A second possibility is to use the CO_2 released during combustion in green houses; this already occurs in greenhouse cultivation: the power station provides electricity, heat and CO_2.

One way of reducing the net release of CO_2 is to make use of alternative energy sources that are available from material sources such as PV cells and wind energy. Energy sources must be used, however, in a sensible manner. An integral evaluation of the positive and negative elements of energy sources (geothermal heat, nuclear energy, solar energy, heat pumps, magnetism, etc.) is always of importance. Nuclear energy is included because this form of energy is still an important source in many countries. This type of energy is not relevant in the Netherlands. Energy must be considered not only from a quantitative standpoint, but from that a qualitative standpoint as well (exergy).

Storing fossil raw materials for use in the chemical industry

If substantial alternatives for fossil raw materials become available as a source of energy, the depletion of fossil raw materials will be drastically reduced; as a consequence, growth in the chemical industry will increase. This will be reflected in higher prices for chemical raw materials because the costs of oil exploitation will increase. The "economy of scale" decreases, however. Alternatives on the basis of agricultural products and biomass materials will, therefore, achieve a more constant price level, providing more continuity in the chemical industry.

4.2 Description

C1 chemistry is based on molecules that contain only one carbon atom (carbon monoxide 'CO', carbon dioxide 'CO_2', methanol 'CH_3OH, etc.). In principle, all carbon-rich materials can be viewed as raw material for these C1-molecules. Methane 'CH_4' is, for example, a C1 molecule, but biomass materials and polymers consist of extremely large molecules. As an illustration, glucose has 6 C-atoms and polymers can be made up of more than 1000 C-atoms. Biomass materials and polymers can be broken down to C1-molecules in a gasifier, for example. Typical gases that result from this process are: CO, CO_2, H_2) and H_2. A mixture of one part CO and two parts H_2 are known as Synthesis gas.

C1 chemistry based on biomass materials was established on the foundation of coal chemistry, which was developed in Europe between 1945-50. One of the most important processes was the synthesis of gasoline by the Fischer-Tropsch method, developed by the Germans during the Second World War and used on a large scale. This process is still being used in South Africa (SASOL). With the help of special catalysts, it is possible to build up a significant number of organic chemicals from Synthesis gas, including the most important plastics and rubbers.

The energy sector uses carbon raw materials for the production of electricity and liquid energy sources (gasoline, kerosene, etc.). This aspect concerns the energy content of the raw materials. The most important products of the (organic) chemical industry are various types of plastics.

An outline of the concept of C1 chemistry is given in figure 4.2. It consists of two parts:

- The conversion of hydrocarbons to Synthesis gas
- The conversion of Synthesis gas to the desired hydrocarbons

Conversion of biomass material and methanol production are further put into focus. By examining figure 4.2, it can be seen that transitions can exist next to each other: in addition to biomass materials, Synthesis gas can be produced from fossil sources. DME and gasoline can also be produced in addition to methanol. Gasification is not

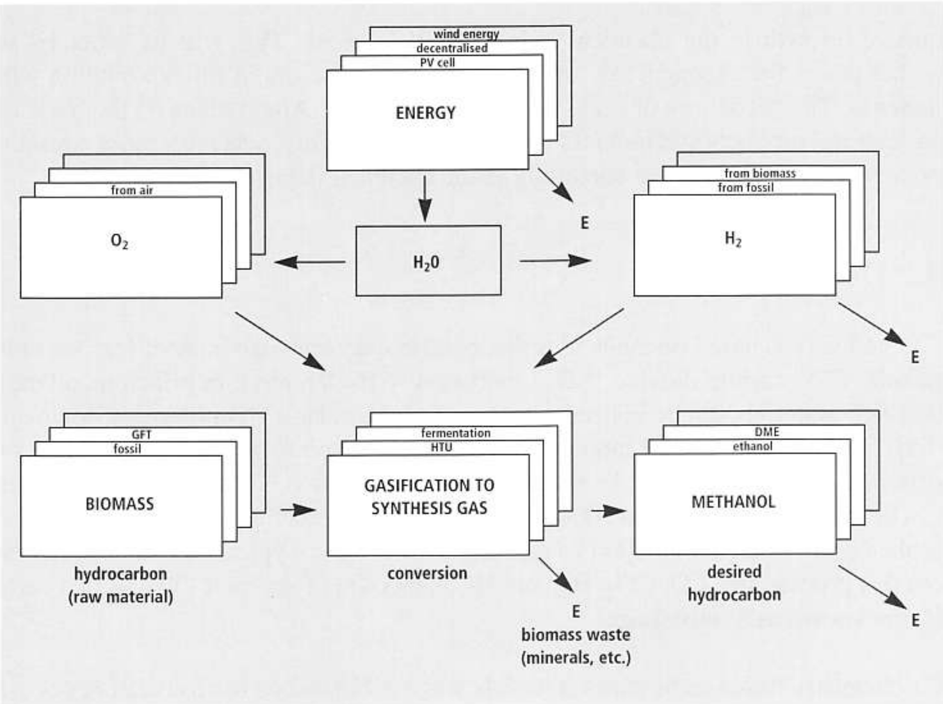


Fig. 4.2: C1-chemistry

the only potential conversion technology; other routes, such as fermentation, are possible for producing ethanol or biocrude from the Shell HTU process. Initiatives have been made to replace hydrocarbons as energy source by hydrogen alone (partial oxidation).

4.2.1 Current technology

Essentially, the goal of the technology is to convert, as efficiently as possible, the available hydrocarbons into desirable materials (such as plastics) and energy forms (diesel, heat, electricity, etc.) via an intermediate C1 basic product. For sustainable considerations, a recyclable process must eventually be developed.

The current hydrocarbon sector is dominated by the petrochemical and the energy/electricity sector. Until recently, combustion and subsequent gasification were the large-scale technologies used for electricity generation. In order to optimise these processes, a number of research initiatives were set in motion. In this discussion they have been limited to the three relevant options.

Developments in biomass conversion:
Biomass conversion as an alternative is not a new concept; there are already many operational examples, but the scale to which they are applied concerns only a fraction of the petrochemical industry.
Examples are:

- Waste wood consumption and gasification in Dutch electricity-producing companies
- Sugar beet projects in Brazil (BG/STEG)
- Wheat and corn fermentation to produce ethanol as an additive in gasoline in the United States

Developments in the area of methanol production:
Methanol is given special attention because it is expected that in the future methanol will be a good intermediate C1-hydrocarbon (intermediate between available hydrocarbons). Methanol must also be viewed as a manageable H_2 source.

Development of fuel cells
The fuel cell is based on the controlled reaction of H_2 and O_2 to give H_2O. In this process an electron stream is released through which an electron can travel. H_2 from gasified biomass, methanol (after catalytic conversion of H_2 and CO_2) or Fischer Tropsch gasoline (after partial oxidation) are significant factors in these developments. Mercedes, Volkswagen, and Chrysler are carrying out extensive experiments in cars.

4.2.2 Economic significance

The technology area described in this chapter is concerned with three sectors:

Petrochemistry/energy:
In view of the fact that the current economy is controlled for a large part by the need for fossil raw materials, a switch to biomass materials will not be without consequences for the global economy. This influence applies not only to the supplier market for energy, but also for consumers: energy is an important production factor. The most important participants in the hydrocarbon market are the petrochemical sector and the energy/electricity sector. Concurrent with the trend towards sustainable development is the liberalisation of the electricity sector in many countries. In this regard, it is becoming more attractive for companies, especially for the large transnationals that are concerned with supplying energy, to speculate in this area. For example, Shell has plans to expand into the electricity sector in the near future. The hydrocarbon market has a strong international bent.

Agriculture:
Agricultural expertise is currently more relevant than production capacity. The cultivation of energy crops followed by compacting will take place in countries that have more agricultural capacity. Biomass materials can subsequently be transported to regions with harbours and conversion capacities.

Methanol
The current world market for methanol is 25 million tons. Europe accounts for 6 million tons of the total, half of its needs are primarily for the production of formaldehyde and acetic acid. The production process relies mainly on Synthesis gas created from natural gas. If methanol becomes a significant factor in new processes, this will mean an enormous growth in the methanol sector.

Production methods of C-raw materials

Gasification

One method of producing C-raw materials is by the gasification of biomass materials to give Synthesis gas. The majority of organic chemicals can be derived from this method.

Gasification of the biomass is comparable to the way in which gas was produced from coal. That process has been exploited since the sixteenth century, first for the production of coke for blast furnaces, later, in the last century, to supply houses and factories with gas (city gas, a mixture of carbon monoxide and hydrogen). At the end of the last century, a chemical industry based on producing gas from coal was created. Before and during the Second World War, Germany was at the forefront of C1-chemistry. With the arrival of cheap petroleum, C1 chemistry lost ground in relation to the ethene-based C2 chemistry.

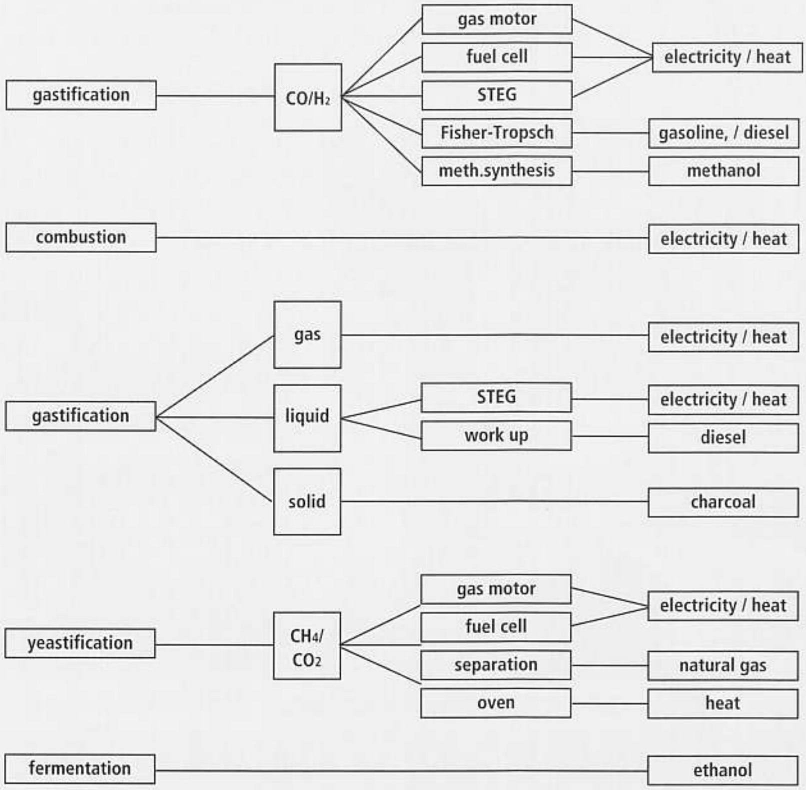


Fig. 4.3: Biomass processing techniques [J. van Doorn, 1992]

Because the gasification process releases a great deal of energy, it is a good method for the co-production of energy and Synthesis gas. For this purpose, a collaboration between the energy sector and the chemical sector in their search for alternatives to fossil raw materials is necessary. Gasification of biomass materials can be done in two ways:

- with oxygen, at temperatures of 900 °C (biomass) to 1300 °C (coal), to produce Synthesis gas that can be further processed to give methanol and hydrocarbons, from which electricity is produced.
- With air, at temperatures of 600-900 °C to make fuel gas, from which electricity and heat can be produced.

If the goal of the production of Synthesis gas is additional processing to produce basic chemicals, it is better to carry out the reaction with pure oxygen, due to the large amount of nitrogen in air. Pure oxygen, however, is more expensive than air. Therefore, to produce Synthsis gas (2H2, CO), extra H2 must be made. This is achieved by spraying high temperature water into the system. The water decomposes to H2, in which CO is converted into CO2 (Water-gas-shift). This reaction requires heat.

Gasification of biomass materials is an environmentally friendly process in which the efficiency for conversion to electricity is high. An example of a promising and modern process is the circulating fluid-bed reactor (CFB). Currently there are ten of these in use in Europe, most of which are used for the production of energy on a small scale. Large installations are still in the planning phase. In combination with steam turbines, in which the gas produced is converted into electricity, a system is created, the so-called BG-STEG (biomass gasification with steam turbine).

Combustion

The class method of biomass conversion is by combustion. Biomass material is burned either in a columnar bed, on a grate or in a powder flame. Steam, created from the heat generated, is used to drive a steam turbine and an electrical generator. The net efficiency of combustion is relatively low. This technology is well developed and is frequently used even though the potential for large-scale application is limited.

HTU process

HTU is an abbreviation for Hydro Thermal Upgrading and is a process that is similar to the natural occurrence of oil from biomass material. Biomass material is treated as a watery slurry at 200 °C and 30 bar. Subsequently, it is converted to "biocrude' in a series of reactors. This occurs at 330 °C and a pressure of 200 bar. In this way, a process that would normally take millions of years is complete in a few minutes. The efficiency of the conversion is approximately 40%. The 'bio-petroleum' contains little oxygen, nitrogen and sulfur. It is easily converted to diesel oil (for transport), but also into high quality naphta, a raw material for basic chemicals. From this naphta it is possible to produce the same series of chemicals as from the naphta derived from petroleum. An added advantage of the procedure is that different types of biomass materials can be used including wood, GFT and sewerage.

Pyrolysis

In pyrolysis, biomass material is thermally decomposed in the absence of air, steam, or other materials. In this way, the organic material is converted into charcoal, bio-oil and pyrolysis gas. Bio-oil can be used as a fuel oil after the necessary adjustments to combustion facilities. The bio-oil contains a large assortment of chemicals such as acids, alcohols, aldehydes, ketones, aliphatic and aromatic hydrocarbons, furans, naphtans, and phenols. A number of these products are of interest from an economic standpoint. The yields of these products can be influenced by varying the process parameters or by using appropriate catalysts. Investigations are underway to determine whether or not this bio-oil can be processed in a conventional oil refinery. Pyrolysis, is still quite expensive, however, particularly in hydrogenation processes, and the conversion efficiencies are disappointing.

Yeastification

Another method for producing basic chemicals from biomass material is by anaerobic yeastification to produce methane. In this process, CO2 is also formed.

Fermentation

A third route from biomass to basic chemicals is by fermentation. In this process biomass material is converted by micro-organisms in a solution of 10% ethanol in water. Further separation by distillation, membranes, or zeolites, can yield pure alcohol.

4.3 Long term view

4.3.1The future

The long term view is complex. As described in paragraph 4.2 there are several potential ways of converting biomass material into energy or raw materials for the chemical industry. It is difficult to say at this time, however, which method is best. A starting point for the future is the decision to concentrate on supplying raw materials and energy that are completely independent of fossil raw materials. A system in which both of these aspects are combined is the GSHPC (see 4.3.2). An important point to consider is the relation between energy source and the role of raw materials for the chemical industry.

4.3.2 GSHPC

The GSHPC (Green synthesis heat power coupling) is suggested as a potential system for future energy and raw material supplies. This model has not been completely thought through, but is a concept for further development.
In general, in can be stated that the overall efficiency can be improved by optimising a number of integrated technologies, in comparison with the optimisation of separate technologies. GSHPC enables the production of energy (biomass gasification with heat power coupling) integrated with the synthesis of a C1 raw material (methanol), see figure 4.4. This C1 raw material can subsequently serve as a raw material for the chemical industry, a storage medium for energy or as a transport fuel.

What is the idea behind GSHPC?

GSHPC is a concept for large-scale energy and raw material production. Combination with decentralised small scale installations is possible (it is expected that the increase in decentralised energy generation will be large).
Biomass (imported, due to insufficient space in the Netherlands, reason for the importance of having a good harbor) is gasified through the combination of water-gas-shift to yield Synthesis gas.
Synthesis gas can be converted for example into methanol that can serve as the starting material for important basic chemicals such as ethene, propene, and butene. Furthermore, methanol can act as a starting material for dimethyl ether (DME, a fuel for diesel motors), Methyl-tertiary-butyl-ether (MTBE, a lead replacement for gasoline), formaldehyde and acetic acid.
By splitting water electrolytically, hydrogen and oxygen can be obtained. The oxygen can be used to gasify biomass material and the hydrogen can be used to improve the quality of Synthesis gas. The energy needed for the electrolysis could come from PV cells, (off-shore) wind energy, water power, etc.

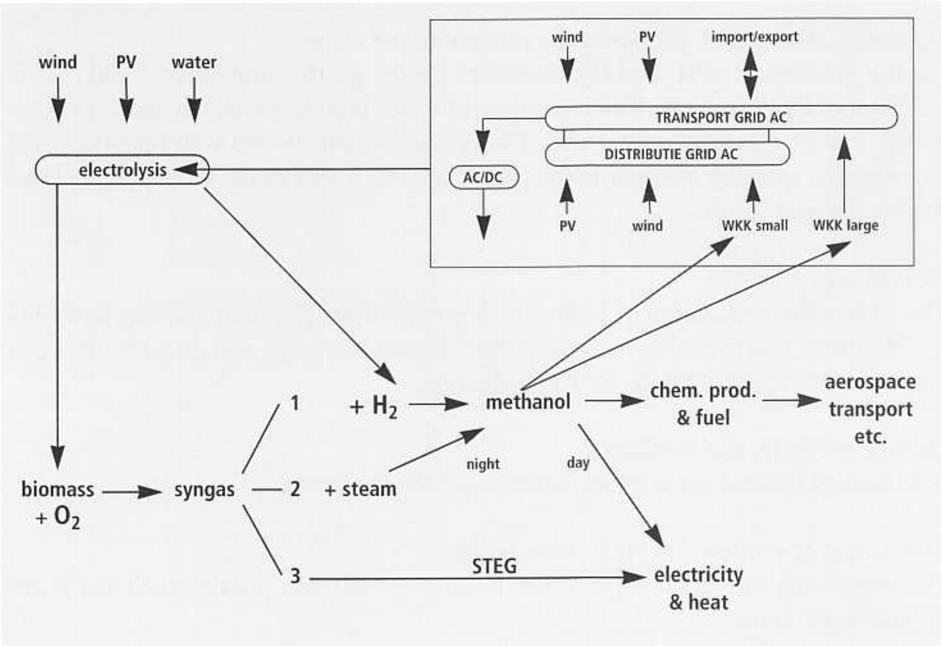


Fig. 4.4: Schematic diagram of GSHPC system

4.3.3 Enabling Technologies

The following list is a summary of technologies necessary for achieving GSHPC.

Integral technology
The GSHPC concept, as introduced in this chapter, needs to be detailed and evaluated on the basis of its subsystems.

Biomass conversion, primarily gasification
Technologies for the conversion of biomass material for the production of Synthesis gas (or fuel gas). Gasification of biomass material is one of the most important methods for success. Biomass energy will only be efficient when it is integrated with the production of other products derived from biomass material (integral yield approach and cascading, see Chapter 3, Integrated Plant Conversion). Establishing crops purely for energy production is less efficient in this country. In countries with soft currencies (no dollars), the situation is completely different. The production of energy from rape seed, after 35% of this crop is used as oil, offers, however, a good and efficient possibility for use of the whole plant. In this way, the waste is valorised, for example by gasification of the HTU (Hydro-Thermal Upgrading) process.

H_2 and O_2 production, primarily the electrolysis of water
For the production of H_2 and O_2, necessary for the gasification process and the enrichment of Synthesis gas, the electrolysis of water is an important technology. Currently, however, it is too expensive. The previously mentioned water-gas-shift, the endothermic splitting of water in the presence of CO, will be the most practical method in the near future.

Methanol production
The large scale production of methanol from Synthesis gas is an existing technology. Methanol will probably be an important source of energy and therefore it is crucial to develop new methods for its production.

Storage of H_2, O_2 and methanol
Safe storage technology is an important topic for the future.

Processing of methanol to yield other products
The processing of methanol (as a new basic material) into plastics such as PE and PP is already known.

PV cells
One of the aspects of the GSHPC concept is the coupling of decentralised sustainable energy sources, such as wind energy and PV cells. In the long term it is expected that PV cells will have increasing importance. The PV electricity is either used directly or used for the electrolysis of water to produce hydrogen. The hydrogen can be stored to make methanol or Fischer Tropsch gasoline that can be stored in existing tank facilities.

Silt/slag processing
In the future, it will be necessary to have adequate methods for processing by-products such as silt and slag that are produced in the gasification facilities.

Biomass compacting
For the transport of biomass materials over long distances, compacting of the material is of great importance in view of the need for a low storage weight.

4.3.4 The road to the future

There are two parallel pathways of development, namely the long-existing development of the conversion technology for fossil fuels and the more recent development of sustainable energy conversion. On the basis of biomass materials, both pathways can reinforce each other.

In the development of electricity production from fossil raw materials a number of efficiency improvements can be reported: with combustion, a changeover to gas turbines has been made, in which STEG and the HPC (heat power coupling) were made possible.
The route of coal gasification with consequent electricity generation was also opened up. The next step is to produce methanol or gasoline in addition to heat and power. In the parallel route, coal is slowly replaced by biomass materials; the same route is further followed by STEG, HPC and co-production of renewable energy sources. In figure 4.5, the development over time is plotted against the sustainability contribution. It is clear that both pathways can lead to GSHPC. Further developments of the old combustion process should not be neglected, however. For a time, it will remain an important competitor.

4.3.5 Technological prerequisites

For the development of GSHPC, a number of technological prerequisites must be taken into account:

- Technologies must be rationalised and developed from an integrated systems standpoint, using water, carbon dioxide, oxygen and sunlight as essential building blocks.
- The underlying connection between the subsystems (PV, H2, biomass, Syngas, etc.) is crucial.
- A mega-system is vulnerable. Decentralised units are important and fit into the GSHPC concept.
- For the development of these technologies, the size of the scale must be taken in to account. For the supply of electricity, the macro-scale (biomass gasification), the micro-scale (PV cells) and the meso-scale (those that fall in between) are of importance.
- The system must be dynamic to be able to handle fluctuations in energy/electricity demands (day/night; summer/winter). Storage technology is, therefore, an important point of consideration in the development phase.
- The system must be able to be modified and added to according to geographic region, independent of available resources, energy demands, infrastructure, etc.
- Central to this system is the production of methanol. A critical topic is the coupling of methanol/Synthesis gas. It is important to obtain a better idea of the possibilities and limitations of methanol production and processing.
- Optimisation of energy and exergy production of the whole system deserves attention in relation to determining the temperatures required by the various gasification processes.
- The limited availability of space must be taken into account.

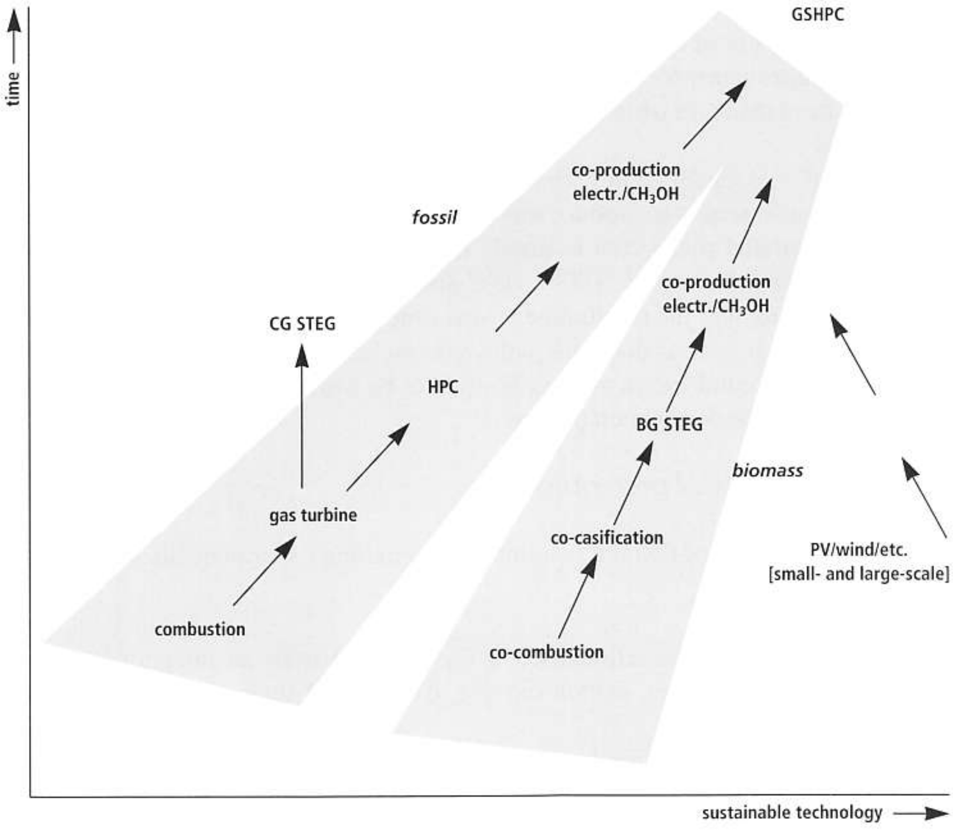


Fig. 4.5: Development of the GSHPC process from fossil and biomass material combustion

- The system must be feasible in the short term in terms of the individual technologies (PV for electricity) and be able to be integrated into the system in the long term (PV for hydrogen production, among other things).
- For the GSHPC concept, all the necessary building blocks (biomass, water, sun) must be available in sufficient quantities at the same place.

4.4 R&D Agenda

The R&D agenda was established to evaluate the feasibility of GSHPC and its sub-elements:

4.4.1 Studies

System study GSHPC

Development in the U.S. (Liquid Phase Methanol Process on the basis of coal gasification) and the numerous initiatives that exist in the area of biomass gasification indicate that GSHPC has a strong potential for supplying energy and raw materials in the future. In a system study, the current GSHPC scenario must be further developed. An energy/exergy analysis is of great importance in this regard. In addition, the scale size must be taken into account. The already existing process developments must be built upon. A combination of the bio-STEG with the LPMEOH could already be a GSHPC.

Comparison of H_2 production technology

In the GSHPC process biomass material is gasified with pure oxygen and hydrogen is added to the gas. For enriching pure H_2 and O_2, the electrolysis of water has been proposed. An investigation will be carried out to determine if this is the best method. There has already been evidence for the feasibility of the water-gas shift and also developments with photo-catalysed conversion of water with Pt/TiO_2 as catalyst.

Internationally co-ordinated R&D of sustainable energy

In the Netherlands NOVEM is a focal point for sustainable energy. A number of universities and the institutes ECN and TNO-MEP have relevant research in this area. In the fifth programme, sustainable energy has been identified as a focal point (EU-Joule). The following is a brief description of developments in the Netherlands:

The energy policy of the Netherlands recognises three main areas:
- reduction of energy use
- development and application of sustainable energy sources
- infrastructural system integration

The goal is to achieve a 33% improvement in energy efficiency by 2020 compared to that of 1995 and for a contribution of 10% to come from sustainable energy. In order to achieve these aims, an ambitious European policy is a necessary prerequisite.

For electricity production, several possibilities can be considered:

- concurrent heating of biomass material in coal installations
- concurrent heating of biomass material (after gasification) in gas installations
- gasification and combustion of biomass material in new independent installations
- on shore wind energy
- off shore wind energy
- PV cells
- increasing energy retrieval from waste
- water power
- environmental heat

Due to the limited amount of space in the Netherlands, importation of cultivated crops for biomass material will be an important consideration. In this regard, it must be emphasised that a great deal of logistical and technological research is necessary. For wind energy an increase of power of 100 MW is expected to occur each year to approximately 1500 MW (200 to 300 turbines). The bottleneck is space. The potential of external wind energy, perhaps in an international context, must be examined.

For the long term, the highest expectations are with PV cells, primarily as a result of decentralised use by current homeowners. The potential for the Netherlands is estimated to be several thousands of MW. The main focus rests on research, development and pilot projects directed at cost reduction, efficiency improvement and increasing production volume.

For the supply of heat, there are several possibilities:
- thermal solar energy
- geothermal heat and heat pumps in combination with storage in aquifers
- heat from biomass installations, waste combustion installations and electricity plants

In view of the fact that sustainable energy at present is relatively expensive, there are regulations necessary to promote an accelerated introduction of these technologies. The regulations that have already been put into effect are insufficient, however, to reach to target of 10% sustainable energy by 2020. Therefore, the Plan of Action for Sustainable Energy is being developed. The plan creates a stimulus for investment in sustainable energy and methods for creating the necessary infrastructure. The goal of the plan is to increase the contribution of sustainable energy to the energy supply in the Netherlands to 10% of the total use by the year 2020.

Intrinsic cost analysis of ethanol, methanol, bio-oil, etc.

It is still not clear what the best choice is for the carbon source / energy source of the future. Methanol is a good option in many instances, but whether or not it is always the best choice requires an extensive cost analysis study. It is important to develop several options at the same time. Other interesting options (non C1) are ethanol and bio-crude (produced through the previously mentioned HTU process). The potential of processing raw materials for the bulk chemical industry (ethene, propene) must be taken into account, as well as storage possibilities for the energy sector. In addition, connecting the supplies to the transport sector is an important factor that needs to be investigated.

4.4.2 R&D options

Pilot projects GSHPC

On the basis of the system study of GSHPC (see 4.4.1), it can, on a pilot scale, be coupled to and tested in already existing installations.

Storage technology

The supply of energy, in the form of PV energy, wind energy, and biomass material, will vary strongly over different periods. There are day/night differences, summer/winter differences and variations in quality. Furthermore, the energy sector must deal with variable patterns of demand. Due to this highly variable supply and demand situation, there is a great need for the storage of energy. For this purpose, various methods have been investigated (aquifers, weirs, etc.). An interesting way of storing this energy is in the form of a liquid such as methanol, ethanol, pyrolysis oil and biocrude, that can be stored in existing tanks. The storage technology of H_2 must be further developed.

Biomass gasification to give Synthesis gas

The reactions given for Synthesis gas (see p. 83: Methanol) are completely different and occur at different temperatures. This has an effect on the gasification process. The whole process of converting biomass to methanol (or Fischer-Tropsch gasoline) must be optimised in an exergetic way.

A step in which much is still unknown is the introduction of biomass material into the reactor. A number of projects have begun in which biomass material is mixed in with fossil fuels during combustion.

Other problems are caused by nitrogen, sulphur, and phosphorous compounds as well as metals that are present in biomass material. Even though the concentrations of these elements in the biomass are fairly low, the absolute amounts can quickly add up. The possibility of NO_x, SO_2, phosphorous, and heavy metal exhaust, caused by the presence of these spoor elements must be examined.

Optimisation of methanol synthesis

There are several ways of making methanol: from CO/H_2-gas, through dry-formation and by means of electro-chemical production from CO_2. The production of methanol from CO/H_2-gas is the most popular method. This occurs, for example, at Methanor in Delfzijl (the Netherlands) and at the Air-Products/ Eastman LPMEOH process in Kingsport (U.S.A.). It is important to choose the proper route. For this purpose an initial screening of the most promising routes is necessary. The production of methanol will probably take place with the help of newly developed catalysts and reactors. Because this involves an exothermal process, a high temperature conversion is desirable. In the development of catalysts, this must be taken into account. This goes against the trend of low-temperature catalysts.

Conversion of methanol into raw materials for the bulk chemical industry

The end product of the GSHPC process must be able to serve both as an energy source and a raw material for the chemical industry. It is naturally extremely important that the right product is chosen for these ends. The new raw material will eventually be a replacement for the currently used fossil raw materials. The chemical production that is currently used must also be able to be produced from the new raw material. Methanol appears to be a good possibility. From the study, it will become apparent if this is the case.

Methanol

Types

A distinction can be made between methanol as a raw material for electric energy, transport fuel and chemistry. Methanol as a chemical raw material must be of very high purity. Methanol as an energy source is not further purified. Small amounts of water, higher alcohols and organic impurities are acceptable. Methanol used as fuel is a mixture of higher alcohols and can be used as an additive to gasoline without resorting to expensive purifying procedures. Methanol should be thought of as a good way of transporting H_2 that is deliverable upon demand by simple catalytic conversion.

Routes:

Methanol 'CH_3OH' can be made from Synthesis gas. The conversion of Synthesis gas into methanol is described by the following reactions:

$CO + 2\ H_2 = CH_3OH$
$CO_2 + 3\ H_2 = CH_3OH + H_20$

A number of side reactions occur, namely:
$CO + 3\ H_2 = CH_4 + H_20$ (methane formation)
$CO_2 + C = 2CO$ (Boudouard reaction)
$CO + 2H_2 = (-CH_2) + H_2O$ (Fischer-Tropsch reaction)

Due to the large number of side reactions and by-products, the choice of catalyst is important for achieving an optimal process. In addition, natural and process conditions such as temperature and pressure play an important role. These are dependent, however, on the choice of catalyst.

A promising new process is:
Liquid Phase Methanol (LPMEOH ™) Process

The LPMEOH process was developed in the 80s in the United States by the Eastman Chemical Company and Air products. The process uses a slurry bubble column reactor to convert CO-rich Synthesis gas into methanol. The process can be combined with an 'Integrated Gasification Combined Cycle (IGCC) electricity plant. The process converts a part of the CO-rich Synthesis gas into methanol, and the non-reacted gas is conducted to the gas turbine with 'combined cycle.' The combined IGCC with LPMEOH allows for energy storage, peak leveling, clean fuel for export and/or the sale of methanol. The concept has been tested in a factory with a capacity of approximately 100,000 tons/year of methanol in Kingsport, Tennessee in the United States. Using this process it is possible to produce methanol at a cost of 46-50 $ct per gallon (US).

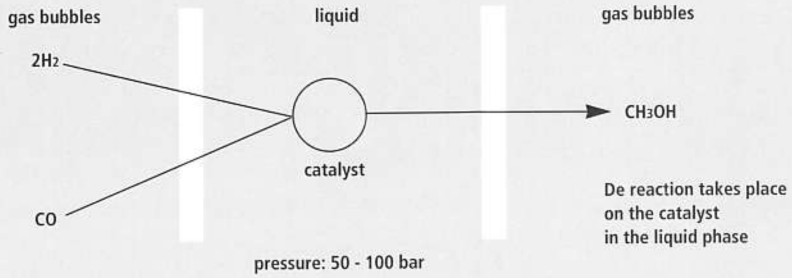


Fig. 4.6: Principle of the liquid phase Methanol (LPMEOH™) Process

Fuel cells

In a fuel cell chemical energy is directly converted to electrical energy by electro-chemical reactions. During the generation of energy, no polluting materials such as carbon monoxide, sulfur dioxide or NOx are released. In addition, the fuel cell can operate quietly.

Currently, fuel cells are used in space vehicles, decentralised energy generation and co-generation of heat and power. Examples of fuels that can be used in a fuel cell are: methanol, natural gas, coal and gasoline. The fuel is first converted to hydrogen (H_2), then subsequently oxidised with O_2 in which water is formed (H_2O). As a result of this electro-chemical conversion, energy is released in the form of electricity.

Compared to what happens in a conventional combustion chamber, in a fuel cell the fuel and oxidiser do not come into direct contact with each other, but are separated by an electrolite. A number of subsystems are necessary for a fuel cell to function. One of these systems is a fuel reformer, which converts the fuel into hydrogen by coal gasification or steam reforming, for example.

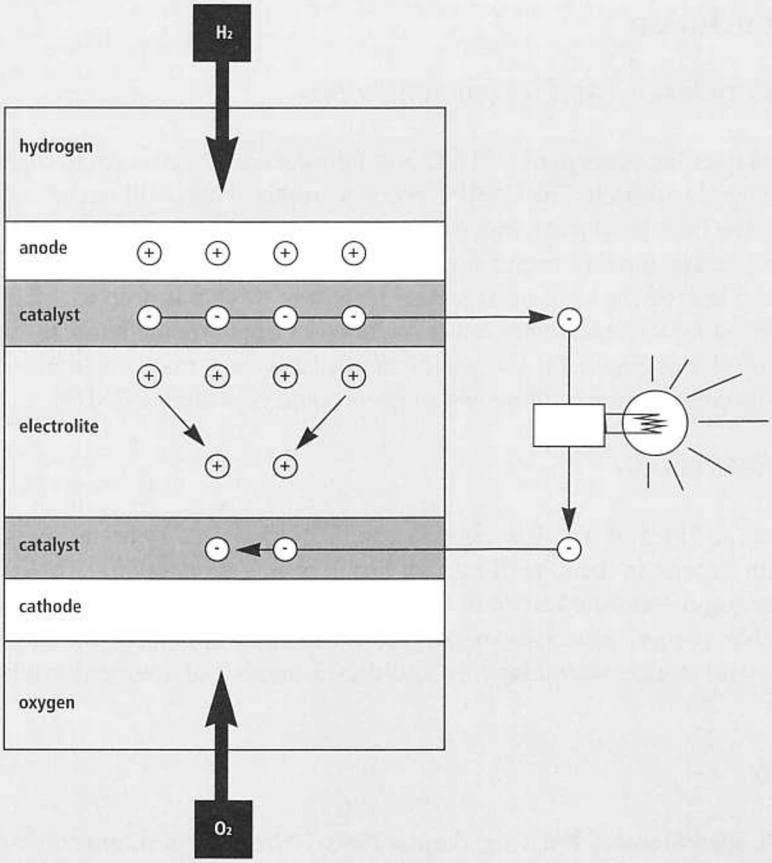


Fig. 4.7: Operation of a fuel cell

The ion exchange between fuel and oxidiser creates a charge difference between two electrodes; furthermore, heat is created as a by-product. By connecting the two electrodes the charge can be used. The by-product heat can be used as a high value process heat for a high temperature fuel cell or be used for heating a low temperature fuel cell.

4.5 Conclusion

4.5.1 Conclusions and recommendations

In this chapter the concept of GSHPC was introduced. The concept is characterised by an integral approach. The GSHPC process proposed here will not be achieved all at once. The individual parts, however, can be tested on a pilot scale. In the U.S.A. a pilot project has already begun for the co-production of methanol and electricity, power and heat on the basis of fossil raw materials. With this process, methanol can be produced for a considerably lower cost then in conventional units. In England, a pilot project has begun for the gasification of biomass material in an electricity plant. The combination of these two projects could constitute a GSHPC.

4.5.2 References

To obtain and idea of the view regarding hydrocarbons, a number of sessions were held with experts in the area of energy with a chemistry coupling. The ideas from these sessions contributed an extra dimension to the current initiatives in the area of sustainable energy, especially regarding the integral approach, the development pathway and storage technology. In addition, a number of sources have been consulted:

Reports:

- Derde energienota, 1996, vergaderjaar 1995-1996; Tweede Kamer der Staten Generaal.
- Duurzaamheid en chemie, Een bundel essays; Interdepartementaal onderzoekprogramma Duurzame Technologie; 1996.
- De haalbaarheid van de productie van biomassa voor de Nederlandse energiehuishouding, NOVEM, 1992.
- The Shell hydrothermal Upgrading Process, a Shell/Comprimo publication, Jan. 1995.

Various articles:

- Biomassa tussen zon en wind; Gas; May 1995.
- Vergassing en synthese voor energievoorziening op middellange termijn; NPT Procestechnologie; Feb. 1995.
- Abrado M., Air Products and Chemicals Inc. V. Khurana, Kinetics Technology International Corp.; Hydrogen technologies to meet refiners' future needs; Hydrocarbon Processing, Feb. 1995.

- Drown David P., et al., Fuel and power co-production, The Liquid Phase Methanol (LPMEOH™) Process Demonstration at Kingsport; Air Products and Chemicals Inc., Air Products Europe, Eastman Chemical Company, U.S. Department of Energy; Fifth annual DOE Clean Coal Technology Conference, Tampa, Florida; January 7-9, 1997.
- Tindall B.M., M.A. Crews Alternative technologies to steam-methane reforming; Howe-Baxter Engineers, Tyler, Texas; Hydrocarbon Processing; Nov. 1995.
- Trimm D.L., Methanol synthesis and water-gas-shift reactions on raney copper catalysts; M.S. Wainwright; pp. 29-42; Catalysis Today 23; 1995.
- Xiaoding Xu and J.A. Moulijn; Mitigation of CO_2 by chemical conversion: plausible chemical reactions and promising products; Energy & Fuels, volume 10, number 2, pp. 305-325, 1996.

Chapter 5: Photovoltaic Cells

Technologies for the conversion of solar light into electricity

5.1 Introduction

The sun is an important energy source. The development of economically feasible methods for using solar energy on a broad scale has attracted intense interest. In this chapter, the techniques behind the current application of photovoltaic (PV) solar cells are described. It is clear that solar cells have a future, but to what extent and what role they will play, is not yet certain. The vision of the future for solar energy is outlined in paragraph 5.3. The R&D agenda is based on existing lines of research in the field of PV solar cells.

5.1.1 Justification

From a chemical standpoint, there are a number of reasons for focusing on the photovoltaic (PV) effect:

- developing solar cells for energy will reduce the use of (dwindling) fossil fuels;
- the chemical industry is a potential producer of the starting materials for solar panels or even for the cells themselves; chemistry is used in the production of solar cells;
- the chemical industry consumes a great deal of energy; solar cells could provide a large fraction of the energy necessary, or even lead to the selective addition of energy to chemical reactions;
- the possibility of producing H_2 with solar cells for the production of methanol (long term option);
- (indirect) reduction of CO_2.

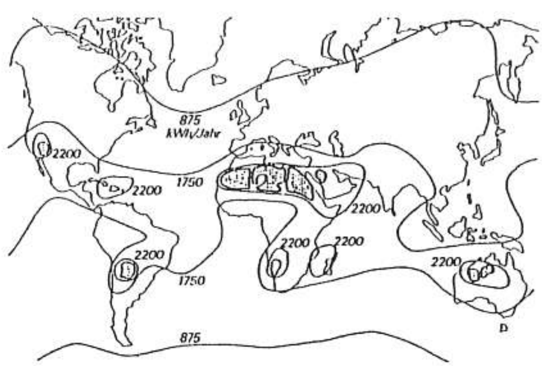


Fig. 5.1: World sunshine map - kWh/year must be read as kWh/m²/year

5.2 Description

5.2.1 Solar energy

The energy received by the earth from the sun is thousands of times higher than the amount of energy consumed. It is therefore of considerable interest to make use of this sustainable energy source. There are many ways of converting solar energy into usable energy:

- Photosynthesis, such as that which takes place in plants. The efficiency in which plants convert sunlight into biomass that can be used as a chemical building block is low (0.5%); on the other hand, they are spread out over a large surface area;
- Solar collectors, in which solar energy is converted into heat;
- Chemical reactors, in which the energy from sunlight is converted into chemical energy, for example for the production of fuels, H_2 or other (temporary) energy carriers;
- Photovoltaic cells, in which electricity is made with the current (record) efficiency (depending on the material used) of 25-34%.

One of the most elegant and potentially interesting sources of sustainable energy is the last option, the conversion of sunlight into electricity with the aid of photovoltaic solar cells.

The various sources of data regarding the amount of solar radiation and worldwide use of energy are not in agreement with each other. These divergent data are shown in table 5.1.

Even though the data presented below do not differ that widely from each other — the NOVEM estimate of radiant energy concerns that which reaches the surface of the earth, i.e., the radiant energy minus the absorbed and reflected energy — there is still no agreement by scientific experts concerning the amount of sunlight that, within a reasonable assumption, can be trapped and used. Estimates concerning these numbers range from 600 to 3000 EJ/y (1EJ = 1x 10^{18} J). In general, it can be

	Okkerse & van Bekkum	Turkenburg	Novem
incoming radiant energy	$2,8 \cdot 10^6$	$3,0 \cdot 10^6$	$0,54 \cdot 10^6$
world energy consumption	350	400	338

Table 5.1: Incoming radiant energy and energy consumption, global, in EJ/y.

argued that PV is capable of contributing greatly to world energy production.
The amount of incoming radiant energy is not the same everywhere on earth. The "world sunshine map" is shown in figure 5.1 from which it can be seen that the amount of radiant energy per square meter per year is the highest in the Sahara and in parts of North and South American and Australia. That doesn't mean that it is not possible to make use of radiant sunlight in other parts of the world. Even with limited radiant sunlight, energy supplies are sufficient; in addition, indirect sunlight (for example, on a cloudy day) provides energy. In the Netherlands, 60% of the energy comes from indirect radiation. The total yearly sun availability in the Netherlands amounts to approximately 3600 MJ/m^2. This is approximately 45 times the total energy consumption in the Netherlands and approximately 500 times the country's electricity consumption.

5.2.2 Solar cells

In general, PV cells can be divided into two types: organic and inorganic. These two types can be further divided as shown in figure 5.2. The current generation of solar cells is based on inorganic materials.
A standard silicon solar cell is made up of a layer of p-type silicon and a thin top lay-

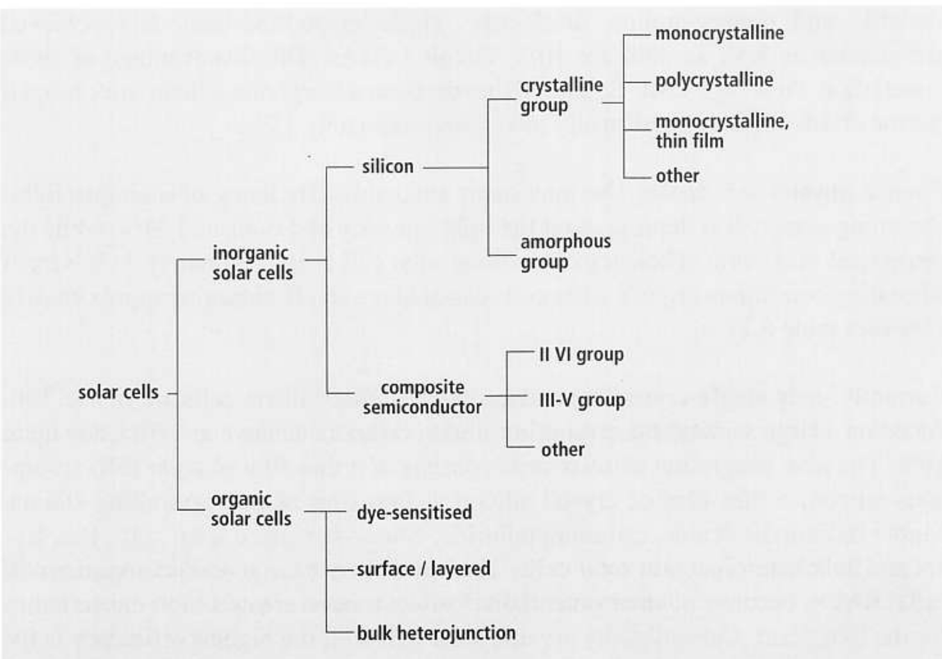


Fig. 5.2: Distribution pv cells

er of n-type silicon. Excitation of an electron by a photon transforms an electron from the valence state to the conducting state. In the p-type crystalline silicon solar cell, the attacked electron diffuses to the interface with the n-type material. The electric field present ensures that the electron crosses the interface and ends up in the n-type material (front side of the cell). Through normal Ohmse conduction, the remaining hole ends up on the backside of the cell. After connecting electrical cables on the front and backsides of the cell, the energy from the sun, stored in the electron, can be used in the external electrical circuit: in this way electrical power is generated.

The band gap of the semiconductors must be between 1.1 and 1.7 eV (1100 to 700 nm) in order to absorb the sunlight as efficiently as possible.

5.2.3 Current technology

The principle of the PV cell was discovered in 1839 by the French physicist Becquerel. But it was only after the Second World War that serious work was carried out to develop his idea. Initial investigations were carried out primarily for use in space travel and, after 1970, as an alternative source of energy. The first generation of solar cells were made of crystalline material such as silicon, gallium-arsenide and copper-indium diselenide. These crystalline materials achieved efficiencies as high as 30% for III/V GaInP / GaAs. The disadvantage of these materials is their high cost. Solar cells made from amorphous silicon are cheaper, but the efficiency is proportionally lower, approximately 15%.

From a physics standpoint, the maximum attainable efficiency of a simple light-absorbing solar cell is dependent on the light intensity and is around 34%, while the theoretical maximum efficiency of a silicon solar cell is approximately 31%. Under laboratory conditions organic solar cells can achieve an efficiency of approximately 11% (see table 5.2).

Currently, only single-crystalline and multi-crystalline silicon cells are in use. Produced on a large scale, these crystalline silicon cells can achieve an efficiency up to 16%. The new generation of solar cells consists of a thin film of solar cell, amorphous silicon, a thin film of crystal silicon, a thin film of polycrystalline silicon, copper indium diselenide, cadmium telluride, colour-sensitised solar cells, flat, layers and bulk heterojunction solar cells. The last three are the so-called organic solar cells, which, because of their potentially lost-cost, have created high expectations for the long term. Currently, the organic solar cell with the highest efficiency is the Grätzel cell. This type of cell uses a ruthenium bipyridine dye as its basis, that is absorbed onto a nanostructured semiconductor. The absorption of a photon causes

type pv-cell	commercia l	laboratory
crystalline silicon	13 - 16%	24,5%
polycrystalline silicon	12 - 15%	18,6%
thin film crystalline silicon	-	19,2%
amorf silicon	4 - 7%	13,2%
III / V GaAs / Ge	21% (satellites)	27,3%
III / V GaInP / GaAs	-	30,2%
CIS	8%	17,7%
CdTe	4 - 5%	16,0%
thin film polycrystalline silicon	-	10,3%
organic	-	11,0%

Table 5.2: Record efficiency of PV cells (early 1998)

excitation of the dye, after which an electron is directly transferred to the semi-conductor. Because the semiconductor surface is nanostructured, the effective surface is increased by 800 to 1000 times in relation to the geometric area. It is sufficient, therefore, to use a monolayer or a few monolayers of dye to achieve complete light absorption. The energy efficiency of this cell is 11%, comparable to that of an amorphous silicon cell.

The cell from the Netherlands' consortium, Interdisciplinary Research Group on Organic Solar cells, is based on an antenna layer of dye molecules on which light is absorbed. This antenna layer does not require the use of a solvent. The layer is attached to either a flat or microstructured semiconductor. A growing number of research groups in the Netherlands are working together on the development of a "plastic-PV." The PV active layer of the cell investigated by the "Polymer Solar energy Initiative (PSI) consortium consists of a nanostructured composite of polymer dye and a derivative of [60] fullerene (C60, "bucky ball"). In the thin donor-acceptor composite layer, there is a very large contact surface between the polymer donor and the fullerene acceptor. The components are present in a particular ratio such that two interpenetrating networks are formed (the so-called bulk heterojunction). The transport of the holes and the electrons to the electrodes takes place separately in this network.

5.2.4 Economic significance

By the end of 1997, a total of 4.0 MWp (peak power) of PV cells had been installed. In the third energy report from the Dutch Ministry of Economic Affairs (1995), it was proposed that 10% of the energy in use by the year 2000 be sustainable, of which 10 PJ must come from PV cells, accounting for 17% of the electrical power.

The large grid-coupled applications of solar cells in the Netherlands involve three residential projects:

- Amsterdam: 72 residences, 4400 solar panels 250kWp.
  The energy is brought to the central grid.
- Amersfoort: 50 residences, 2214 panels 110kWp.
  The energy is taken up in the central grid.
- Apeldoorn: 100 residences, 2200 m^2 of solar panels 230kWp
  The residents individually own the solar cell system and the electricity.

In addition to these applications there are several other large and small applications including:

- PV sound barrier. Along a distance of 550 m, PV, with a capacity of 55kWp, combined with a sound barrier.
- PV systems for existing houses in Leiden. For a restoration project, a grid coupled PV system was installed on five houses. The 2.3kWp system with individual converters is the property of the homeowner and delivers, in the case of excess capacity, electricity to the grid at the normal energy rate.
- Two "zero-energy" houses exist in the Netherlands. For the energy needs of these houses, use is made of solar panels and collectors.

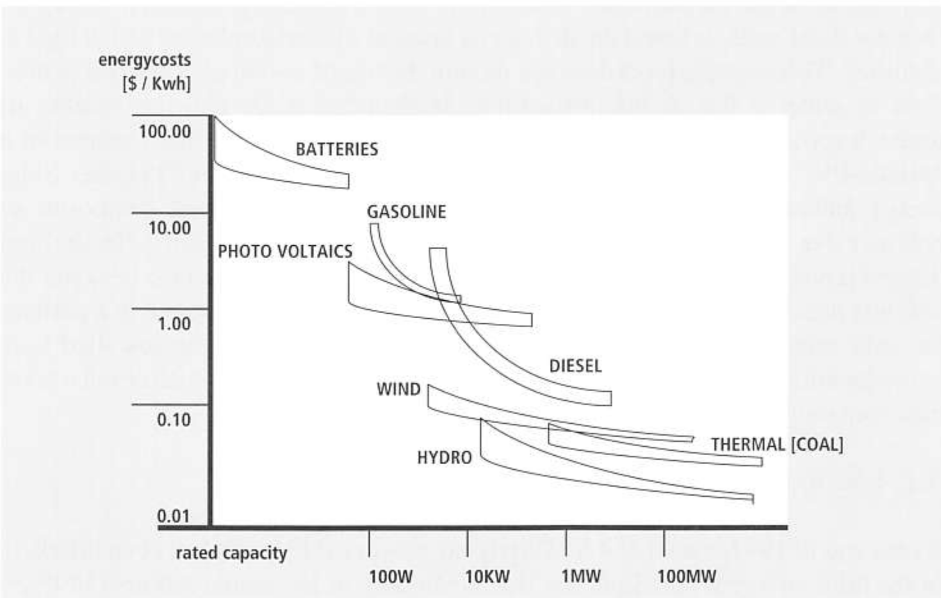


Fig. 5.3: Comparative electricity production costs, 1987

Shell Solar Energy b.v. in Helmond is currently the only producer of PV cells in the Netherlands.

Costs

PV cells can best be compared to other forms of energy by determining the cost per kWh. Additionally, the scale must be taken into account (see figure 5.3). In spite of the fact that this figure was determined in 1987, it still gives a general view of the effect of scale size. Electricity from solar energy is still much more expensive than that derived from fossil raw materials (see figure 5.4). That photovoltaic electricity can still be competitive cost-wise, can primarily be explained by its lower distribution costs.

The solar cells currently in use in Apeldoorn in the residential project (1996) provide an indication of the current cost: $22m^2$ of solar panels cost fl. 40,000.

From several sources it appears that the costs of a kilowatt of electricity, derived from solar energy, sometime between 2005 and 2010, must be reduced by 70% in relation to the costs in 1996.

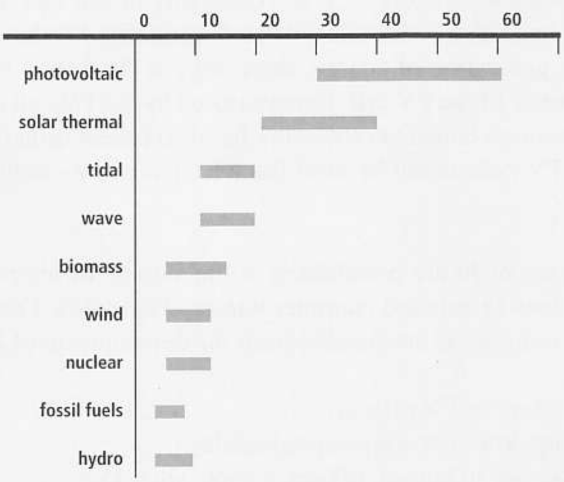


Fig. 5.4: The generation gap; price range of electricity generation, 1993

The use of solar cells is being promoted by a number of organisations in the Netherlands. Four of them are listed here:

- NOVEM manages the national research programme solar energy photovoltaic

conversion (NOZ-PV) under the auspices of the Ministry of Economic Affairs.
- NOVEM stimulates activities that may lead to future large-scale applications of PV in the Netherlands.
- Holland Solar, industrial society of the solar energy industry, whose goal is the promotion of solar energy in its broadest meaning.
- ISES-Nederland, the Dutch department of the International Solar Energy Society, whose goal is the application of solar energy in all forms and promotion by the exchange of expertise and experience.
- ODE, the national organisation for Sustainable Energy, serves the interests of people who use, or will use, applications of sustainable energy. ODE is planning to specialise in the establishment of PV-societies.

5.3 Long term view

5.3.1 The future

It is expected that photovoltaic energy will play an important role in the future. The approach will be decentralised and will take place within different users groups (households, industry, transportation, etc.) and differ according to region, depending on the regio-specific factors such as availability of sun and wind. Decentrally generated energy must also be introduced in a decentralised fashion.
In addition to the generation of energy, there will, in the future, be more complex uses for the chemistry of the PV cell. Energy stored by the PV cell could be used for redox reactions in the so-called photoelectrochemical cells. Furthermore, it is not inconceivable that PV cells could be used for selective energy transfer to a reaction mixture.

An important aspect of future possibilities is the storage of generated energy that can handle variations in demand (summer/winter, day/night). The development of good storage technologies is inseparable from the development of PV cells.

Concepts for the future of PV cells are:
- modular build up, low cost, easy, reproducible
- decentralised service in houses, offices, remote sites, etc.
- central coupling (dynamic / storage
- simple to use, for example, as adhesive foil
- integral approach

5.3.2 Enabling Technologies

The following is a summary of technologies that are important for achieving viable PV systems.

Integral PV technology in application
Currently, the principal problem of solar cells is the high cost. It is expected that new technologies will lead to a considerable decrease in costs.

Semiconductor technology
The PV cell is based on semiconductor technology. The material can be either inorganic or organic.

Cell technology
Cell technology is aimed at developing new concepts for solar cells that have a long lifetime and a high efficiency.

PV foil laminate technology
For commercially viable PV cells it is necessary to be able to laminate PV sensitive materials by a simple method. New pressure techniques for simplifying the lamination of PV materials will play an important role.

Cell production technology
Production technology is of great importance for lowering costs.

Installation technology
In addition to PV cells with a high efficiency and a low cost, the installation must also be inexpensive.

Charge-transport technology
Charge-transport is coupled with energy loss. These losses are caused by switching from constant current to alternating current and vice versa. If used on a large scale, in which excess electricity is delivered back to the electricity grid, which serves as a backup during cloudy days, for example, then there will most likely be problems when switching from the constant current grid (PV cells) and the alternating current grid (large electricity stations) and vice versa. A possible solution to this problem is the establishment of a large-scale, constant current grid instead of the alternating current grid that is currently in use.

Storage technology
Energy storage is needed to span the time between the production and consumption

of energy. In chapter 4 a solution to this problem (GSHPC) was discussed. Additional storage technology will involve batteries, for example.

5.3.3 The road to the future

The future of PV cells and systems is not yet clear. The following is a sketch of a step-wise trajectory towards sustainable energy with the help of PV cells.

In the Netherlands, three concepts will be considered since 1995 for the decentralisation of energy generation by PV cells:
- The decentralised concept. The electricity plant is the owner of the system and uses the roofs or facades of buildings.
- The PV system is the property of the homeowner, who also controls it. The homeowner has a contract with the utility company to deliver excess electricity to the power grid.
- The service concept. The system is managed and operated by the utility company and is leased or rented by the homeowner. The electricity is the property of the homeowner.

In the Netherlands, current total energy use per year is approximately 2,900 PJ. In the year 2000, that number will increase to around 3000 PJ. The policy of the Dutch government aims at a goal in which 10% of the energy consumed in the Netherlands in 2020 is sustainable. In this regard, it is expected that an important role will be played by photovoltaic solar energy. The main emphasis is on research, development and demonstration projects, increasing efficiency, cost reduction, and increasing production volume. The intended contribution of sustainable energy to total energy use is provided in table 5.3:

sustainable energy sources	1990 (PJ)	2000 (PJ)	2020 (PJ)
wind	0,4	16	45
photovoltaic	0	<1	10
thermal solar heat	0,1	2	10
geothermal heat	0	0	2
cold and heat storage			
aquifers	0	2	15
heat pumps	0,2	7	65
water power	0,7	1	3
waste and biomass	21	54	120
total sustainable energy	22	83	270

Table 5.3: Sustainable energy

According to the World Watch Institute in Washington, a country such as the U.S., using political means and high taxes on fossil fuels, can expect to convert 30% of its electricity to solar energy within the space of a few decades.

5.4 R&D Agenda

From the information in the previous paragraphs it is clear that PV cells can play an important role in providing energy in the future. There is still, however, a great deal of research to be done. The following is an outline of important research areas to be pursued.

5.4.1 R&D Studies

Comparison of silicon cells with organic PV cells
Organic and inorganic thin film solar cells are both very promising. It is, however, not yet clear which of these two types of solar cells has the most potential for the long term. An investigation will be carried out to compare the potential of these two types as well as to determine the advantages and disadvantages of amorphous silicon cells and several organic types which are being developed in the Netherlands.

Study of the environmental gain from the PV chain
A comparison of different types of solar cells can illuminate the competitive advantages of each type. A chain analysis, in which the whole chain from production of PV cells to the waste stage is measured, is necessary. Energy analysis is of particular interest. Energy from the sun is free, the reduction of SiO_2, however, for the commonly used silicon cells, takes energy. The "thick" multi-crystalline silicon cells (300 μm) are, therefore, very expensive. Only after a very long time — several years — will these cells deliver as much energy as was put into them during production.

Considering that the lifetime of these cells is limited (30 to 40 years), the energy from them cannot compete with cheap fossil fuel energy. New generations of silicon cells are, however, much thinner, so that part of the production costs in the energy price can be considerably lowered. The question is whether or not the costs will further decrease as a result of savings in starting materials and energy. There are many ideas for improving PV cells. In this regard, much is expected for the future.

Integral study on integrating the biomass and PV into energy services.
Similar to the comparison of PV cell types (see above. Comparison silicon cells with organic PV cells), a comparison between alternatives, such as using biomass

material, is of interest. There are still differences of opinion about the most efficient means of converting sunlight to a useable energy form.

5.4.2 R&D Options

Further development and scaling up of PV cells
Solar cells are receiving attention in a number of programmes:
- National research programme solar energy photovoltaic conversion (NOZ-PV), administered by NOVEM;
- EC-JOULE programme
- NWO, priority programme "solar cells for the 21st century;
- research programme of institutes (ECN) and universities;
- EET programme of the Dutch government
  The most obvious approach at this point is to further stimulate activity within these existing programmes. The research into different solar cells is currently focused on cheap PV cells that have a high efficiency.

Research in the Netherlands can be divided into three categories:

A *Current generation solar cells*:
Support of market development in the short and long term.
- Improvement and cost reduction of production technologies of multi-crystalline silicon.
- Research into high efficiency scenarios for multi-crystalline silicon.

B *Next generation solar cells:*
Research into concepts with potentially low costs.
- Inorganic thin films
- Thin films

C *Long term studies into alternative concepts on the basis of high efficiency and hybrid systems*

In the Netherlands research is being carried out, among others, by:
- SHELL SOLAR ENERGY B.V. R&D department,
- ECN, department of sustainable energy, PV cells, and modules
- LU Wageningen organic chemistry,
- University of Utrecht atom and interface physics
- TU Delft applied inorganic chemistry
- Dutch Interdisciplinary Research Group on Organic Solar Cells
- Debye institute (University of Utrecht),

- TU Delft DIMES,
- TNO-TPD

World-wide, an immense amount of research is being carried out on solar cells. The following is a brief overview of a number of universities, institutions and companies participating in solar cell research.

Japan:	NEDO,
Switzerland:	Grätzel, Ecole Polytechnique Federale de Lausanne
United States:	University of Notre Dame,
	California Institute of Technology,
	Polaroid Corporation
	Eastman Kodak Company,
	Columbia University,
	National Renewable Energy Lab,
	Northwestern University,
	Johns Hopkins University,
	Rutgers University,
	Colorado State University,
	Xerox Webster Research Center,
	University of Texas at Arlington,
	University of California,
Germany:	ISFH,
	Fritz-Haber-Institute,
Sweden:	University of Uppsala
Ireland:	University College,
France:	NAPS France,
Finland:	Microchemistry

Fundamental research on organic PV cells
A representative overview of fundamental research into organic solar cells is difficult to present. For antenna-layer cells the current research is directed primarily at:
- Understanding of the processes that occur after photon absorption in heterogeneously layered systems: exciton transport, charge transport, energy transfer, interfacial energetics, and electron transfer as a function of the interfacial energetics on an electrode or contact.
- The formation of charge carriers after photon-excitation.
- Charge transport.
- Which type of contact do the carriers come up against at an interface, organic/organic or organic/metal.
- What is the role of crystallinity, and what is the optimum crystallinity.

- The development of new analysis techniques.
- Purity of the dye. (Among other things, reactive train sublimation is being looked at).
- New organic materials that not only have the desired physical properties in terms of light absorption, excitation energy transfer and electron/hole conduction, but also have highly ordered and thin organic films that can be formed in a sandwich structure between semiconductor and opposing electrode.
- Can the required crystallinity be achieved in large scale production. Can the existing inexpensive techniques be improved so that they provide a good quality cell or must new production techniques be developed.

One production method for organic solar cells involves the sequential evaporation of layers of dye pairs in which a junction is formed with a space of 500 to 600 Å. The dye absorbs light in the range of 400 to 700 nm and achieves a quantum efficiency of 20% with monochromatic light. An improvement is expected, if the impurities found in the dye can be removed.
The method being investigated by the Netherlands' research consortium for the production of organic solar cells with antenna-structured organic dye, is based on the liquid crystalline properties of the molecules used. When they are in the isotropic fluid phase, the materials are introduced between the electrodes by means of capillary filling. Subsequent cooling to the liquid crystalline phase results in a highly ordered film.

Storage and transport technology
If PV cells are to be used in the future for generating energy, then this will most likely happen in a decentralised fashion (on roofs, sound barriers, etc.). Due to the day/night and the summer/winter variations in the supply and demand of energy there will be a need for some kind of energy storage. A solution to this problem might be the generation of H_2 gas by PV cells when there is an excess of electricity. The gas is stored and, during a shortage of electricity, it is converted to electricity by a fuel cell. The bottleneck in this process is the production of a high efficiency fuel cell at a low cost. In addition, the high- efficiency conversion of electricity into hydrogen and its storage will have to be improved.

There is a "solar-hydrogen" pilot factory in Bavaria (Germany) with a capacity of 200 kW, in which this process has already taken place. Storing energy in the form of methanol is another possibility (see chapter 4). Seasonal influences are a bigger problem than day/night differences. Possible solutions for these variations include the thermal storage of solar energy. In this scenario, water with a temperature of 90°C is pumped during the summer into aquifers at a depth of 3 km. Because the temperature at this depth is also 90°C, the energy content of the water will not decrease. In the winter the energy is recovered, for example, by Organic Rankine Cycles (ORCs), that makes use of the inverted refrigerator effect. The storage capacity of these aquifers is approximately 20,000 PJ. Drilling these aquifers is currently still expensive, but thanks to recent developments in horizontal drilling techniques, the prospects are very promising.

Total concept of solar cells in application

Inexpensive, high efficiency PV cells are only useful when integrated into a system. At the very least, a PV system consists of a panel of solar cells, equipment to control the system, and a battery or connection to the electricity grid. If the system must provide electricity for households in the Netherlands, there must also be an inverter that converts the constant current to 220V alternating current. A distinction can be made between an autonomous system and a grid-coupled system. Autonomous systems need to be adjusted to user needs. The batteries, for example, must have sufficient capacity to handle several dark days.

The quality of the grid-coupled system is dependent not only on the efficiency of the PV cells, the slope and orientation of the panel, etc. Losses that occur during electricity transport, mismatch, kWh-meter and invertor also play important roles. The yield factor is defined as delivered kWh per kWp, divided by the radiant solar energy in kWh/m^2. In the Netherlands, in 1995, grid-coupled state-of-the-art PV systems were made with a yield factor of around 75%. In 1992 that figure was only 60%. It is expected that the yield factor around the year 2000 can be increased to 80%.
In addition to the user situation, research must also be done into the shaping of the PV foil and the installation of the PV systems. It is in the interests of small and medium-sized businesses to be involved. Furthermore, PV systems should be considered from an integral standpoint. Improving the overall efficiency will also involve the possibility of integration of the PV cells with other systems and should be investigated. The solar boiler is a good example of this. In the PV cell, not all the energy is converted to electricity, a great deal is lost as heat. The produced heat can be used by a solar boiler, so that the overall efficiency is increased.

In order to increase the types of use, new applications will have to be developed. One possibility is the integration of the PV systems in windows, the so-called “smart windows.” Even though these windows absorb a portion of the incoming light they allow sufficient light to pass through. The absorbed light is converted to electricity. Roofing tiles are another possible application.

5.5 Conclusion

5.5.1 Conclusions and recommendations

Intensive research is being carried out on PV solar cell technology. It is important to stimulate and administer the already established R& D lines and to focus attention on further developments of a broader vision.
Regarding this vision, companies and institutes will set up R&D projects. The most important recommendations are:

- Study the international position of research and industry in the Netherlands. Due to the enormous global interest in sustainable energy sources, the international context of the research is important. This study can be carried out by the Ministery of Economic Affairs. The weak and strong points of the Netherlands' investigation into PV cells must be established. From this information policy standards can be outlined.
- Continuation of existing research programmes in the area of solar cells (NOVEM, NWO, EET, EU, etc.). In order not to get behind the rest of the world, at least the current level of research should be maintained. It is very important that not too many different goals are pursued, but to focus only on those that appear to be promising for the future. Amorphous silicon and organic cells appear to have very good potential for commercial success.
- Evaluate solar cell pilot-projects for their optimisation aspects. The most important aspects appear to be: SEP, electricity distribution companies, the government, large consumers (industry).
- Stimulate research programmes that focus on storage technology (see also chapter 4).
- This stimulation is in conjunction with Senter, NOVEM, NWO, etc., industry and research institutes should then take up the challenge.
- Comparative study of PV cells that will enable a choice to be made in the long-term regarding energy aspects. On the basis of the results of this study, the direction for the future can be determined. Together with the study of the international position of research in the Netherlands, this input can be used for establishing direction in the various research programmes.
- Involvement of small and medium-sized businesses in the Netherlands in the development (primarily with shaping and installation) of PV cells.

5.5.2 References

Reports:

Derde energienota, 1996, vergaderjaar 1995-1996, Tweede Kamer der Staten Generaal, October 1995.

Duurzaamheid en chemie, Een bundel essays; Interdepartementaal onderzoekprogramma Duurzame Technologie; 1996.

Various articles:

J.A.M. van Roosmalen: Thin Film Solar Cells, (ECN-AC-95-107); (ECN, Petten NL).

J.T.N. Kimman, E.W. ter Horst, L.A. Verhoef, E.H. Lysen, The new pv-programme in the Netherlands, a balance between R&D market development and pilot projects, Novem; 13th European photovoltaic solar energy conference; Nice, France; 23-25 October 1995.

E.W. ter Horst, J.T.N. Kimman, E.H. Lysen, Large scale urban pv-projects in the Netherlands, four pilot projects in urban areas, Novem; 13th European photovoltaic solar energy conference; Nice, France; 23-25 October 1995.

Organic solar cells and other photoconductive systems, internet:
http://www.er.gov/production/bes/chm/photochem/panela 1.html; 10-9-96.

George R. Bird, Organic semiconductors.

A critical test of organic p-n photovoltaic cells, internet: http://www.er.gov/production/bes/chm/photochem/bird.html; 9-25-96.

Chapter 6: Process Technology of Fine Chemicals

Methodology of Manufacturing Processes for Fine Chemicals

6.1 Introduction

The fine chemicals industry is a clearly-defined sector where major, rapid improvements could be made and which can also serve as a model of sustainable development for other sectors. This chapter presents the interpretation of 'fine chemicals' in this context, and how the fine chemicals industry can contribute to sustainable development. The future perspectives and requirements imposed on process technology in the fine chemicals industry are discussed. The R&D Agenda in section 6.4 emphasises the further development of the fine chemicals sector. The activities of the multi-disciplinary Programme for the Development of Sustainable Technology (DTO) in the Chemical Industry project in 1996 provided a solid foundation for this in the form of the Fine Chemicals Forum. This has received strong support from the fine chemicals industry in the Netherlands.

6.1.1 Background

Why does the fine chemicals industry serve as a model for sustainable technological development? Links between the fine chemicals industry and sustainable technological development are:

- *Wastes:* the fine chemicals industry produces relatively large quantities of waste compared to the end-product volume. The effects of scaling-up and the period during which plants are operational are also relevant.
- *Model:* the fine chemicals industry can provide an example of sustainable development to the bulk chemicals industry.
- *Quality of life:* the high added value of the products means that the fine chemicals industry improves the quality of life.
- *Fine chemicals research:* there is clear interest in this field and there is and attractive outlook for the future.
- *Expertise:* the high added value and complex, small-scale operations and technology require great expertise and skills.

ad: Wastes
It is widely recognised that the fine chemicals industry produces large volumes of wastes compared to the end-product volumes. The volumes handled in the fine chemicals industry are relatively small, but there are relatively large waste streams that are sometimes harmful to the environment.

ad: Model
Given the small scale of the fine chemicals industry compared to the petrochemicals industry, the fine chemicals sector produces little pollution in absolute terms. However, in relative terms the fine chemicals industry produces a large amount of pollution (volume of waste per unit of end-product).

An important reason to designate fine chemicals technology as sustainable technology is that it could serve as a model and lead to spin-offs of new technology to the bulk chemicals industry. It has been shown on several occasions that the fine chemicals industry is open to large-scale innovation. Examples of this are provided by biotechnology and biocatalysis.

A few years ago, most bulk chemicals companies bought biotechnology and plant breeding companies. They are now disposing of them as it is thought that biotechnology will not develop into a fundamental technology for the chemicals industry in the near future. In contrast, biotechnology is increasingly applied in the fine chemicals sector. This is partly due to the investments of venture capital companies in small biotechnology businesses in the US. However, the fine chemicals industry is also turning towards the bulk chemicals sector, e.g. for enzymes (washing agents, foodstuffs), process technology and equipment. Other bulk chemicals technology such as chemical catalysis has not yet been successfully transferred to the fine chemicals industry. At present, chemical catalysis is not well-suited to the fine chemicals sector. The reasons for this include the high temperatures associated with these catalysts, which fine chemicals cannot withstand.

Fine chemicals for the pharmaceutical industry amount to about half the production volume and can therefore serve as a guide to future developments in this industrial sector. This is particularly relevant for the Netherlands as Dutch companies, with a market share of about 4%, are important players on the world market, and have an 8% share of the market for fine chemicals for the pharmaceutics industry, where they are leaders.

This area also appeals to other professional and consumer target groups if examples of applications can be provided, such as pharmaceuticals, fragrances and flavourings.

ad: Quality of life

The fine chemicals sector improves the quality of products and processes and therefore contributes to the quality of life. Health throughout the world is an important element of sustainable societies. The same applies to personal care products. Fine chemicals can also extend the life of products. Furthermore, fine chemicals can directly improve sustainability, for example, when used as additives in plastics.

ad: Fine chemicals research

Due to the relatively recent recognition of fine chemicals as a separate industrial and academic subject, knowledge and expertise are still being developed at a rapid pace, particularly regarding the underlying chemistry and catalysis, while other areas are still largely undeveloped (e.g. appropriate fine chemicals process technology). It is expected that it will be possible to make a fairly significant advance towards sustainability in the near future, for example through the use of biocatalysis. However, it is quite possible that other technology pathways could lead to greater advances in the period up to the year 2050. Confidence about the technical feasibility of more selective and effective fine chemicals processes is warranted in view of the rapid development of biocatalysis and the wide range of technological concepts for improvement, most of which are currently limited to the academic world. Because the price of fine chemicals is often high, it is likely that a stepwise R&D approach (converting long term goals into short term interests) can be formulated. As far as innovation is concerned, it is reasonable to expect that the disciplines in which the Netherlands is strong (fine chemicals, agricultural sciences, chemical and biological expertise at the universities, process technology) can co-operate to create innovative added value.

The fine chemicals industry has a significant presence in the Netherlands (DSM-Life Science Products, Akzo Nobel, Quest, Solvay, IFF, etc.) and has shown itself to have a positive attitude to sustainable development.

ad: Expertise

The fine chemicals industry fits in perfectly with the goal of developing knowledge-intensive industries through high added value and products dependent upon special expertise.

6.1.2 Delineation

There is a need to distinguish between the areas covered by the applications side (e.g. pharmaceuticals) and the fine chemicals side (building blocks). Starting points for advancing sustainability in the fine chemicals industry are:

1. Applications industry:
   a. Increasing the quality of life through product innovation;
   b. More effective use of products.

2. Fine chemicals industry:
   c. Plant-based raw materials
      (closing the materials cycles)
   d. More efficient and flexible processes
      most relevant to sustainable development in the fine chemicals sector

ad 1a and 1b: Applications industry
In this context, the developments will be autonomous, the commercial interests are so great that industry will have to initiate this development itself. In certain areas government intervention will be necessary to ensure a sustainable future. There are many examples of rapid advances in the pharmaceuticals industry. Where a few years ago several grams of certain drugs were needed, better results are now obtained by doses of around 10 mg (a hundred-fold improvement in just a few years). Similar developments are underway in the agrochemicals sector where pesticide doses have been reduced from 10 - 100 kg/ha to 100 - 1000 g/ha.

Potential developments include:
- providing the required function with the use of fewer raw materials;
- alternatives to existing fine chemicals: e.g. ultrasonic cleaning or biological control methods;
- obtaining better results through using more effective substances (better understanding of the mechanism);
- more effective use of substances (only to be used if they are effective);
- preventing the use of substances.

ad 2c: Plant-based raw materials
The use of plant-based raw materials is likely to be the area of the chemical industry where the greatest developments will occur over the next 50 years. These developments will be based on modern biotechnology and metabolic engineering as well as more conventional methods such as homogeneous catalysis and biocatalysis (enzymes) combined with bioprocess engineering. In short, plants, bacteria or cells will be used to produce raw materials or even fine chemicals.

ad 2d: More efficient and flexible processes
The major contribution to sustainability in the fine chemicals industry will be provided by fine chemicals process technology. This will be discussed in greater detail below.

6.2 Definition

6.2.1 Fine chemicals process technology

In this context we refer to 'fine chemicals' in a broad sense, i.e. the production of defined chemicals or mixtures which are produced to set specifications on a small scale. These chemicals may be organic or inorganic. To some extent, the distinction between commodities, fine chemicals and specialties has been abandoned. As an example two common classification methods will be discussed below.

The characteristics of commodities, fine chemicals and specialties are listed in figure 6.1 and table 6.1 below. Another characteristic of the fine chemicals sector is that products are replaced relatively quickly (short product life-cycle: products 5 - 25 years, processes 5 - 15 years).
Important applications of fine chemicals include pharmaceuticals, agrochemicals, flavourings and fragrances (F&F) and additives. Other types of important fine chemicals include high performance polymers and monomers, plastics additives, dyes, catalysts, cosmetics ingredients and photographic chemicals.

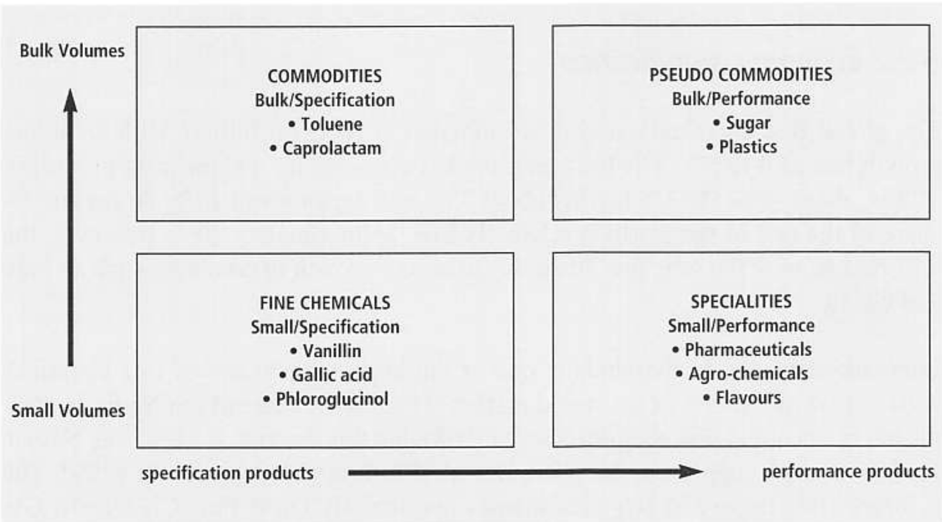


Fig. 6.1: Kline's quadrant

Fine chemicals may also be classified by the function they perform:
- bio-effect (pharmaceuticals, agrochemicals);
- monomers for specialty polymers (e.g. biodegradable, absorbent, gas permeable,

electrically conductive, high strength, temperature resistance);
- photochemical and chemical effects;
- flavour and fragrance effects;
- physical effect (e.g. adhesion promoters, surfactants, antistatic compounds);
- chemical effect (e.g. anti-oxidants, curing and drying agents).

	commodity chemicals	fine chemicals	specialty chemicals
Product assortment	small	very large	very large
Product differentiation	none	small	very large
Volume	> 10.000 ton / year	< 10.000 ton / year	variable
Price	< ƒ 5 / kg	ƒ 10 - 1000 / kg	variable
Added value	low	high	average / high
Product life cycle	long (> 30 year)	average (10-20 y.)	short (< 10 year)
R&D focus	process development	process development	product development
Production	continuous	batch	continu / batch
Profit / investment	< 1	± 1	> 1

Table 6.1: Characteristics of commodity, fine and specialty chemicals (source: Frost&Sullivan).

6.2.2 Economic significance

The global fine chemicals market is estimated at NLG 50 billion, with an annual growth rate of 4 to 5%. The European market accounts for a significant proportion of this, about 40%, the US market about 35% and Japan about 15%. At present the share of the rest of the world is relatively low, approximately 10%. However, this will change over the next few years due to strong growth in countries such as India and China.

Internationally, the Netherlands is one of the largest producers of fine chemicals with a share of 4 to 5% of the world market. The market share of the Netherlands in the pharmaceutical fine chemicals sector is double this amount, 8-10%. The Netherlands is a major supplier to the pharmaceutical industry throughout the world. This is largely due to several large companies, particularly DSM Fine Chemicals, Gist Brocades, Chemferm (now DSM-Life Science Products), Akzo Nobel-Diosynth and Solvay-Duphar. A favourable development in this area is the strong trend, particularly in the pharmaceuticals industry, to dispose of fine chemicals activities to reliable, certified fine chemicals companies. The industry is highly fragmented, there are over 5000 companies in the world producing over 10,000 products. Consolidation, in the western world, has started however.

There are two developments: the development of fine chemicals activities by chemical companies, and by applications companies, such as in the pharmaceuticals industry.

Independent fine chemicals activities are disappearing due to the high R&D costs. Small companies are coming back in the biotechnology industry. Small-scale plants are often set up in newly emerging economies, to supply regional industries. The rise of South East Asia in the fine chemicals sector is largely due to specialist independent manufacturers. In Europe, the USA and Japan these two types of supplier are becoming integrated, combined with the withdrawal of integrated end-users from the fine chemicals sector. In the context of sustainable development, the emerging markets, and competition, in countries such as China and India should also be considered.
The Netherlands fine chemicals industry could develop into a major world-wide supplier to the pharmaceuticals industry.

The world market for fine chemicals can be divided by application:
- Agrochemicals
- Fragrances and flavourings
- Food additives
- Miscellaneous
- Pharmaceuticals

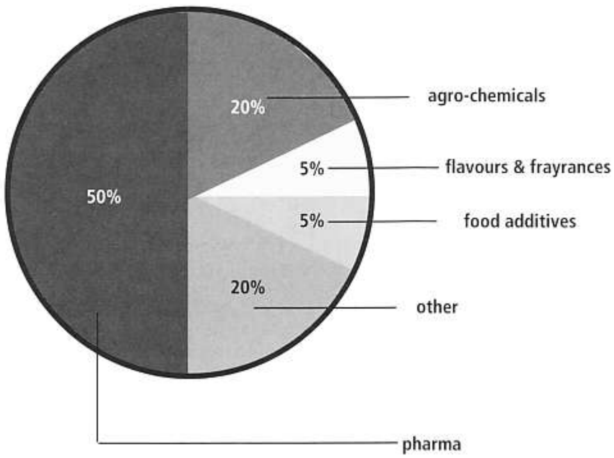


Fig. 6.2: The world market for fine chemicals according to application in the fiscal year 1990 (source: Flemings)

6.2.3 Current Technology

In most cases, fine chemicals manufacturing uses flexible, multi-purpose, small-scale batch production. The main characteristics of the current production processes are:

- Feed: organic
- Process batch, stoichiometric
- Reaction environment solvents
- Reactor type multi-purpose batch reactor

Research and development in the fine chemicals sector focuses on process development and improvement, making extensive use of classical organic synthesis, bio-organic synthesis. The use of biocatalysis is increasing, while little use is currently made of chemical catalysis.

The fine chemicals sector includes a number of business areas and disciplines, these are illustrated in Figure 6.3.

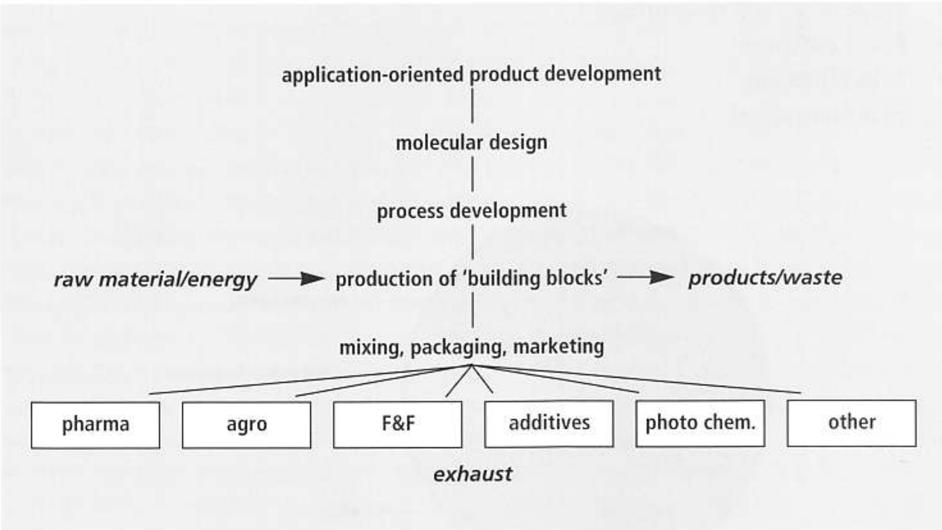


Fig. 6.3: Fine chemistry chain of events

Catalysis is becoming more important, but there is still room for significant development in this area. The distinction between continuous and batch processes is becoming less clear cut. Currently biocatalysts are only used in some processes. Only a few amino acids in these biocatalysts are functional while the rest are not. There is

a trend towards reducing these biocatalysts to their basic chemical structures. Thus, it could be said that biological and chemical catalysis are converging.
Research and development is so capital intensive that little capital is left for production and purification. Downstream processing is not particularly well managed. Greater attention should be given to process technology aspects.

Some trends in technology include:
- Biocatalysis (enzymes) will continue to play a key role in organic synthesis.
- Chiral processes are important because chirality is relevant in almost all natural processes. Chiral products are attractive in view of the increasing interest in and need for targeting, specificity and minimising the use of substances and maximising their effect.

On the basis of extrapolation it may be expected that the ratio between stoichiometric organic chemistry and biochemistry, currently 80:20, will be reversed. However, in view of the overall growth, stoichiometric chemical processes will maintain their current volume.

There is no specific fine chemicals discipline at universities in the Netherlands. However, all chemistry faculties teach supporting disciplines such as organic chemistry, catalysis, process engineering, etc. and fine chemistry is taught as an optional subject at some universities (Nijmegen, Amsterdam and Eindhoven).

6.2.4 Present environmental aspects of the fine chemicals industry

The production of fine chemicals results in the generation of considerable waste volumes as syntheses generally include a number of steps. The yield of each of these steps is rarely 100%, 60 - 90% is common and 10% is not unusual.
For example, if five steps are needed to produce product A and each step has a yield of 50% then 16 kg of raw materials will be needed to produce 1 kg of A. In other words, 1 kg of end-product leads to the generation of 15 kg of wastes.
Furthermore, the solvents and large number of intermediates also generate wastes and acid/base reactions and separations are widely used, hence large quantities of salts are generated as wastes.

A major cause of the large waste volumes is the use of sometimes greatly outdated processes, focused more on the production of the end-product and less on efficiency and process costs. In the past this was quite acceptable because, until recently, there were sufficient facilities for landfilling wastes and were, therefore, no incentives for improvement. The problem, primarily, is that salts are created as by-products, which cannot be reused and which are currently discharged to surface waters. In the past, recovery plants, e.g. for bromides, were offered on the market, but they were not adopted by industry. At present there are almost no truly effective concepts for syntheses in which little or no salt is generated.

Heavy metals are often used in fine chemicals manufacturing, for example as catalysts. Owing to the limited development of downstream technology it is often difficult to separate the products. This often requires the use of large volumes of volatile solvent. These volatile solvents and heavy metals greatly increase the environmental impact.

- The application of fine chemicals also frequently leads to emissions.
  An example of this is the incineration of additives during the thermal recycling of wastes from the fine chemicals industry. After use, all substances reach the environment.
- Safety, noise, odour, energy and water consumption are other important environmental aspects associated with the fine chemicals industry.

In the course of recent years the volume of waste per kg product has already been reduced significantly. However, this was largely offset by the growth of the production volume. Hence, in absolute terms waste volumes were only slightly reduced. Table 6.2 shows that the production volume of the fine chemicals industry rose from 0.5 to 2 mln./ton i.e. a factor 4. This covers 1975-1995, i.e. 20 years. If this trend continued over 50 years this would result in a factor of 10. Hence, the desired factor 10 over the coming 50 years is not unfeasible, given historic extrapolation.
The major elements associated with sustainability throughout the fine chemicals sector are:

	Increase in production volume (mln./ton)	Decrease in waste production (kg/kg)	Decrease in waste volume (mln./ton)
Petrochemistry	100 ➤ 250	0.1 ➤ 0.01	10 ➤ 2.5
Bulkchemistry	10 ➤ 25	1 ➤ 0.01	10 ➤ 2.5
Fine chemistry	0.5 ➤ 2	10 ➤ 2	5 ➤ 4
Specialty chemistry	0.1 ➤ 0.5	50 ➤ 10	5 ➤ 5
Total (rounded off)	100 ➤ 300		30 ➤ 15
Production + waste	130 ➤ 315		
Production / waste	100/30 ➤ 300/15		

Table 6.2: Development of waste volume in various chemical industries between 1975 and 1995

- Wastes: leaks and other losses of raw materials and process materials during production should be reduced, in recent years the emission problem has largely been reduced to a waste problem (salts).
- Harm to the ecosystem: ensuring that substances can be incorporated in life-cycles, particularly after emission.
- Development: effects on sustainability have to be considered during process and product development (laboratories, emissions and risks associated with experiments, etc.).

6.3 The long-term perspective

6.3.1 Perspective

The question arises how the fine chemicals industry will develop in the future.
There are several relevant developments:

- It is most likely that the global demand for fine chemicals will rise by at least a factor of 10 over the coming 50 years. This is also to be expected on the basis of historical extrapolation.
- A fall in demand through the development of products which are not fine chemicals (e.g. bioactive substances such as pheromones or fungi which may be used as pesticides) and more effective products. However, these new products will also generate a demand for new fine chemicals.
- New markets will be developed, such as the electronics industry or organic solar cells (polymers with special properties). Innovation will continue to be important in order to tie in with new developments (diseases, telecommunications, environment, etc.).
- It is likely that the relative market shares of the various types of fine chemicals will change although pharmaceuticals will remain the largest market.
- Continuing differentiation in the end-use markets and an increasing demand for products with specific effects, smaller volumes and reduced environmental impact. Shorter product life cycles due to an increasing product range which will lead to:
  - greater product differentiation;
  - greater product development efforts.
- The fine chemicals industry will be characterised by increasing complexity, diversification (e.g. additives), more complex molecules and an increasing range of processes.

In the longer term, the aim should be to make the applications more effective and processes more selective, to lead to major reductions in the use of raw materials.

The fine chemicals plant of the future will also have to be increasingly flexible. All these considerations are summarised below.

Fine chemicals in the future

- Selectivity: improving the selectivity of processes (less raw material/product).
- Effectiveness: making the applications more effective (fewer mg/function).
- Quantity: meeting the increasing world-wide demand (factor 10 over 50 years is likely).
- Flexibility: meeting the growing need for flexibility:
  - differentiated and increasingly complex product range;
  - shorter product life cycles, hence shorter runs.
- Innovation: developing new applications (disease, telecommunications, environment, etc.).
- Safety: managing the risks of processes and products (safety considerations are an obstacle to modification - this conflicts directly with the other demands), meeting future GMP and GLP requirements.

Indicators towards these improvements (as identified in the DTO essay) include:

- Raw materials: new raw materials such as proteins, carbohydrates, cellulose, lignin, plants, bacteria, biomass.
- New processes:
  - catalysts: enzymes, immobilised enzymes, immobilised chemical catalysts;
  - new conversion techniques: photosynthesis, micro-organism genetic engineering.

	raw materials	process	equipment	waste
NOW	• petrochemical • organic	• stoichiometric • reaction aids • reactor	• multi-purpose	• generic
FUTURE	• bio • agro	• biocatalysis • chemo-catalysis	• discrete • small scale • dedicated	• molecular recognition

Fig. 6.4: Development of process technology

- New equipment: small-scale (may be down to microchip-size), dedicated equipment, new process pathways.
- New separation and downstream methods: membrane technology, electrophoresis, selective adsorption, supercritical extraction. See also Figure 6.4.

This also extends to product and process development for the fine chemicals industry. Such developments should not lead to worse environmental impacts than at present: increasing differentiation and shorter product life-cycles are likely to lead to more product development. The effective use of laboratory facilities and the environmental impact of experiments may become relevant - although the quantities are small the materials may be harmful.

6.3.2 The road to the future

The envisaged path, with the aim of radically changing the current trends in efficiency, towards the development of 1:1 fine chemicals processes, is described below.

6.3.3 Enabling Technology

The major new techniques for future fine chemicals plants are listed below. Current techniques are not included, although they may be relevant. The new techniques will be discussed in greater detail in the R&D Agenda.

Fine chemicals enabling technology

- Integrated technology
- New scale-up tools
- Closed synthesis steps
- New discrete process engineering techniques
- Molecular separation technology
- Catalysis & biocatalysis (enzymes)
- Biotechnical manufacturing methods
- S-S, S-G reactions, solid phase chemistry
- Chiral synthesis methods
- Multiphase reactions

6.3.4 Expected Implications

Economic structure:

Compared to the current fragmentation in the fine chemicals sector it is to be expected that it will be even more fragmented in future. An even more specific and integrated approach will have to be taken to the availability of feedstock and the required application properties. These properties will be defined with increasing accuracy.

The role of the chemical industry need not necessarily change. Some likely developments include:

- In some cases specialist farming operations (plants, insects, animals) may replace chemical reactors.
- In some cases specialist raw materials will be obtained from non-traditional sources (oceans, rain forest, or even outer space, etc.).
- Shift in employment towards specialist R&D: operators in future fine chemicals plants will be more like laboratory technicians or engineers.
- More product development facilities and diversified production units.

Environment:
In view of the potential to optimise the environmental impact of current technological concepts it is to be expected that the positive environmental impacts will become dominant. The scale of the operations will also be reduced and modular, dedicated production methods are likely to be introduced, which will benefit life-cycle management.

6.4 R&D Agenda

The R&D Agenda is primarily focused on implementing the second stage of the road to sustainable development, as set out in the preceding section. In addition to this essential step, parallel studies will have to be carried out to identify 1:1 technology and to develop it.

In the development of super-selective fine chemistry there will be a need to establish fine chemistry and technology as distinct disciplines. The fine chemicals industry will change in terms of process selection and manufacturing methods. The adoption of scale-up tools will lead to more, quicker and better options, in terms of the environment, quality, speed and cost. New principles (pipeless plants, discrete manufacturing, semi-continuous operations) will make it possible to optimise each technique. Hence the following research areas are relevant:

R&D Agenda
The next generation of process technology for the fine chemicals industry

Area 1: methodology and design tools
A. Improvement of the technical implementation of various reaction types.
B. Developing a knowledge-based system for interactive process synthesis.
C. Development of process technology and engineering for the fine chemicals industry.

Area 2: plant layout
A. Rationalisation of existing plants in terms of selection and layout of equipment.
B. Feasibility study of dedicated continuous processes, bench scale.
C. Pipeless plants/discrete production.
D. Customised production.
E. Optimisation of discontinuous processes.

Area 3: integration of new technologies and disciplines
A. Molecular separation systems.
B. Catalysis, biocatalysis (enzyme technology).
C. New techniques.
D. Integration

Area 4: long-term technology (1:1)
Chemistry and biotechnology

6.4.1 R&D Area 1: Methodology and design tools

Historically, developments in the chemical industry have largely arisen in the large-scale process sector: the production of basic chemicals and other basic materials. More recently, an intricate product and process development network of technology for fine chemicals developed in these industries, thereby creating the fine chemicals industry. Owing to this historical development no dedicated fine chemicals process engineering was developed, instead the large scale process technology practices were followed. As the fine chemicals sector has built up its own identity, over the years this has resulted in some problems, in particular with regard to sustainability. Some suggestions for improvement are given below.

Differences between basic chemicals and fine chemicals
The development of fine chemicals and associated products differs from basic

chemicals product and process development in the following respects:

A. The range of reactions is much larger than in the basic chemicals industry.
B. The number of reaction steps is generally much higher.
C. The production volumes (tonnes per year) are much smaller. In this sector, 1000 t/year of a product is a high volume.
D. The lifetime of a product is already short compared to the basic chemicals industry.
E. The time to market, from the start of a development project, is essential and is much shorter than in the basic chemicals industry.
F. In general, the technical implementation of the processes is much less sophisticated than in the basic chemicals sector.
G. The large volumes of raw materials and auxiliary materials, including solvents, used per kg of product, which have to be disposed of as wastes, is a special problem of this sector.

The combination of items C, D and E above in particular means that product and process development in the fine chemicals industry has to be approached completely differently than in the basic chemicals industry. In the basic chemicals industry it is normal practice to set up development projects and commit significant human resources and expertise to them. There is also an extensive infrastructure of expertise: contractors, engineering companies, research institutes and universities. Developments in the fine chemicals industry cannot support this approach as the costs would never be recovered and the process would take too long. This could lead to a vicious circle: insufficient development capacity will lead to processes which are not carefully designed hence the costs will be too high and the competitive position will be weak, particularly in comparison with low wage countries. As a result, the approach of the fine chemicals industry is much less sophisticated than that of the basic chemicals industry. A dedicated process technology for the fine chemicals industry is lacking.

Opportunities for improvement

Improvements could be made by operating differently. As the human resources which can be deployed will always be limited there will have to be rapid interaction between chemists and process engineers. This requires the availability of a broad general knowledge. This points to the following topics:

Application-focused product development

During their development work chemists should be able to rely on expertise of the reaction pathways and their implementation in process plant. This expertise has to be available in generic form. As there is a trend towards increasingly complex products the emphasis will be placed on better reaction techniques such as the use of catalysts (homogenous, heterogeneous, enzymes, metabolic production techniques, etc.). This will demand greater cooperation with research institutes and universities where such techniques are, or could be, developed. The same applies to the purification of products (downstream processing). There is a need for better, cheaper purification methods, resulting in less waste. This means that new techniques will have to be implemented operationally.

Product and process development

During the development of a product/process there will have to be intensive, daily co-operation between chemists and chemical engineers. The chemists' ideas should be immediately interpreted in terms of a potential process path and the associated advantages and disadvantages in terms of yield, investment, safety and wastes. This approach means that the development can be steered at an early stage. However, this means that the process engineer (joint developer) should have access to a generic knowledge base in a system, this information should not be locked away in the heads of dozens of experts. Hence, a knowledge system will have to be created which, when fed with limited information, will be able to make suggestions about the engineering options and their implications, and which also asks questions interactively to improve the concept.

Scaling-up

More than at present, the process parameters critical to the scale-up should be identified at the laboratory scale. Hence, it would be desirable to modify the laboratory rigs to improve the scale-up step. Eventually there would be no need for pilot plants. In this context, the best possible configuration set and appropriate functionality of large-scale reactors and auxiliary equipment in a multi-purpose environment will also have to be considered to accommodate the large number of new processes more easily.

The experience obtained with the scale-down approach to existing processes can be applied and increased in the fine chemicals sector through the scale-up and scale-down of new processes. An analysis of common scale-up problems (non-flyers) indicates that materials transfer and heat exchange require modifications in about half the cases. Other matters, such as inappropriate equipment, quality of the raw materials, process stream stability, cleaning, solvent recycling, etc. are relevant to the other half of the problems.

These modifications will have to be recorded systematically to facilitate scaling up. The drafting of a development checklist for the fine chemicals sector could be considered in this context.

6.4.2 R&D Area 2: plant layout

The availability of the equipment, as well as the layout of the equipment of the plant is an important consideration in the fine chemicals industry. Most high-cost process equipment will have a lifetime longer than the products. Production is often undertaken in campaigns, hence the equipment has to be multi-purpose. As a result, production planning is subject to many constraints, hence batch production is widely used which leads to many movements and complicated logistics within the plant. This problem requires further study. Potential solutions include:

Multi-purpose equipment
This applies, for example, to multi-purpose reactors and multi-purpose distillation plants. Decisive aspects include the range of equipment in terms of size, compatibility with the reaction conditions (temperature, pressure), available instrumentation and control systems and layout in the plant (scheduling, logistics). Generally production is carried out in batches and there is extensive handling of the product streams. It is becoming increasingly difficult to combine this approach with c-GMP requirements and the ability to demonstrate with certainty that cross-contamination of chemicals and process streams is impossible.

Dedicated product lines
These lines are used for one product only. However, this approach means that wherever possible production should be undertaken continuously and that the equipment will have to be dimensioned appropriately. For products produced in very small volumes (up to several tens of tonnes per year) there are some developments towards continuous production in a miniature plant (bench-scale plant). Such a plant would occupy little space, have a modular structure and would require little direct supervision. Such plants may be attractive in the future as there is a general trend towards modular process equipment, i.e. process equipment with instrumentation and control using a DCS (distributed control system).

Pipeless plant
In this approach the process media (solid, liquid, gas) are not conveyed between the equipment (reactor, separation, conditioning) through piping and containers. Instead the process vessel moves through the plant, between specialised processing stations. Such a plant would not suffer from a myriad of piping and large product inventory. This are important issues in the context of GMP and quality assurance.

Discrete production
This is the ultimate consequence of the previous option, i.e. moving from batch production to discrete production. This approach is similar to the unit production in-

dustry, e.g. the car industry. In this case the plant is laid out as a production line and the various products travel down the line in small vessels and are processed by robotised stations. (Similar to producing several makes of car of different types, interiors, colour, etc. on a single line.) The advantage of such a plant would be that scale-up problems are eliminated, that production could be carried out in flexible quantities and that a new product can be implemented through process control. The disadvantages are the large initial investment in the plant and the complex measures to be taken to prevent contamination.

In general, it should be noted that the reduction in the use of auxiliary materials, solvents, etc. is an important issue in the development of new processes.

R&D options Area 2

A. Rationalisation of existing plants in terms of selection and layout of equipment.
This study should address chemical, process engineering and operational aspects and result in a cost/benefit analysis. Co-operation between a chemicals company, engineering firm and a university of technology is an obvious option.

B. Feasibility study of dedicated continuous processes, bench scale.
An initiative for this has been taken in an EC network (process intensification).

C. Pipeless plants/discrete production.
Firstly, the opportunities and problems will have to assessed, and whether or not these will affect the implementation of this concept.

D. Customised production.

E. Optimisation of discontinuous processes.

6.4.3 R&D Area 3 Integration of (new) technologies and disciplines

The implementation of more specific processes requires different conversion and downstream techniques. Catalysis, specifically homogeneous catalysis and biocatalysis aimed at defined conversions, will play a major part in this.

R&D options Area 3

A. Molecular separation systems
A process engineering turnaround will be needed to raise efficiency. Where conver-

sion and downstream processing/purification are now largely separate steps, these will have to be integrated in the future. Multi-phase systems will be useful in this regard, particularly gas or liquid reactions with solids (solid phase chemistry). Membrane reactors, in which the conversion occurs on the membrane and where the reaction products are immediately removed, would also be attractive. At present, substances are often obtained from plants by solvent extraction or steam distillation. The disadvantages of this are that the extraction process is not particularly selective and downstream processing has a high energy consumption and uses large volumes of chemicals. Supercritical extraction and product-specific recovery methods (e.g. using membranes) may solve these problems.

B. Enzyme technology; catalysis

Modifications can easily be made using enzyme technology and biosynthesis. An example of this is the production of aspartame, a sweetener which consists of the amino acids phenylalanine and aspartic acid. Both the production of phenylalanine and linking it to aspartic acid are mediated by enzymes. Other examples of enzyme technology are the conversion of sugars to lactic acid or ethanol. A prominent example is the production of penicillins and cephalosporins. Multi-step traditional stoichiometric chemical processes have been shortened considerably by the introduction of biocatalysis, i.e. a 10-step process for cephalexin without any (bio-) catalysis has been replaced by a 6-step process scheme including three enzyme-catalysed steps.

New areas of (bio)catalysis will have to be developed, for example, in which a set of catalysts performs a multi-step process (cascade catalysis). Directed alteration of enzymes and the development (genetic engineering) of new enzymes will be another area. New, fast screening techniques should allow for a quick analysis of (bio-) catalyst capabilities. Formulation, i.e. immobilisation, of (bio-)catalysts tuned to the process and down-stream conditions could become a new area of specialisation.
The use of new technology will make it possible to replace organic solvents by water.

C. New techniques

Embryonic techniques will have to reach maturity to serve a sustainable fine chemicals industry. Whereas biocatalysis enables us to prevent the use of solvents, it might also be the entry to reactions in aqueous slurry's and (almost) solid phase chemistry. Extremophiles have been found to be able to function under unthinkable conditions. The use of supercritical solvents will open up other vistas.
A very important area for future research should be the avoidance of salt formation in the fine chemicals industry. In multi-step fine chemicals processes generating 10-30 kg of waste per kg of product, over 80% is mostly inorganic salts. The introduction of bio- and chemo-catalysis does not solve this problem. New reaction schemes

and down-stream procedures will be needed. Electro-chemistry and membrane technology might be a promising route.

D. Integration

Whereas some new specialties might be needed to sustain the R&D Agenda of the future, integration of disciplines will be the key towards a sustainable industry. This encompasses profound changes. Academic education, university research, public and private R&Ds will have to change focus and direction. The vertical specialties-oriented approach to research and education must also adopt a horizontal direction that covers more disciplines and results in a lateral movement. Teamwork, already a common practice in industry, must be introduced at universities and public R&D facilities.

Ingredients for an integrated approach required for a sustainable (fine-) chemicals industry are (bio-)organic synthesis, catalysis, chemical technology and bio-process technology. Attention to quality (GMP, GLP etc.) and customer orientation will be desirable assets for future R&D workers in the fine chemicals industry.

Integration should also allow for an interactive approach of process development in which scouting out synthesis routes, catalyst development, down-stream processing, plant lay-out and QESH-aspects (quality/environment/safety/health) are treated as a whole.

6.4.4 R&D Area 4 Long-term Technology (1:1)

An approach which should be initiated now, especially at the universities, is the identification and development of technology that can lead to major, rapid changes. Metabolic engineering might provide such an opportunity. High throughput screening and experimentation techniques might be another area of keen interest.

The production of chemical specialties - fine chemicals - in 2050 will increasingly be based on the direct or indirect use of natural substances. Secondary metabolites, i.e. substances which are found in plants in small quantities, have pharmacological activity or can be activated through modification. Taxol, from the yew tree, which is used to treat breast cancer, is a good example of this.

Existing plants and micro-organisms provide an enormous reservoir of chemicals. Biotechnology can be used to tap this reservoir more efficiently. Appropriate organisms can be genetically modified to produce the required substance as their metabolite. For example, taxol can now be produced by micro-organisms.

Commodities could also be included in this group. Starch and proteins are attractive raw materials for resins, unsaturated oils are used for a range of 'natural' paints and hemp and flax fibres can be used as reinforcement.

Metabolic pathway engineering, followed by metabolic flux analyses, as well as more conventional techniques such as homogenous catalysis and biocatalysis, combined with process engineering is the area where the major developments are expected to occur in the next 50 years. New secondary metabolites will be synthesised to our requirements using modified micro-organisms or plant cells. It is also to be expected that during the course of the next decades complex molecules which are currently produced by complicated syntheses will increasingly be recovered as secondary metabolites. A new fermentation industry might emerge.

On the other hand, increasing knowledge of the biosynthetic schemes will enable the development of highly efficient and specific chemo-catalysts. Exploitation of combinatorial techniques will speed up this process.

These developments apply in particular to products in which regio- and stereospecificity are required. Following the present trends, this will apply to the great majority of fine chemicals in the next century. Current (bio-)catalysts have to become much more efficient (kg of product/volume), more specific and, most importantly, much easier to develop. Integration of disciplines, as discussed in the previous section, is again of pivotal importance for these R&D directions.

6.5.1 Conclusions and recommendations

The fine chemicals industry has a number of promising options for more sustainable production methods. The approach taken by the fine chemicals sector should serve as an example to the rest of the chemical industry.

Considerable development work will have to be undertaken to meet these objectives.

The first important instrument to realise the objectives of an innovative and new fine chemical process technology is to set up a forum with representatives from this industry. This forum should continuously work on the definition of R&D projects needed to develop technology for major, rapid changes. This forum will help to shape the fine chemicals industry.

The first impetus for the creation of such a forum was provided by the meetings organised by DTO in 1996 and 1997. During these meetings it became apparent that there is a clear support for such a forum within the fine chemicals industry, appraising the need for technological breakthroughs towards sustainability. The main reasons for this are defining the objectives for a long-term approach and pre-competitive information exchange enables efficient operation of this platform. The first joint industry-university research projects have already been defined.

The policy outlined with respect to the R&D Agenda has been described in detail in an STW proposal.

6.5.2 References

We would like to acknowledge the assistance of the participants in the fine chemicals forum for their support in writing this chapter. The essay by Fortuin and Boelhouwer written for DTO provided the basis. DSM provided information on this branch of industry for the general description of the fine chemicals sector.

Chapter 7: Sustainable Construction Materials

7.1 Introduction

Many sustainable construction materials are made of fibre-reinforced composites. Fibre-reinforced composites are prepared by combining fibres and a binder. The choice of fibres and binder, as well as the manner in which they are combined, determines the strength, the rigidity, and the mouldable qualities of the end product. Frequently used materials are polypropylene, polyethylene, PVC or polyester, strengthened by glass fibres. Due to the irritation caused by glass fibres, however, their use is associated with health risks.

An alternative to glass fibres is flax or hemp. These fibres can be combined with a biopolymer binder to create a composite end-product that is completely biodegradable. Furthermore, working with polymeric materials and natural fibres poses no health risks. Natural fibres are used on a large scale in 'classic composites' such as paper and board. New applications are being developed by automobile manufacturers, among others. Important points to consider are the elementary strength of the fibres, the moisture sensitivity of natural fibres and the bonds formed between the fibres and the plastic matrix. The flax fibre appears to match the qualities of glass fibres.

A frequently used composite of completely natural origin is wood. Wood is easy to work with and has favourable material qualities. A disadvantage, however, is that wood, softwoods in particular, is unable to withstand water, changing weather conditions and micro-organisms. The properties of wood can be improved by the use of resins. Materials made in this way are resin-based board materials such as triplex, MDF and HDF. For these applications, resins are made on the basis of phenol formaldehyde, ureaformaldehyde and melamine. To make the material water resistant, environmentally unfavourable impregnating materials such as lacquer and stains are often used.

7.1.1 Justification

Fibre-reinforced polymer materials are a good addition to currently available materials and can absorb the growing demand for materials of this type. Furthermore, fi-

bre-reinforced polymer materials are considerably lighter than metals so that transport and building applications, as well as energy and ergonomic advantages can be achieved.
Justification for fibre-reinforced polymeric materials as an important technology for sustainable development:

Lighter materials
Fibre-reinforced polymeric materials result in lower weight, which is an advantage in the transport sector, for example. In this way, energy consumption can be significantly reduced. In the construction industry, ergonomic considerations are worth considering in that lighter materials reduce the physical stresses on builders.

Contribution to a growing need for materials and fibres
Due to population growth and an increase in standards of living, a large increase in the need for fibres and materials is expected (for construction, textiles, consumer products, paper, hygiene, furniture, etc). By seeking alternatives now, a head start can be made in reducing the threat of scarcity. At the same time, inroads into optimising new materials can be made.

Alternatives for hardwood
Tropical hardwood is currently used for many applications. This type of wood combines good mechanical properties with a reasonably good resistance to wood rot. It is, however, a slow growing wood type. The pace at which it is consumed is high, complicated by slash and burn agricultural practices. In spite of the fact that wood is a renewable resource, in principle, there is a potential for a non-sustainable consumption of this material. The current sustainable techniques of softwood are quite damaging, in practice, even though they do not appear to have negative effects in life cycle analyses in relation to other materials. This is due to the toxic materials used, often chromium compounds. Alternatives that other technologies use for prolonging the life cycle are already available. Some examples are: Plato-process, acetylation, plastification. In the meantime, there has been a great deal of attention paid to managing hardwood sources by renewed plantings. The replacement of hardwood is relatively inexpensive.

Renewable materials
The majority of metal-based materials currently in use is not renewable. Adequate recycling is therefore an important consideration. By making use of biomass based materials, however, as a source for (composite) materials, a closed cycle can be achieved when after use the consistuent molecules of CO_2 andH_2O combine again with sunlight to biomass.

7.2 Description

To obtain a relative sense of the value of fibre-reinforced polymeric materials, an insight into the criteria established for these materials is necessary.

7.2.1 Material prerequisites

Every application asserts particular demands on a material. The material properties that can be important in this regard have been divided into the following categories:

- Low cost
- Primary properties (mechanical); in particular, strength, toughness, resistance to breaking and deformation, weather resistant, and water resistant
- Secondary characteristics; in particular, chemical (corrosive resistant, UV stabile), and physical (density, conductability, colour). Ageing
- Sustainable characteristics; in particular renewability, energy consumption (during production and use) and recyclability.
- Application-specific characteristics (a universally superior material does not exist!)

For most applications, the specific strength and specific rigidity (strength and rigidity divided by density) are important parameters in the choice of material. They indicate the characteristics of certain materials through unit of weight. This information is especially important for transport considerations. In figure 7.1a, this information is given for different materials. Although expensive, carbon fibre-reinforced plastics have very good properties. When the costs of the materials are taken into consideration, the relationship is shown in 7.1b. It should be noted that the costs considered here are the material costs only; production costs can vary considerably.

7.2.2 Composites

Combining materials results in a combination of their characteristics. Examples of this are reinforced concrete and reinforced glass. Plastics to which fibres are added are referred to as composite materials. The fibres increase the rigidity and strength of the material, while the plastic matrix ensures that the material is water tight, consistent and flexible. If the matrix and the fibre are made of natural materials, a biocomposite is created. A good example of a natural biocomposite is wood, paper and board material. Wood and the woody parts of plants are responsible for the rigidity of trees and plants.

Two qualities of composites:

1. Low tech, large market, low costs, natural and synthetic materials
2. High tech, specific market, high prices, synthetic materials

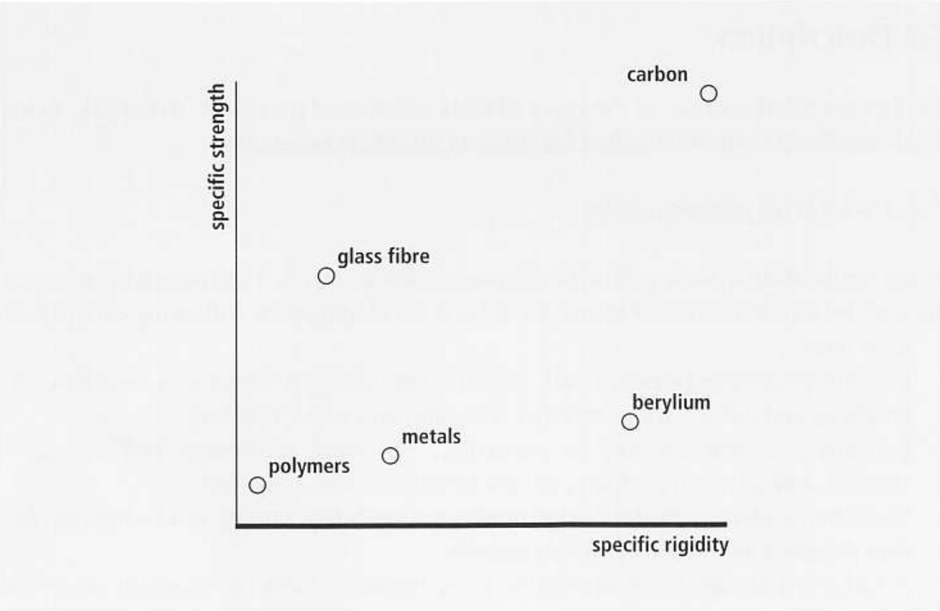


Fig. 7.1a: Specific strength vs. specific rigidity

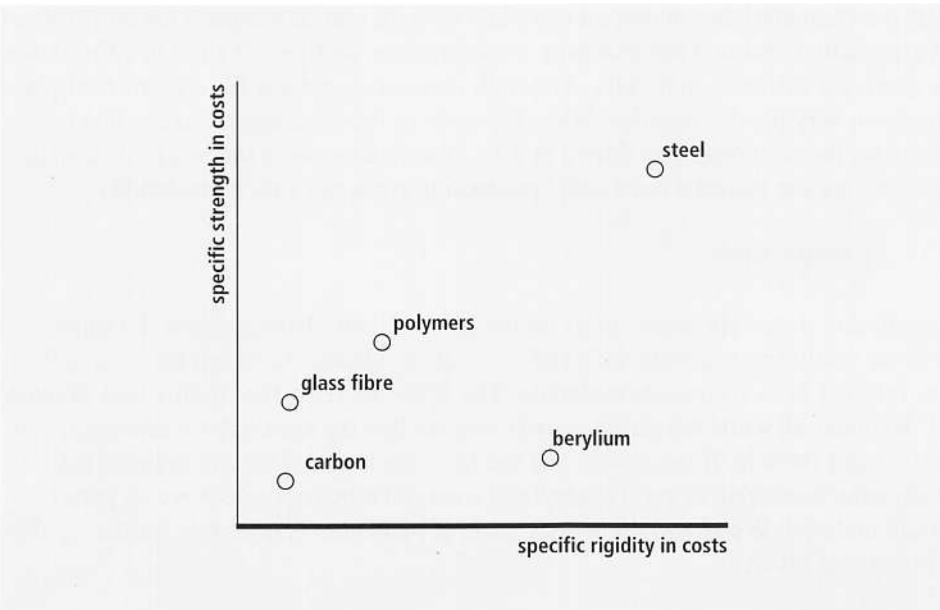


Fig. 7.1b: Specific strength vs specific rigidity in costs

Fibres

Fibres can be divided into three groups: natural fibres, semi-synthetic fibres (made from natural materials) and synthetic fibres (made from petroleum). An overview of these types is shown in figure 7.2.

The properties of these types of fibres differ vastly from one another. Currently, synthetic fibres often have many advantages over natural fibres in terms of their material characteristics. Poor strength, durability, resistance and water retention are some of the disadvantages of natural fibres.
Semi-synthetic plant-derived fibres are made up of cellulose and to some extent have less desirable properties than synthetic fibres. Cellulose is a natural polymer that occurs in the cells of all plants. It is the most ubiquitous and renewable biopolymer on earth.

As a result of increased research, the properties of plant-derived fibres are continually being improved, and natural fibres appear to offer good possibilities for the future. Even though fibres can be extracted from all plants and trees, only a small number have commercial potential. A summary of fibres that are used in commercial applications (in addition to deciduous and evergreen wood), are listed below:

- wood
- jute (for textiles)
- ramie (for textiles)
- kenaf (for textiles)
- hemp (for textiles and paper)
- flax (for paper, rope, building materials and linen)
- kapok (for paper, rope, building materials)
- sisal (for paper, rope, building materials)
- coconut fibre (for paper, rope, building materials)
- manilla abaca (for rope)
- reed (for paper, rope, building materials)

Fibres used in the Netherlands are wood, hemp, reed, flax

Currently, the most important applications of plant-derived fibres are wood-products, paper (including paper for hygienic products), and textiles. In addition, fibres are also used as rope, but this application is decreasing in favour of plastics. In building materials, many plant-based fibres are used in hard-board, sheet-rock, insulation materials, and cement, for example. In addition to wood and plant fibres, inorganic fibres are also used for these applications. New applications are in the areas of board material for the building and construction industry, geotextiles, and as substitutes for asbestos.

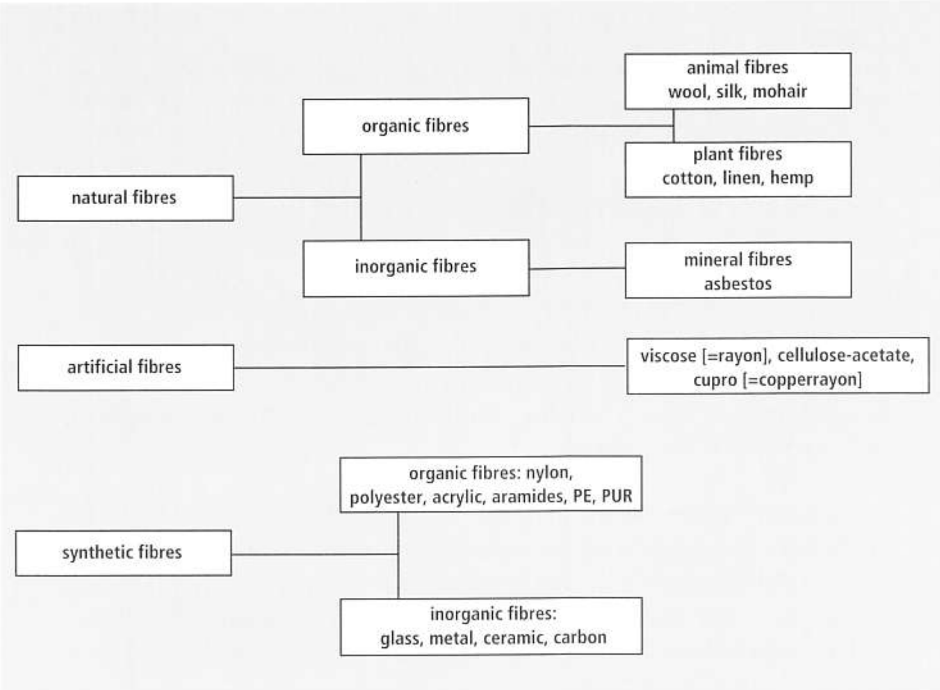


Fig. 7.2: The three main fibre groups [source: STT Publication, Plant-derived raw materials for industry, 1991]

	Thermosets		Thermoharders	
	1992	1995	1992	1995
Aerospace/military	6,8	8,3	0,7	1,3
Transportation	232,9	284,2	178,9	332,1
Building/construction	204,6	249,7	3,2	5,9
Electrical	184,7	225,4	151,2	280,7
Marine	95,6	116,7	n/a	n/a
Sport/leisure	54,8	66,9	3,2	5,9
Other	47,8	58,3	30,7	57,0
Total	827,2	1009,4	367,9	543,7

Table 7.1: West European consumption of reinforced composites according to end use (in thousands of tons)
(Source: Reinforced Plastics, March 1997, from the handbook Plastcs Federation, BPF)

7.2.3 Economic aspects

As was previously stated, a distinction must be made between low-value and high-value applications of composite materials.
The low-value applications involve the wholesale market of moulded and sprayable compounds, laminates, powders, MDF, triplex, OSB, hardboard, Trespa, plastic wood, etc. Natural fibres are being introduced into this market on a large scale. Triplex is cheap, MDF is more expensive. Paper can also be included in this group.

Examples of applications for high-value fibre-reinforced composites include:

- construction: corrosion and heat-resistant materials, high-voltage cables, light dividing walls,...
- machine construction: weight-bearing constructions, fatigue-resistant materials, transport belts,...
- sport and leisure time: tennis rackets, golf clubs, F1 racing cars,...
- biomedical: orthopaedic aids
- automobile: interior panels, bumpers, leave springs
- aeroplane: interior, many secondary parts (flaps,...), some primary parts (vertical tail piece), helicopters,...
- fibre-reinforced wood for bridges and weight-bearing constructions.

Market figures covering a number of aspects have been recorded in order to give an economic indication of the subject of this chapter. It includes tables in the areas of:

Market development of composite materials:
It is expected that the European market for fibre-reinforced plastics will continue to grow throughout the 90s, albeit at a slower pace than in the last few decades. According to the statistical handbook of the British Plastics Federation (1996), the average growth after 1994 was 5% a year. The market for reinforced thermal plastics grew

Application	Price (EURO / kg)
PMCs (polymer matrix composites)	0.690
IMCs (inorganic matrix composites)	0.650
MCs (matrix composites)*	0.549
textile	0.616
paper and pulp	0.352
total average	0.547

Table 7.2: Indication of end users prices for euro/kg dry goods (DG XII publication)
**MC is a group in which the trial was not reported whether it was PMC or IMC.*

somewhat faster than for reinforced thermoharders. An indication of the market growth in Europe is shown in table 7.1.

Fibre prices:

Shown in table 7.2 are the average prices of fibres used in applications. The data come from the report Industrial Fibre Crops from the EC (1994). The sample was small, however, and the prices show a broad distribution. The prices given here, therefore, can only serve as an indication.

Production of (man-made and) textile fibres:

An overview of the world production of textile fibres is presented in table 7.3.
A distinction is made between 'man made' fibres (synthetic and cellulose), cotton, wool, and silk. It primarily concerns fibres that are not used in composites. In addition, a geographic distribution of the production of 'man made' fibre is shown (table 7.4).

	1993	1994	1995	95/94: ±%	1995: share (%)
Man-made fibres [1]	19,781	21,050	21,741	+3,3	52
Synthetics	16,652	17,908	18,471	+3,1	
Cellulosics	3,129	3,142	3,270	+4,1	
Cotton	18,494	18,394	18,602	+1,1	44
Wool	1,687	1,736	1,767	+1,8	4
Silk	68	69	92	+33,3	
Total	40,030	41,249	42,202	+2,3	100

Tabel 7.3: World production of textile fibres (in 1000 ton), Source: Man made fiber year book, September '96

	synthetics	cellulosics	total	share (%)
Asia	10,218	1,308	11,526	53
USA/Canada	3,313	240	3,553	16,3
Latin America	988	98	1,086	5,0
Western Europe [2]	2,697	543	3,240	14,9
Eastern Europe	1,028	263	1,291	5,9
Africa	220	13	233	1,1
Australia	9-	-	9	-
World, total	18,472	3,260	21,741	100

Tabel 7.4: Geographic distribution of the production of man-made fibres (in 1000 ton/in 1995) Source: Man made fiber year book, September '96

1) excl. polyolefin fibres, textile glass fibres and acetate cigarette filter tow; 2) incl. Turkey

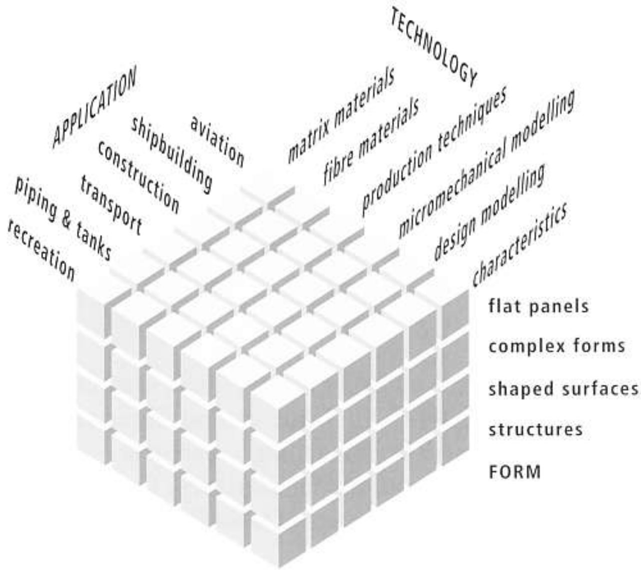


Fig. 7.3: Material matrix [© Willems & v. d. Wildenberg, the Hague]

7.2.4 Current technology

Composites have made a place for themselves in the use of materials. There is, however, vast room for improvement. In this chapter, two approaches are outlined for achieving fibre-reinforced composite materials:

From (organised) fibres and a binder, construct a suitable material

The first approach involves preparing a suitable material from fibres (even if they are not organised) and a binder. Several combinations of fibres and binders are possible. Organising the fibres contributes greatly to the performance of the material, but this process is expensive. Many natural and synthetic fibres are anisoptropic. This means that the material does not have the same properties regardless of the orientation of the fibres. The efficiency of strengthening with fibres is expressed as efficiency factors. These factors are dependent on the packing direction and the direction of force. Orientating the fibres in the proper direction can result in 'textile' construction. Fabrics and knits are good examples of this, but they have only been used in limited applications.

In figure 7.3 composites are illustrated in terms of their different possible applications, the shapes and the supporting technologies. The field of high value composites and the accompanying research is presented. In the priority program of the Netherlands Scientific Research Organisation (NWO), however, little attention is paid to these materials. A few examples of Dutch and Belgian organisations that are active in the area of composites: DSM, DAF, Akzo Nobel, Vredenstein, GEP, ATO-DLO, FOM, TNO, TU Eindhoven, TU Delft, SHR Wageningen, TU Twente and KU Leuven. The Eindhoven University of Technology, is one of the most active in this area.

Natural fibres

A number of examples of applications of natural fibres used in the European Union are given in the following table (7.5). While natural fibres are increasingly being utilised, they are seldom used in demanding construction applications. Natural fibres often do not have the appropriate characteristics. The following list contains a number of disadvantageous characteristics of natural fibres.:

- too hygroscopic
- not resistant to molds and fungus
- poor bonding with matrix material
- sometimes insufficient chemical resistance
- poor moisture resistance (lifetime)

country	amount [ton]	fibre	application
SP	300000	wheat straw (110000), eucalyptus (180000), flax, hemp, abaca, sisal kenaf	pulping
NL	3500	flax, hemp, abaca	bank notes
F	7000	cotton litter, abaca, jute, sisal, kenaf	specialty paper
GE	2000	flax, miscanthus, bamboo, kenaf	pulp and paper
I	3000	starch fibres	paper
UK	8000	wheat straw	compressed board
GE	5000	wood and paper	ecological building materials
GE	4000	cotton (recycled clothes)	car seat filling
I	50	cellulose	fibre reinforced cement
DK	12000	flax	fibre reinforced cement
B	200	flax, jute, sisal, ramie, abaca	fibre reinforced cement
UK	15	jute	fibre reinforced PMCs
NL	1000	jute	non wovens and technical textiles
	500	cotton	laminates
	3500	cotton	moulding compounds

Table 7.5: Examples of applications of natural fibres.

The application of plant-derived fibres has received a great deal of interest in recent years. Plans for flax and hemp, in particular, are extensive. These crops are desirable due to their long bast fibres, which can sometimes be a meter long. According to ATO-DLO, there is room in Europe for an additional 50,000 hectares of flax, a significant addition to the current area. From the 100,000 tons of fibres that this would produce, 40,000 tons would be used for building and insulation material, 10,000 tons as geotextiles, 10,000 tons for babies' nappies and fabric and 40,000 tons as a replacement for glass and other synthetic fibres in fibre-reinforced plastics.

From natural composites (wood), construct suitable materials

A second approach to producing composites is the adaptation of wood. Wood consists of a honeycomb structure, in which the cell walls are built up from cellulose, hemicellulose and lignin.
The problem with softwood grown in the Netherlands is that it isn't as hard and sturdy as hardwood, it absorbs too much water, and is poorly resistant to changing conditions and micro-organisms. The properties of fast-growing wood—resistance to wood rot, for example—can be artificially improved. There is already a number of technological solutions for this problem, such as improved binding, chemical modification of the fibres, inclusion of biocides in sheet materials (see also the table 'new wood preservation techniques'). Sometimes the improvement of certain characteristics leads to a worsening of others.

7.3. A look toward the future

7.3.1 The future

The future view is that fibre-reinforced composite materials are the most important materials for a broad range of applications, particularly for construction and transport needs, but also in consumer goods, furniture, sports articles, etc.

7.3.2 Enabling technologies

Listed below are ten 'enabling technologies' that are important for achieving improved composite materials:
1 Integral technology
2 Fibre processing
3 Fibre properties
4 Composite behaviour
5 Composite production

6 Application development
7 Preservation techniques
8 Replacement of heavy metals
9 Textile technology
10 High-tech wood

7.3.3 The route to success

As previously outlined, the future view involves using different materials in conjunction with each other. See figure 7.4 for the relative importance of these materials over time.

The following quote characterises the expectations in terms of the future of materials.
'Ten years ago, it was thought that new materials such as ceramics, plastic composites and superstrong fibre would replace older metals and materials. Until now, that hasn't happened. New materials just about never replace the old, but are added to the other offerings on the market. Furthermore, what is a new material? What actually happens is that the expertise in dealing with 'old' materials is increased, the materials become more high-tech.' (quoted from Technisch Weekblad 16-4-97).

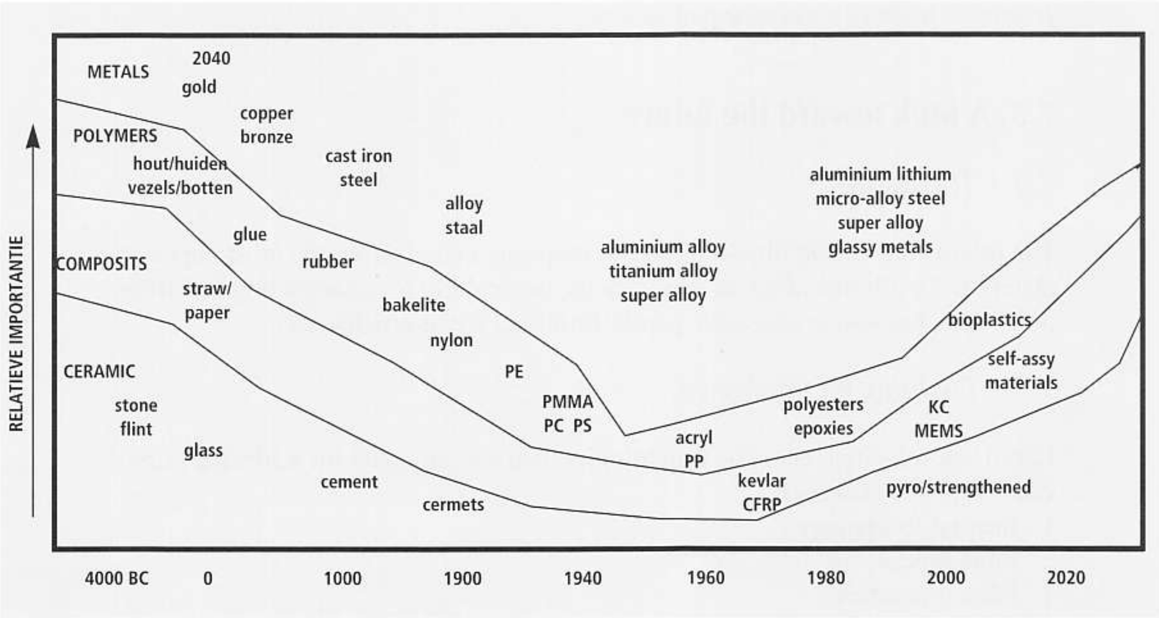


Fig. 7.4: Relative importance of materials over time [from Chemisch Magazine, May 1995]

New Wood Preservation Techniques

The polymeric structure of the wood cell wall mainly consists of cellulose, hemicellulose and lignin. The most reactive sites on these components are the hydroxyl groups. The cell wall polymers (and its reactive hydroxyl groups) are responsible for most physical and chemical properties of wood. By changing the basic chemistry of the cell wall polymers, it is possible to change different undesirable properties of wood considerably, such as durability, dimensional stability, hardness and stability against UV-degradation.

Chemical modification of wood often involves reactions with the hydroxyl groups of holocellulose and lignin. In most reactions of the wood with a modifying chemical the wood polymer itself is an alcohol. Many chemicals have been used to chemically modify wood. Depending on the type of bonding formed during the reaction between the hydroxyl group of the wood polymers and the reacting agent these wood modifications can be classified into several types. This leads to a series of chemical operations. The more important are:

Etherification

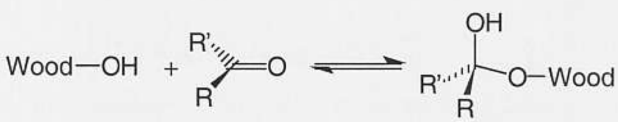
During etherification the hydrogen within the hydroxyl group of a cell wall polymer is substituted by an alkyl group:

$$\text{Wood—OH} + \text{R—X} \longrightarrow \text{Wood—O—R} + \text{H—X}$$

Fig. 7.5.1: Etherification of wood

Acetalisation

By addition of an alcohol (hydroxyl group of the wood cell wall polymers) to a carbonyl group of a modifying agent (aldehyde or keton) a half acetal is formed. This half acetal can further react with a second hydroxyl group of the cell wall polymers (crosslinking) and an acetal bond is formed. Several acids have been used as catalysts as well as sulfurdioxide (SO_2) (Akitsu et al., 1993).



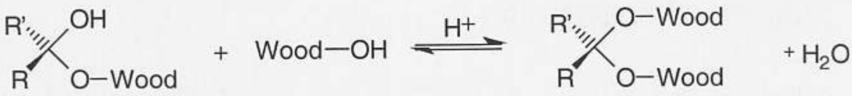


Fig. 7.5.2: The acetalisation of wood

Alkylation

In the reaction of alkyl chlorides with wood, hydrochloric acid is formed as a by-product. Because of this, a great deal of wood degradation takes place during the reaction (Rowell & Banks, 1985). The most simple ether is formed during methylation of wood. This can be achieved by reaction with methylchloride.

$$\text{Wood—OH} + CH_3\text{—Cl} \longrightarrow \text{Wood—O—}CH_3 + \text{H—Cl}$$

Fig. 7.5.3: Reaction of wood cell wall polymers with an epoxide

Epoxidation

Another category of ether bond forming reactions is those between wood and alkylene oxides.

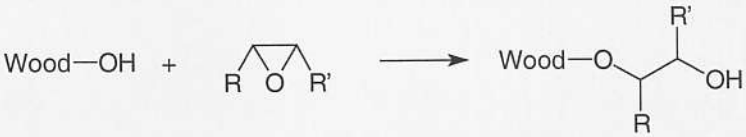


Fig. 7.5.4: Reaction of wood cell wall polymers with an epoxide

Esterfication

Esters are formed by reaction of wood with carboxylic acids or acid anhydrides. Ester bonds are liable to acid or base attack, which leads to hydrolysis.

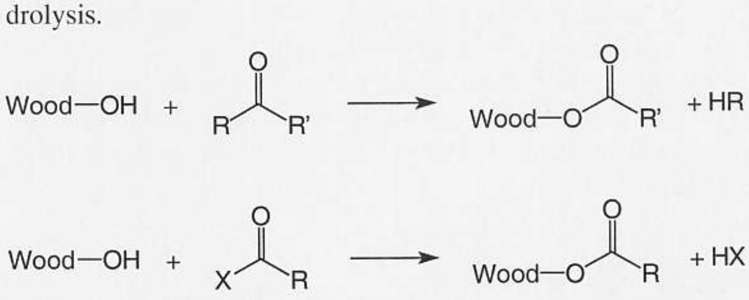


Fig. 7.5.5: Esterification of wood. R: alkyl group or proton (H); X: halogen.

Urethane-formation

Another class of reactive chemicals which has been studied extensively includes the isocyanates. In reaction of wood hydroxyl groups with isocyanate a urethane bond (nitrogencontaining ester) is formed. Unlike mono-isocyanates, a reaction of wood with di- and poly-isocyanates can result in polymerization/bulking.

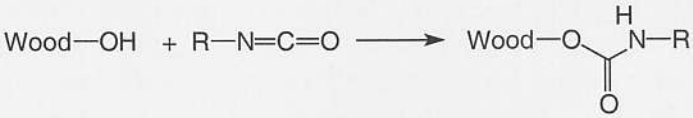


Fig. 7.5.6: Reaction of wood with a mono-isocyanate

Oxidation

Chen & Rowell (1989) and Goethals & Stevens (1994) used sodium periodate and periodic acid for oxidation of solid wood. Wood treatment with aqueous solutions (1-3%) of these chemicals at 25°C for 4 hours, resulted in limited oxidation in the cell wall polymers.

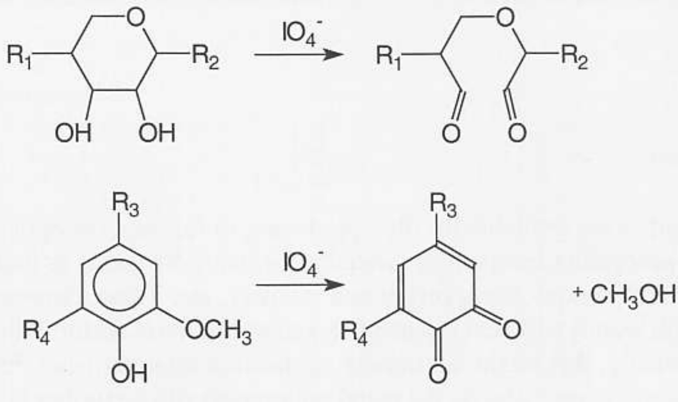


Fig. 7.5.7: Oxidation of wood cell wall polymers (according to Goethals et al., 1996).
Top: holocellulose; bottom: lignin
R1 and R2 = holocellulose unit
R3 = lignin side chain
R4 = H, OCH3 or lignin unit

A different category is the transition of wood in the so-called PLATO-process.

PLATO Process

The PLATO Process (Providing Lasting Advanced Timber Option) was developed by Shell Research to preserve fast-growing softwood (polar, pine, spruce, etc.). If softwood is treated in a steam kettle under a pressure of 10 bar and heated to a temparature of 180°C, the sugar chains in the cellulose depolymerise. Phenol is generated from lignin and the hemicellulose degrades into aldehydes. As a result of this treatment, softened wood is created. The (cellulose) fibre remains nearly intact. In the subsequent phase - hardening - the phenols and aldehydes react to form a water resistant resin layer around the cellulose fibre. The wood cell structure undergoes minimal change, but the hemicellulose is degraded and with it the food sourcr for the micro-organisms that cause wood rot. It is also possible to shape the wood slightly. Further development is now being carried out by the Dutch Cr&dO Credo) compagny, that is focused solely on optimising the PLATO process and improving the quality of flax fibres (Duralin Process).

7.3.4 Implications

Economic opportunities are available for fibre producers, in forestry, the agricultural sector, material-processing companies, producers of transport goods or building materials, transporters (cheaper transport), wood industry, etc. These fibre-sectors (in combination with wood) will develop itself as a new important sector in the coming decades. Currently, this sector is strongly application-related (paper, textile, wood). The influence of composites on the metal sector must still be further investigated.

7.4 R&D Agenda

It is clear that a great deal of R&D must be carried out to make possible a large-scale application of natural fibre composites by the year 2050. For the most part, this will happen autonomously, through the usual innovation framework, because there will be more than just sustainable developments. The following is an additional summary of necessary research to stimulate the use of natural fibres, because they must be supported by sustainability arguments.

7.4.1 Studies

Evaluation of fibres, comparative study

In order to be able to compare the vast variety of fibres to the most important, the wood fibre, data from a number of materials are shown in table 7.6. Included also are carbon, aramide and glass. From this table it appears that flax has extremely good mechanical properties. Hemp is also a good alternative. Hemp can be produced more cheaply than flax. Hemp has high yields, about 14 tons/hectare, and the majority of the plant can be used for applications other than energy. In order to make a good choice, a comparative study of fibres from different natural crops is necessary.

7.4.2 R&D Options

Composites research

A matrix with topics for composites research are shown in paragraph 7.2. An important challenge is the optimisation of textile techniques for new fibres, 3D orientation, constructing integral pre-forms and the possible exploitation of the so-called sandwich effect (for example, by filling with insulating materials, or conferring different properties). Another challenge is the optimisation of the matrix infiltration of the binder (thermoharder, thermoplast). Problems with the implantation of fibres, with glass and cellulose, for example, involves bonding to the binder. It is important that the binder has a high Tg (glass transition temperature).

Improvement of properties of fibres from biomass materials

The negative aspects of natural fibres are listed in paragraph 7.2. Furthermore, the yields per hectare are currently still too low (flax is an exception), and fibre quality is too low. Material properties can be improved by changing the plant, or by carrying out steps in the pre-processing phase. Better cultivation techniques need to be developed. The fibre treatment techniques need to be directed towards good adhesion of the fibre with the matrix and obtaining good moisture and chemical resistance.

Wood research

Wood is a beautiful material. The disadvantage of wood, however, is that it is not isotropic and homogeneous, due to its varying structure and the presence of knots. In addition, the sustainable production of wood is not simple to achieve. For a number of applications, wood is less suitable than plastic because the processing of wood is more expensive than the production of plastic (unless wood technology is further developed, in which the shaping of wood becomes more simpler for larger applications). The big advantage of wood is the low cost compared to its high rigi-

dity.
The treatment of glass fibres with a similar procedure is still in the preliminary research phase, but it appears to be very promising. Another commercial process, developed by Courtaulds Fibres in England, is the Lyocell process. This does not entail a completely new process, rather a greatly improved production method for natural fibres, with better properties, fewer emissions and a reduction in the use of solvents.

The development of new fibre unlocking techniques
Removing fibres from plants and trees requires that they be released from the rest of the plant material. Mostly this involves the release of cellulose. The unlocking of wood and bast fibres (jute, linen from flax, kenaf, ramie, hemp) is fairly difficult to do with traditional techniques. Modern techniques can raise the processing of flax from the level of craftsmanship to an industrial scale. Leaf fibres such as sisal and manilla abaca and seed fibres such as cotton are easy to unlock. The quality of the fibres is often insufficient for composites. Better techniques, geared towards the use of composite fibres, can contribute to the feasibility of natural fibre composites.

7.5 Conclusion

7.5.1 Conclusions and recommendations

The majority of materials in current use are non-renewable, relatively heavy, make use of increasingly scarce raw materials and are probably unable to meet growing material needs. Fibre-reinforced composite materials form an important contribution to the supply of materials. Natural fibres already offer superior performance, albeit in only a few applications. In addition, binders will have to be developed on the basis of natural raw materials. Wood will play a dominant role in a sustainable society. Therefore, development initiatives directed towards the improvement of wood, as well as genetic manipulation and post-treatment of wood should receive a great deal of attention.

7.5.2 Some references

Reports:

- Increased application of domestically produced plant fibres in textiles, pulp and paper production, and composite materials, DG XII report 1994.
- Brouwer W.G.J. (Ed.), Plantaardige grondstoffen voor de industrie, STT publicatie 51, 1991.
- Man Made Fiber Yearbook

Articles:
1 Zuylen A. Van, Platonische liefde voor hout, Chemische Magazine, May 1995
1 Militz H, Beckers E.P.J, Homan W.J.: paper presented in Whistler (Canada), 26-30 May 1997.

Characterising the route to composite materials

Phase 1

large-scale use (current)

Currently, synthetic fibre-reinforced composite materials are already being used on a considerably large scale in a number of high-tech applications (interior doors, dividing walls, military helmets, etc.) or are actively being developed (automobiles, masts, boats, etc.). Natural fibres are being used in 'classic composites' that are more low-tech such as paper and board, but in a limited way are being utilised in more demanding applications.

Phase 2

further development (the near future)

Raw material costs of conventional materials are lower than those of fibre-reinforced materials. As a construction material, steel is by far the cheapest to use. When the processing costs are included in the total costs of the material, however, coupled to the production volume, the cost of steel increases considerably, particularly when the series is small. The investment costs for fibre-reinforced materials are much smaller and the cost per product for fibre-reinforced material and steel will, as a result, become more equitable, especially for products that are produced on a small scale. More expensive materials will be used, therefore, more readily on a small scale than on a large one.

Designers and processors often think in terms of steel. As a result, steel is often chosen unjustifiably as a material rather than a fibre-reinforced composite. Therefore, a change in perception is necessary from people who are responsible for making the initial decisions about which materials to use, namely designers and builders.

Phase 3

optimisation (afterward)

On the basis of experience in a number of applications, the large-scale production of fibre-reinforced composite materials that replace steel is a strong possibility: bulk construction material. In this phase the distinction between natural fibres and synthetic fibres is not that important. Furthermore, entry into the market through the transport sector to other bulk applications is a logical move, in view of the high added value in this sector.

Phase 4

large-scale use in high-value applications (2050)

The road to large-scale production of natural fibre-reinforced composites in high-value application is now unobstructed. The expertise about natural fibres has made it possible to process them so that their properties are comparable to those of synthetic fibres.

Chapter 8: Epilogue

Current state of affairs of the Foundation for the Development of Sustainable Chemistry (DCO): Experiences and Perspective

In this chapter the current state of affairs of DCO as of February 1999 is described. What has DCO achieved, what is DCO doing, and what are its plans and challenges for the future?

The character and nature of the functions of DCO are dynamic: yesterday, today and tomorrow it is demonstrating its goals within an established framework and a common ideal.
As a result of the UN report "Our Common Future" and the report of the Netherlands' DTO program (Developments in Sustainable Technology), 1993-1997, DCO has placed itself at the forefront of public discussion and greater awareness. In recent years DCO has actively contributed to public awareness of the structure and quality of life.

Objectives
DCO strives to reach its goals by:
- bringing together government, industry and institutes of higher learning;
- showing that technological solutions can be found for the challenges of the future, under the condition that the triangle, government-industry-educational institutes, will offer its co-operation. The public sector (government and private citizens), in particular, is essential for the financing of R&D and pilot projects.
- believing that sustainability and the economy are not enemies of each other, rather they are allies.
- understanding that sustainable developments can only be achieved if they fall within an acceptable economic framework. Signals from within society can indicate the economic prerequisites that need to be changed, for example, by paying more attention to quality and less to quantity.

DCO has chosen five areas of research that have been described in the previous chapters. Each area is outlined by a position paper and an oriented study.
A position paper is a working document of a forum (so-called platforms) established on the basis of:
- a literature study;
- a specialist point of view from the forum;
- a discussion in the forum meetings.

A position paper describes the actual situation and state of affairs of the forum in question with special attention paid to:

- gaps in the chain of expertise;
- insufficient data for comparing process and production technologies;
- new ideas.

Before a comprehensive research proposal can be formulated, an oriented study must be carried out to precisely define the relevant gaps and ideas. For a number of areas, oriented studies have either been or are being carried out. Research proposals for large projects have been submitted or are in preparation and in a few cases research has already begun.

DCO has established an organisation and working style that is operational and sufficient for its needs (fig. 8.1). In this regard, the following has been taken into account:

- the specific role and interest of the partners: government, industry, educational institutes. The government cannot establish long term plans, but it must carry out a long term policy;
- industry doesn't look further than the short or middle term; they now have the possibility of considering long term perspectives, collectively and in a precompetitive relation to minimum costs.
- universities acquire the opportunity for challenging fundamental work in project form with long term perspectives.

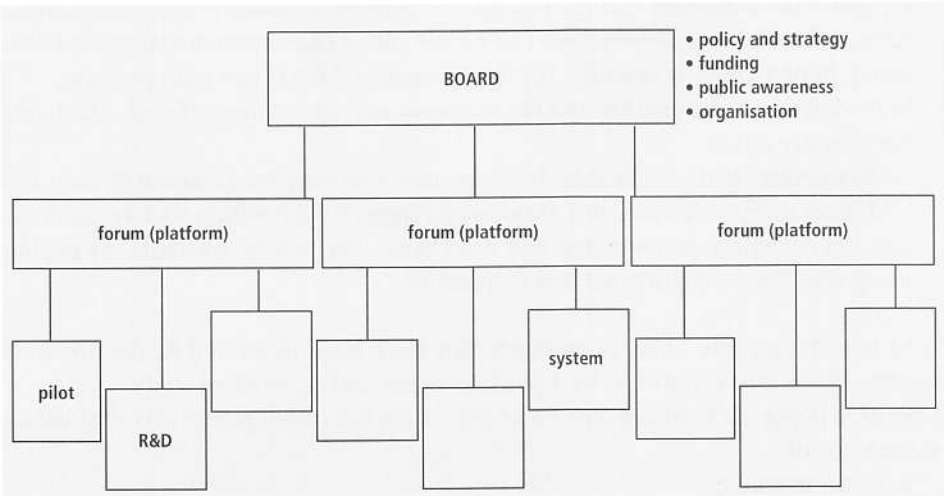


Fig. 8.1: Existing organisation for Sustainable Chemistry

Criteria for sustainability
DCO has established initial criteria for project selection and is involved in further refining and testing this practice. DCO is extremely grateful for the contribution of Dr. Siep E. Schaafsma of DSM Research (Head of R&D planning and Evaluation). Starting from the DSM Research managed system for R&D Portfolio Analysis and Selection, Dr. Schaafsma has proposed setting up projects directed towards sustainability, using an analogue method that groups data into a sustainability-economic matrix. As an example, a matrix for the project 'oxidation technology in the fine chemicals industry' is shown in figure 8.2

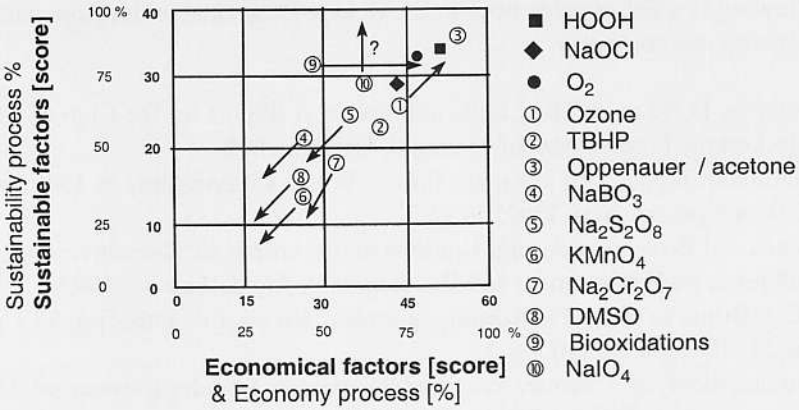
Project Financing
One of the functions of DCO is to help projects make use of existing subsidy channels:
- for fundamental research, the research sector CW of NWO;
- for applied research, EET and STW.

The future
DCO has made a start in the Netherlands. The goal of this book is make the work of DCO available to interested parties in the European Union and the United States. For this purpose, contacts were made at the ACHEMA 1997 and with the EFCHE (European Federation of Chemical Engineers). The EFCHE has declared sustainability to be one of its strategic targets.

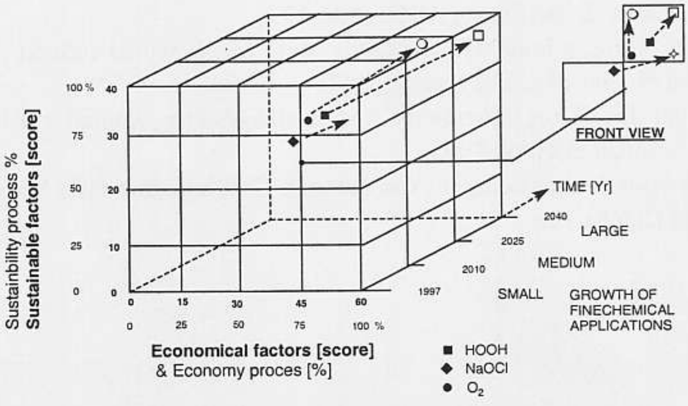
DCO Organisation

Name	Composition	Responsibilities
General Administration	Representatives from: industry (3) banking (1) government (2) universities (2) research institutes (2) + members of the day-to-day administration (DA) meet 3x per year	Authority for sustainable chemistry in the Netherlands: Tests and initiates activities of DA sounding board for DA Sets standards for the criteria of 'sustainability' takes care of network on a strategic policy level of the triangle: science, industry, government

Day-to-day Administration(DA)	A few seniors part-time from industry and universities (3-5) members; meet 10x per year Time commitment: Chairman, 2-3 days per week Members: 1 day per week	administration of programme office; management of the forums; facilitating projects; PR Network formation in the triangle, industry, government, university; combining a top-down and bottom-up approach
Programme Offices (PO)	Director (full-time) Secretary (part-time) several specialists (controller, project leader), part-time	carrying out on a daily basis the functions of DCO project management of the forum projects
Forums (platforms) *At present, there are five forums. This number can be changed. The composition of a forum must represent a majority of the relevant chemical Industry sector.*	10-15 members per platform a representative forum of experts meet three times a year forum chairman is member of DA	* Networking in the triangle; * chain analysis an identification of gaps; * initiating research projects and studies; * vision development in the area of sustainable chemistry with regard to the platforms * portfolio management in the matrix sustainability vs. economy



Positioning total scores of oxidation inventory upon profile analysis and estimates (arrows) of expected positions in future, when factors such as research commitment and external factors are taken into account.



Fit Sustainability, Economy and Fine chemical applications ● O_2 Oxidation and (○) growth of fine chemical applications as function of time, ■ HOOH Oxidation and (□) growth ◆ NaOCl oxidation and (✧) growth ...

Fig. 8.2

General References:

The following is a list of references in the fields of sustainable development, long term planning and chemistry.

1 Meadows, D.H., et al. The Limits to Growth. A Report for the Club of Rome's Project on the Predicament of Mankind, London 1972.
2 Brundtlandt report, Our common future, World Commission on Environment and Development, New York, 1987.
3 Agenda 21; Bossenverklaring, Biodiversiteitsverdrag en Klimaatverdrag, U.N. Conference on Environment and Development, Rio de Janeiro, 1992.
4 W.G.J. Brouwer (Ed.), Plantaardige grondstoffen voor de industrie, STT publikatie 51, 1991 (in Dutch)
5 Duurzaamheid en Chemie, Een bundel essays, Interdepartementaal Onderzoeksprogramma DTO, 1996. (in Dutch)
6 E.U. von Weïzacker, A.B. Lovins, L. Hunter Lovins, Faktor vier, Doppelter Wohlstand halbierter Naturverbrauch, München 1995/1996.
7 Chemie in Perspectief, Een verkennning van vraag en aanbod in het chemisch onderzoek, Overlegcommissie verkenningen, KNAW, 1995. (in Dutch)
8 Toekomstig chemisch onderzoek, Universitair fundament voor industriele meerwaarde, KNCV, VNCI, 1994. (in Dutch)
9 Competitiveness of the Dutch Chemical Industry, a report for the Ministry of Economic Affairs, Chem Systems, 1995.
10 Chemistry: Europe & the future, AllChemE, 1996.
11 Scanning the future, a long term scenario study of the world economy 1990-2015, Central Planbureau, The Hague, 1990.
12 L.J.A. Jansen, J.A. Don, Chemistry and sustainability, Annual conference, American Chemical Society, 1995.
13 Technologie voor de maatschappij van morgen, Overlegcommissie Verkenningen, 1997 (in Dutch).

Glossary

ATO-DLO	Agrotechnological Research Institute
CEFIC	European Chemical Industry Council
CPRO-DLO	Centre for Plant Breeding and Reproduction Research
DCO	Foundation for the Development of Sustainable Chemistry
DTO	Netherlands' multidisciplinary research programme for Sustainable Technology Development
EC	European Community
ECN	Netherlands Energy Research Foundation
EET	Subsidy programme for Economy, Ecology and Technology
EFCE	European Federation of Chemical Engineers
FOM	Netherlands' Organisation for Fundamental Materials Research
GFT	Domestic biological waste
GSHPC	Green Synthesis Heat Power Coupling
HPC	heat power coupling
HTU	Hydro Thermal Upgrading
IPC	Integrated Plant Conversion
KNCV	Royal Netherlands' Chemical Society
KUL	Catholic University Leuven, Belgium
KUN	University of Nijmegen, the Netherlands
LEI-DLO	Agricultural Economics Research Institute
NOVEM	Netherlands agency for energy and the environment
NWO	Netherlands Scientific Research Organisation
OCV	Netherlands Survey Consulting Committee
PV	Photo Voltaic
SHR	Foundation for Timber research
STEG	Steam and Gas Turbine
STW	Technology Foundation, the Netherlands
TNO	Netherlands Organisation for Applied Scientific Research
TNO-MEP	Netherlands Organisation for Applied Scientific Research, Environmental Sciences, Energy Research and Process Innovation.
TUD	Delft University of Technology, the Netherlands
TUE	Eindhoven University of Technology, the Netherlands
URC	University Research Centre Wageningen
UT	Twente University of Technology, Enschede, the Netherlands
VNCI	Association of the Netherlands' Chemical Industry

Sustainable Technological Development in Chemistry

Improving the quality of life through chemistry and agriculture

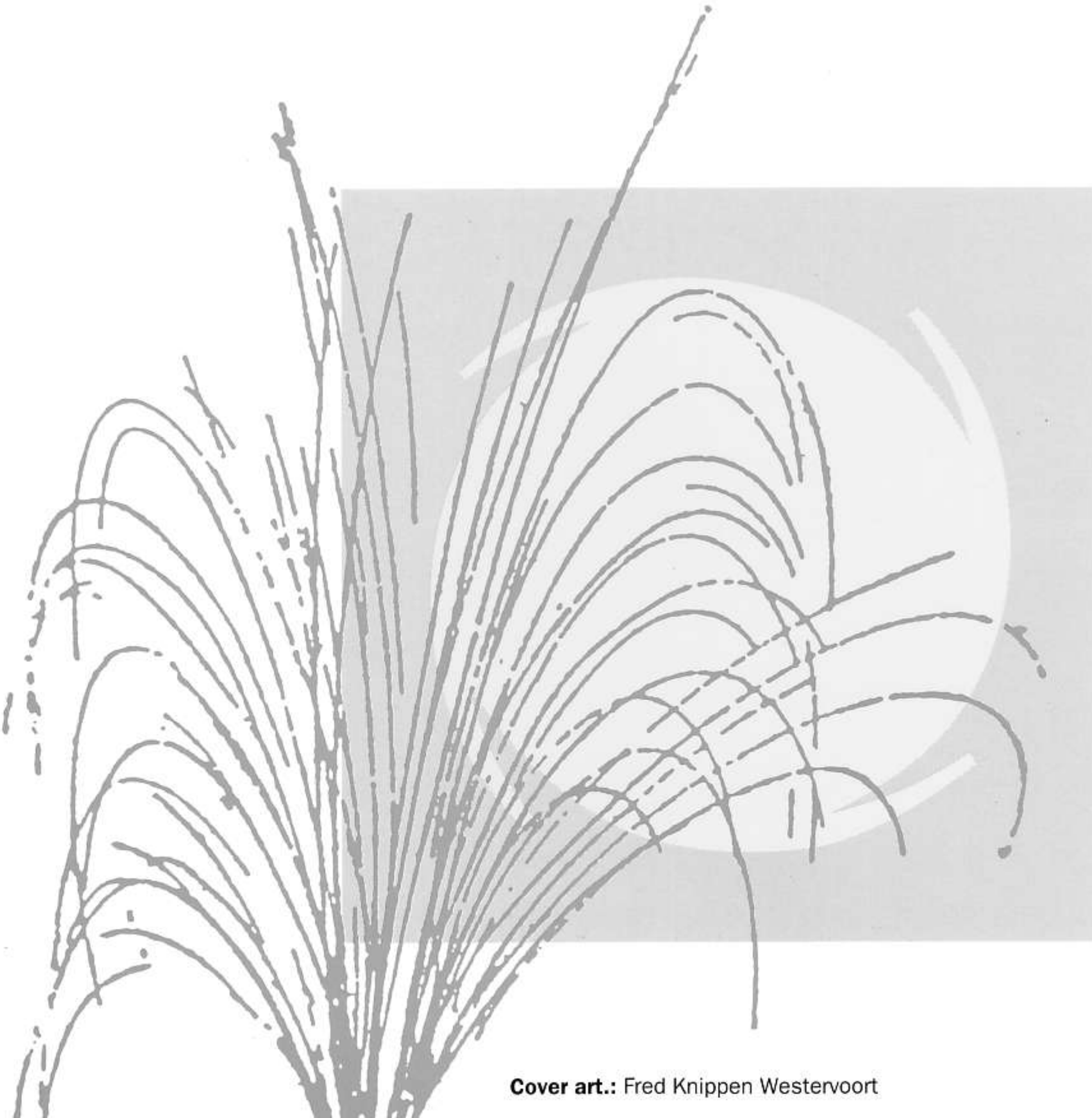
The most important strategy in a sustainable future involves meeting the need for food, housing, transportation and materials by introducing renewable raw materials and non-fossil sources of energy. Essentially, it is a challenge for the chemical and agricultural industry to co-operate in their research for more efficient processes, renewable raw materials and energy sources.

Technological expertise for the short, middle and long term is essential. For the short and middle term, industry, supported by subsidy programmes, has already taken, for the most part, the necessary steps.

For the long term a more fundamental approach is needed. It might be necessary to develop completely new processes for the production and application of alternative raw materials and energy sources. The challenge for the chemical and agricultural industry is to determine the proper direction while keeping in mind a broad range of economic and sustainable interests.

ISBN 90 – 804863 - 0-1

DCO



Cover art.: Fred Knippen Westervoort