The second world summit on sustainable development will be held this year in Johannesburg. The central theme is the conservation and control of resources. A substantial contribution must be made to this by science, whereby the combination of ecological, economical, and social science needs are consolidated to meet the challenges of the future.

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10 Years after Rio—Concepts on the Contribution of Chemistry to a Sustainable Development

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The principles of the United Nations Conference on Environment and Development (UNCED), held in June 1992 in Rio de Janeiro, and Agenda 21, the comprehensive plan of action for the 21st century, adopted 10 years ago by more than 170 governments, address the pressing problems of today and also aim at preparing the world for the challenges of this century. The conservation and management of resources for development are the main focus of interest, to which the sciences will have to make a considerable contribution. Natural, economic, and social sciences will have to be integrated in order to achieve this aim. In their future programs, the associations of the chemical industries in Europe, Japan, and the USA have explicitly accepted their obligation to foster a sustainable development.In this review we investigate innovations in chemistry exemplarily for such a development with regard to their ecological, economical, and social dimensions from an integrated and interdisciplinary perspective. Since base chemicals are produced in large quantities and important product lines are synthesized from them, their resource-saving production is especially important for a sustainable development. This concept has been shown, amongst others, by the example of the syntheses of propylene oxide and adipic acid. In the long run, renewable resources that are catalytically processed could replace fossil raw materials. Separation methods existing today must be improved considerably to lower material and energy consumption. Chemistry might become the pioneer of an innovative energy technique.The design of chemical products should make possible a sustainable processing and recycling and should prevent their bio-accumulation. Methods and criteria to assess their contribution to a sustainable development are necessary. The time taken to introduce the new more sustainable processes and products has to be diminished by linking their development with operational innovation management and with efficient environmental-political control procedures.

Keywords: environmentally friendly synthesis • innovations • oxidations • renewable raw materials • sustainable development

1. Introduction

Principle 1 of the “Rio declaration on Environment and Development”, (Rio declaration) of the United Nations Conference on Environment and Development (UNCED) in June 1992 proclaims: “Human beings are at the center of concerns for sustainable development. They are entitled to a healthy and productive life in harmony with nature.”[1] The world population will rise from the present 6 billion people—1.2 billion of these in the industrialized countries—to 8–11 billion in the year 2050; the National Research Council of the USA considers a population number of 9 billion to be most likely.[2] This growth will unfold nearly exclusively in the developing countries of today, namely in Africa, Asia, and Latin America, thus causing a change in the ratio of the population in the developing countries to that in the industrial countries from 4:1 today to 7:1. The standard of life in the developing countries has to grow and has to adapt more and more to the one in the industrial countries, which must not drop if Principle 3 of the Rio Declaration of a sustainable development has to be met: “The right to development must be fulfilled so as to equitably meet developmental and environmental needs of present and future generations”, or in the frequently quoted words of the Brundtland report: “Sustainable development is development that meets the needs of the present without compromising the ability of

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future generations to meet their own needs".[3] In addition to the demand for food, the demand for other goods will grow substantially. The demand for goods will more than double, and with an increasing adaption of the standard of living it will soon grow by a factor of four and more. Resources will have to be used much more efficiently than today, that is, multiple goods will have to be produced with the same or even a lower quantity of resources. Therefore, measures have to be intensified to lower significantly the use of resources per unit of usage. A lowering by a factor of four will not be sufficient since the existing fossil resources will be increasingly difficult to access.[4, 5] Therefore, it has to be assumed that the oil production will already have passed its maximum in this decade, at the latest by 2015–2020, and will then slowly decrease.[6] The increase in the efficiency of resource usage refers to Principle 8 of the Rio Declaration: "To achieve sustainable development and a higher quality of life for all people, States should reduce and eliminate unsustainable patterns of production and consumption and promote appropriate demographic policies", whereby, as a further essential issue, the protection of the environment addressed in Principle 4 has to be considered: "In order to achieve sustainable development, environmental protection shall constitute an integral part of the development process and cannot be considered in isolation from it."

The Principles of the Rio conference were made concrete in Agenda 21, the comprehensive plan of action for the 21st century which was adopted by more than 170 governments.[7] Agenda 21 "addresses the pressing problems of today and also aims at preparing the world for the challenges of the next century" (Chapter 1.3). The "Conservation and management of resources for development" are the main focus of interest (Agenda 21, Part II). The sciences have to make a considerable contribution if this aim is to be achieved. "There is a need for the sciences constantly to reassess and promote less intensive trends in resource utilization … Thus, the sciences are increasingly being understood as an essential component in the search for feasible pathways towards sustainable development" (Agenda 21, Chapter 35.2) by "integrating physical, economic and social sciences in order better to understand the impacts of economic and social behavior on the environment and of environmental degradation on local and global economies" (Agenda 21, Chapter 35.11c). This, however, means nothing else than requesting scientists to develop basic and applied research topics from the immense catalogue of unsolved problems outlined in Agenda 21.

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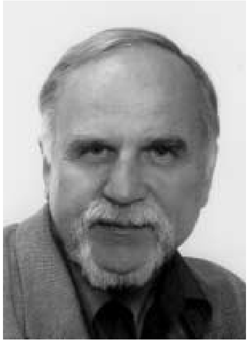

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Jürgen O. Metzger, born in 1940, studied chemistry in Tübingen, Erlangen, Berlin, and Hamburg. He gained his doctorate in Hamburg in 1970 on Ziegler–Natta catalysts. In 1983, he completed his habilitation at the University of Oldenburg on the topic "Thermally initiated intermolecular organic reaction at elevated temperatures and pressures, and reactions under supercritical conditions". In 1991, he was appointed Professor of Organic Chemistry. His work areas include sustainability in chemistry, environmentally benign organic synthesis, renewable raw materials, radical chemistry, and mass spectrometry.

Eberhard Schmidt, born in 1939, studied German Literature, History, and Philosophy at Bonn and Tuebingen, Political Science and Sociology at Frankfurt/M. and Marburg. Since 1974 he has been professor of Political Science at the University of Oldenburg. His central research areas are: Industrial Relations and Environmental Protection, Politics of Sustainability, Work and Environment.

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Though not sufficiently realized to date, this also applies to chemistry.

During the last ten years, essential aspects of the Rio Declaration[1] and Agenda 21[7] have been tackled. The Enquete commission "Protection of Man and the Environment" of the German Bundestag investigated both the prospects for a sustainable handling of the flow of materials and substances[8] and the implementation of the model sustainability into the social reality of the 21st century. It came to the conclusion that the overall objective of the sustainability effort is to secure and improve ecological, economic, and social productivity.[9] The safety of chemicals, which in Agenda 21 is addressed in the separate chapter 19, has been improved significantly by international agreements,[10] to which the worldwide voluntary initiative "Responsible Care" of the chemical industry contributes considerably.[11]

In their future programs, the chemical industries of Europe, Japan, and the USA have explicitly accepted the contribution of chemistry to sustainable development.[12, 13] However, the participation of the chemical industry in the USA in the future program Vision 2020 seems to occur at a lower level than expected, and the Synthetic Organic Chemical Manufacturers Association (SOCMA) has even withdrawn its active support since the interests of smaller sized firms are not met.[13b] In general, it must be said, that the chemical companies are attempting to understand the implications of sustainable development for them.[14]

The principles of production- and product-integrated environmental protection are increasingly accepted and implemented by numerous enterprises.[15, 16] Basic concepts for an environment-oriented design of chemical products and processes have been developed.[17] "Green Chemistry" was proposed as an orientation for basic research in chemistry.[18]

In this review we want to investigate exemplarily innovations in chemistry for sustainable development from an integrated and interdisciplinary point of view at five levels—the process, product, evaluation, organizational, and sociopolitical levels—largely based on the reports presented at a corresponding conference in February 2000.[19a]

Since base chemicals—namely chemicals that are each produced worldwide in more than a million tons per annum (t/a)—are produced in large quantities and important product lines are synthesized from them, their resource-saving production is hence especially important for sustainable development.[19b] This calls for the development of new processes for certain base chemicals or even completely new base chemicals. The base chemicals affect directly the chemical products that are produced from them in one or several steps, they are then processed in fields of industry that frequently do not belong to the chemical industry. These chemical products need to be designed in such a way that they can be processed in a sustainable way. Methods and criteria for the evaluation of their sustainability are necessary at the earliest possible stage of the development process. The time taken to introduce the new more-sustainable processes and products has to be diminished by linking their development with operational innovation management as well as with efficient environmental-political control procedures.

In the discussion on the contribution of chemistry to sustainable development it is often regretted that the term "sustainability" is used in an inflationary way and that there is no longer an exact definition. Therefore, a precise definition of the term is all the more urgent. We comprehend sustainability as the implementation of the Rio Declaration and Agenda 21 including its on-going advancement, such as is planned for the year 2002 in Johannesburg. How chemistry can and must contribute to this is outlined in this review.

2. On the Way to Environment- and Resource-Saving Syntheses and Processes

The energy and environmental profile of the chemical industry in the USA has been investigated and described recently in detail.[20] In 1997, the chemical industry used 6650 PJ (Peta = 10^{15}) of energy, which represents about 7% of all domestic energy used and 25% of the energy consumed in all manufacturing processes. Approximately 51% of the total was used as feedstock for chemical products (non-energetic consumption) and 49% as process energy for carrying out the processes (energetic consumption). The main energy consumption at 2640 PJ is invested in the production of the organic base chemicals (Figure 1).

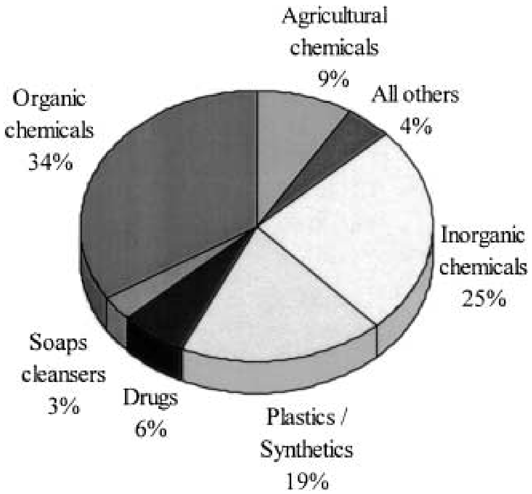


Figure 1. Distribution of gross energy requirements (GER) of the chemical industry in the USA by product groups.[20]

An investigation of the most important value-adding chains based on ethylene, propylene, BTX (benzene, toluene, xylene), and butadiene and additionally comprising inorganic chemicals and fertilizers has shown a consumption of 1690 PJ process energy for these and an estimated potential energy saving of approximately 30%. Analysis of the production output of the chemical industry from 1974–1997 shows, however, that the energy consumption per unit of emission declined by more than 39% between 1974 to 1988 but since then it has stagnated, while the total energy consumption from 1974 to 1997 has risen, as a result of the continuous growth of the chemical production by 80%. This makes us conclude that the relatively low-cost, high-return energy investments have already been undertaken. Further gain will require more dramatic changes in process design and in innovative solutions yet to be provided by research and development. If the intention to reduce by the year 2020 the energy consumption of the chemical industry per product unit by 30% of that at the end of the 20th century[13] can be realized, this will be an important contribution to sustainable development. However, this will not be sufficient, since the total energy consumption of the chemical industry will remain constant or even increase as a result of the further increase in production. Furthermore, chemistry makes major contributions to a more efficient provision of energy[21a] and is also the pioneer of innovative energy techniques.[21b]

An estimation of the material, energy, and CO_2 flows for the chemical industry in Germany in 1995 showed there was a primary energy (see glossary) demand of approximately 1700 PJ, whereof 830 PJ was stored in synthetic organic products (non-energetic use).[22, 23] This value comprises the use of feedstock, the total chain of processing, and waste treatment, and corresponds to 44% of the primary energy use of all manufacturing processes or 12% of the total energy consumption of Germany. A potential saving of process energy of 250 PJ, which corresponds to a total primary energy saving of 14% by the year 2005, was identified. The CO_2 emissions amounted to approximately 57×10^6 t, which is about 20% of all manufacturing and 6% of the total emissions. The potential reduction by the year 2005 was estimated at 16×10^6 t.[23a] With the "Agreement on Climate Protection between the Government of the Federal Republic of Germany and German Business" of November 11, 2000, the specific CO_2 emissions and energy consumption will be lowered by 20% of the 1990 values by the year 2005.[24]

The ratio of the primary energy input in the USA and in Germany corresponds quite well with the ratio of the chemistry turnover in both countries of 733×10^9 DM and 187×10^9 DM, respectively, in the year 1998. It can be assumed that similar data can be obtained for all developed industrial countries. These estimations show that the present processes of the chemical industry can become more efficient, but they also show that it is impossible to produce twice or even four times the present quantity of goods. Basic innovations for the production of the necessary goods combined with a significantly lower need of resources—approximately a tenth—are necessary.[5]

2.1. Catalytic Direct Oxidations

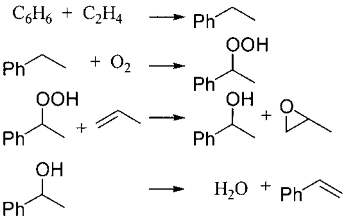
Oxidations belong to the most important reactions in organic chemistry. However, they cause the strongest stress on the environment. It is remarkable how poorly these direct oxidations with oxygen are understood and controlled.[25, 26] Here, as shown by the example of propylene oxide, a breakthrough would be a substantial contribution of chemistry to sustainable development.

Propylene oxide is one of the top 50 chemicals in terms of production: in 1997, 1.9×10^6 t were produced in the USA, about 1×10^6 t were produced in Germany, and approximately 4×10^6 t were produced worldwide. In the USA—and this distribution is typical for the world market—65–70% is reacted via polyether polyols to form polyurethane foams and 22% to form propyleneglycol.[27] Propylene oxide was investigated and described in detail by the Enquete Commission of the German Bundestag as an example of a chlorine-free end product produced using chlorine.[8a] Industrial processes used are:[27]

- chlorohydrin processes (Scheme 1)
- oxirane processes with isobutane or ethylbenzene (Scheme 2).

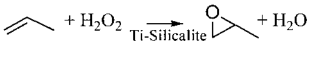
Scheme 1. Production of propylene oxide by the chlorohydrin process. The masses of compounds per ton of propylene oxide are: propene: 0.763 t, chlorine: 1.285 t, sodium hydroxide: 1.4 t, sodium chloride: 2.01 t; byproduct: 1,2-dichloropropane: 0.102 t; necessary process water: 38 t.[27]

Both are indirect processes and the first one in particular is extremely polluting. The oxirane process is a rather more indirect process for the synthesis of *tert*-butyl alcohol and styrene; economically, it can only be done if these coupled products can be sold (Scheme 2). At present, this is the case with styrene, but this is no longer the case with *tert*-butyl alcohol since *tert*-butyl methyl ether is no longer used as an additive to gasoline. However, since additional process steps are required, a compulsory formation of coupled products is always less advantageous than a direct process.



Scheme 2. Production of propylene oxide by the oxirane process with styrene as a coupled product. The reaction sequence starts with the production of ethylbenzene. The masses of the substrates and of the coupled product per ton of propylene oxide are: benzene: 2.11 t, ethene: 0.7 t, propene: 0.88 t, styrene: 2.54 t.[27]

During the last few years, the epoxidation of propylene with titanium silicalite/hydrogen peroxide (yield > 90%) has been developed. (Scheme 3) This process requires hydrogen peroxide, which is both a more reactive but also a more expensive surrogate for oxygen. Hydrogen peroxide can be formed by the alkyl anthrahydroquinone/alkyl anthraquinone process in situ, whereby only water is generally formed as "waste" and yields of propylene oxide of up to 57% have so far been obtained.[28]

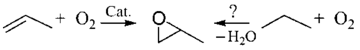


Scheme 3. Oxidation of propylene with H_2O_2 to propylene oxide using Ti-silicalite as a catalyst.[28]

In its investigation in 1994, the Enquete Commission of the German Bundestag has pointed out that there would be a new investment cycle for the existing propylene oxide plants at the beginning of the new millennium.[8b] This is in fact the case:

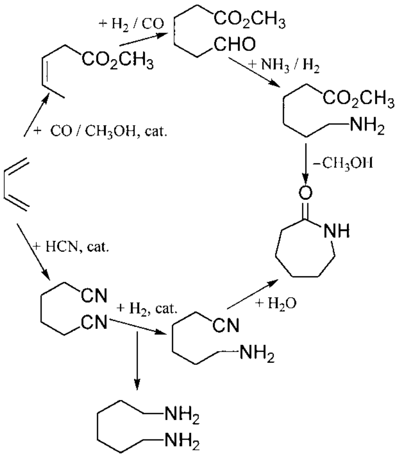
most of the chlorohydrin plants will be closed down. Bayer and Lyondell have announced the construction of a propylene oxide plant in Europe based on the oxirane procedure with an annual output of 285 000 t of propylene oxide and 640 000 t of styrene.[29] New plants using this procedure are also being built in the USA. A Sumitomo Chemical propylene oxide plant that is set to open in Japan in 2003 is based on the use of cumene in the oxirane process. The dimethylbenzyl alcohol coproduct will be dehydrated and hydrogenated back to cumene.[29] Degussa, however, will start a large-scale catalytic oxidation of propylene with hydrogen peroxide.[30]

It has finally become very clear that the direct oxidation of propylene or, even better, of propane with oxygen from the air has to be developed for the next investment cycle (Scheme 4). An interesting attempt carried out with oxygen is the oxidation of propylene to propylene oxide with gold catalysts on a titanium oxide support.[31] It is a disadvantage of this procedure that hydrogen for the reaction of the second oxygen atom has to be added and that more than stoichiometric amounts of water are developed, and hence, the catalyst also catalyzes the oxyhydrogen gas reaction. Other catalysts, for example, bimetallic M/Ti-silicalites (M = Pd, Pd-Pt, Au) have also been described.[32, 33] So far, no attempt has been made to achieve the direct oxidation of propane to propylene oxide with oxygen from the air, a process which would be extremely interesting from energetic and feedstock points of view. As long as propylene oxide is used, it is absolutely necessary to thoroughly investigate the direct oxidation of alkenes or alkanes in order to introduce a new, more-sustainable process over the years to come. Additionally, alternatives to propylene oxide have to be investigated.



Scheme 4. Direct oxidation of propene and propane with oxygen to propylene oxide.

Caprolactam and adipic acid are further important base chemicals produced by oxidation that have a high demand in resources and whose synthetic processes should be improved to be environmentally more benign. ε-Caprolactam (world capacity approximately 4.4×10^6 t/a) is produced on the C_6 route from cyclohexanone oxime by Beckmann rearrangement, whereby two or three moles of ammonium sulfate are formed. In the Enichem procedure of oxidation of ammonia with H_2O_2 on titanium silicalite, hydroxylamine and hence cyclohexanone oxime are obtained without the necessary formation of ammonium sulfate.[34] The Sumitomo process makes possible the heterogeneous catalyzed Beckmann rearrangement in the gas phase without formation of ammonium sulfate.[36] The C_4 route of DuPont leads from butadiene via adipic dinitrile, partial hydrogenation, and gas-phase rearrangement to ε-caprolactam.[36] This route also enables the production of hexamethylenediamine for nylon 6.6 through a complete hydrogenation of adipic dinitrile. Alternatively, butadiene can be selectively carbonylated and hydroformylated in two catalytic steps. In this way, caprolactam is obtained in a four-step process (Scheme 5). However, a comparison of the different processes which are currently under realization shows that only rather small innovative steps are being made. The major breakthrough is yet to be achieved in this area.



Scheme 5. C_4 route of butadiene to ε-caprolactam and hexamethylenediamine.[36]

Adipic acid, which is produced industrially by oxidation of a mixture of cyclohexanone and cyclohexanol (obtained by catalytic air oxidation of cyclohexane) with HNO_3 under formation of the coupled product N_2O and different nitrogen oxides, is also a basic chemical, the production of which should be improved to be more sustainable[35] (see Figure 5). The process was improved by use of the coupled product for energy production[16b,c] and for the oxidation of benzene to phenol.[36] However, it should be possible to obtain adipic acid by direct oxidation of hexane with air. Recently, there has been a breakthrough in this field. It was possible to oxidize hexane with air directly to adipic acid by means of an aluminum phosphate molecular sieve supported by cobalt(III) on the inner walls of the cage.[37] Immense progress has also been made in the catalytic oxidations of cyclohexane[38] and cyclohexene[39] to adipic acid. The advantages of the catalytic process compared to the classical process have recently been discussed by Thomas et al.[40]

All these examples substantiate that the development of more effective catalysts and more selective catalytic processes that lead to the desired product as directly as possible plays a key role.[41] An excellent overview on the relevance of catalysis for carbon management has recently been published.[26] High-throughput syntheses of catalysts and for the fast testing of very small amounts of catalysts in the various processes are necessary for the effective development of catalysts. Electrospray-ionization mass spectrometry is a very promising technique for monitoring homogeneous catalytic processes.[42]

2.2. Use of the Synthesis Output and Synthesis Methods of Nature

The encouragement of environmentally sound and the sustainable use of renewable natural resources (Agenda 21, Chapter 4.18, 16.1a) and biotechnology (Agenda 21, Chapter 16) is one aim of Agenda 21.

2.2.1. Renewable Raw Materials

At present, the share of renewable raw materials in the feedstock consumption of the chemical industry in Germany and in the USA runs to approximately 10%; in Germany, this amounts to 1.8 million t. It is assumed that this percentage will increase notably.[43] In the long run, renewables are the only workable solution, and their catalytic processing will make it possible to replace oil and coal as basic feedstocks.[41] The National Research council of the USA has recently presented its investigations on the estimated development of renewable feedstocks up until 2090. In 2020 25% of the production of organic chemical products is expected to come from renewable feedstocks (Figure 2).[44]

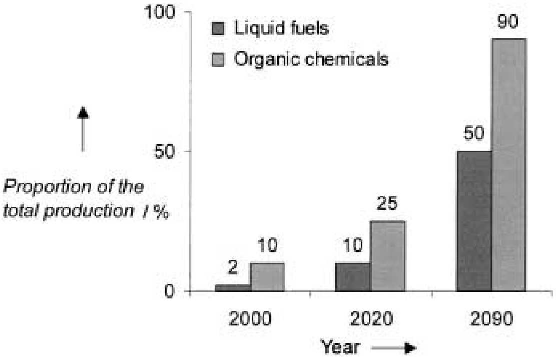


Figure 2. Targets of the National Research Council of the USA for the biobased production of organic chemicals and of liquid fuels by the year 2090. The proportion of the total production of each is given in percent.[44]

Approximately 51% of the renewable raw materials used at present in Germany are fats and oils. Carbohydrates constitute the second largest portion at 43%, while a further 6% is made up of other renewables such as proteins and protein surfactants.[43, 23e] When renewables are used as base chemicals for organic synthesis, nature's synthetic input has to be used to obtain from the natural chiral pool in one or only a very few chemical reaction steps those complex molecules which petrochemically are only accessible in multistep reaction sequences (see Section 4).

In contrast to the fossil raw materials, renewables are more or less highly oxidized. Therefore, it is clear that for base chemicals that are obtained petrochemically through nonsustainable oxidation reactions, alternatives need to be developed from re-growing raw materials.[45, 46] Many highly oxidized industrial chemical products based on starch are available and are further developed.[47] Alkyl polyglucosides are a good example; they are produced as skin-compatible, environmentally benign tensides on a scale of 70000 t/a.[48] Only recently, a review of new syntheses with oils and fats as renewable raw materials for the chemical industry was presented.[49] The transition metal catalyzed metathesis of unsaturated fatty acids produces ω-alkenoic acids; for example, 9-decenoic acid is obtained from oleic acid and 12-tridecenoic acid is obtained from erucic acid.[50, 51] The catalytic oxidative cleavage of unsaturated fatty acids yields dicarboxylic acids such as azelaic acid.[52, 53] All these chemical compounds are potential base chemicals. The epoxidation of unsaturated fatty compounds leads to epoxides of fats which can be used as coating binders, and once ring-opened by water as polyol components for polyurethanes.[54] The oxidative cleavage of petroselinic acid (6-octadecenoic acid), the main fatty acid of the seed oil of coriander, gives access to adipic acid and a coupled product lauric acid. Adipic acid is also accessible from glucose in a biocatalytic process.[55]

Most products obtained with these syntheses from renewable raw materials are at present not competitive with the products of petrochemistry, a circumstance that will change rapidly when oil resources diminish and the oil price rises. Therefore, it is high time to expand basic research to achieve substitution processes and products.

2.2.2. Chemical Biotechnology

"Chemical biotechnology" is the quickly spreading application of biotechnology in chemical production.[56] The estimated annual market share of biotechnological procedures in the chemical industry of Europe, Japan, and the USA amounts to 1–2%, in which biotechnological procedures are mainly employed for the production of fine chemicals and pharmaceuticals.[57] The use of biocatalysis for the industrial synthesis of fine chemicals is increasing rapidly.[58] Here, the driving force is certainly not sustainability but the fact that a nonbiocatalytic process is not possible or would be extremely disadvantageous economically. The production of base chemicals using biotechnology is only gaining recognition at a slow pace. Besides the classical procedures for ethanol (world production in 1991: 12.6 million tons[57]), sorbitol, and citric acid, only the lipase-catalyzed hydrolysis of acrylonitrile to acrylamide by the Nitto Chemical Company with 30000 t/a has been achieved. The production of bio-ethanol will first increase considerably in the USA from the present 6×10^6 t to 10.5×10^6 t in 2003 by the substitution of *tert*-butyl methyl ether (MTBA) as a gasoline additive.[59] It is remarkable that the addition of ethanol to gasoline as an antiknock compound was already known in 1917 and that in 1923, however, General Motors, DuPont, and Standard Oil pushed for the use of tetraethyl lead—despite its long-known toxicity—for patent reasons.[60] It must be assumed that the biotechnological production of base chemicals would be much more developed today if the sustainable decision had been made for ethanol in 1923. Moreover, the fine distribution of millions of tons of lead all over the world—7×10^6 t in the USA alone—would have been prevented. The amount is increasing still further since tetraethyl lead is still produced and sold to Third World countries.[60] This is an impressive example that clearly shows how important it is to steer towards the aims of sustainable development, especially in the highly developed countries, as defined in the Rio Declaration and Agenda 21.

2.3. Separation Processes

A chemical process consists of the pretreatment of the substrates, the reaction, and the separation and purification of the product. The importance of separation technologies for the chemical production processes cannot be emphasized highly enough. In chemical production, the separation processes require 43 % of the consumed energy and 40 – 70 % of the investment and running costs.[61] Therefore, its optimization is of utmost importance. The chemical process should be developed in such a way that separation processes are either not necessary at all or that they are simple and require as low an amount of energy as possible. One solution is to couple the reaction and separation, as is the case in reactive distillation and in absorption, adsorption, and membrane reactors.

In contrast to the classical chemical plant, reactive rectification is characterized by the combination of reaction and rectification in one apparatus unit. Conversions far above the equilibrium conversion (in an ideal case 100 %) and significantly higher selectivities can be reached by the direct rectificative removal of the products from the reaction zone. In the ideal case, further processing steps and recirculating flows are no longer necessary.[62] The heterogeneously catalyzed reactive rectification, for example, of methyl acetate is especially advantageous, since here the separation of the catalyst does not apply.[63] For all other separation methods, for example, adsorption, crystallization, extraction, membrane procedures, and ion exchange, essential improvements are necessary to achieve a 30 % reduction in material and energy consumption, water consumption, and emissions that are toxic to humans and the ecosystem by the year 2020.[61]

3. Products of the Chemical Industry

The products of the chemical industry display a great chemical diversity. Agenda 21 assumes there are approximately 100 000 chemical substances on the market worldwide. Approximately 1500 compounds make up about 95 % of the total world production. (Agenda 21, Chapter 19.11). The challenge for chemistry is to realize the manifold and different product characteristics of the mass products of the chemical industry with as few chemical base products as possible. An effective and large-scale recycling ought to be feasible and economic with only a few base products. The numerous fine and special chemicals have to become more effective, that is, the desired effect needs to be achieved with significantly lower amounts of substance. They need to be mineralized quickly when emitted into the environment. After all, it has to be possible to process chemical industry products in an environmentally benign way.

3.1. Enlarging Chemical Product Diversity and Reducing Compound Diversity Simultaneously

At present, a great number of chemically different monomers are used for the synthesis of plastics in order to obtain the necessary material characteristics. This makes the effective recycling of plastics very difficult. Moreover, there are a number of monomers, for example, isocyanates, ethylene- and propyleneglycol, and acrylates, used for the synthesis of bulk plastics that rank comparably highly in the value-adding chain. The generation of a large variety of material characteristics from as few monomers as possible by a specific and new coupling, as well as by the combination of polymers with themselves as well as with other materials, such as natural fibres, would be an important contribution to sustainable development.[64]

The polymerization of olefins, especially of ethene and propene, with organometallic catalysts has over the last few years developed into one of the largest industrial processes in the chemical industry. Approximately 66 million tons of polyolefins—polyethylene, polypropylene, copolymers, and polydienes—were produced worldwide in 1997. This value amounts to about 44 % of the total production of plastics, and is rising sharply: In 1990, it was still 43 million tons (corresponding to 43 %) and in 2005 it will probably be 100 million tons of polyolefins (corresponding to 45 % of the total production of plastics). The reasons for this development are clear. The new metallocene catalysts have opened up the possibility of varying the structure of polymers and their characteristics considerably.[65] Moreover, they make a detailed understanding of the mechanism and the stereochemistry of the polymerization of olefins possible.[66–69] By using metallocene catalysts, plastics can be made for the first time whereby their characteristic profile of properties, such as temperature resistance, hardness, shock resistance, and transparency, are precisely and largely controllable.[70]

Such new polyolefins could eventually substitute plastics derived from monomers, which are produced with higher resource usage and are less ecologically benign. One example is polyvinyl chloride (PVC) which is increasingly being queried socially, since it is produced from a toxic monomer and contains a large amount of plasticizers which can be washed out. Toxic waste is produced during its production and its disposal causes problems since hydrogen chloride is produced during combustion.[8c] PVC is now gradually being substituted by polyolefins. This is also the case with other special plastics, for example, polycarbonates, polyaziridines, and polyimides, the production of which requires a high amount of material and energy.[65]

3.2. Product Design[17]

The protection of water resources, of water quality, and aquatic ecosystems is of highest priority for sustainable development (Agenda 21, Chapter 18). Chemical compounds, which as a result of their product characteristics enter the aquatic environment, should not endanger this environment and need to be biologically degradable. Persistent and semi-persistent chemicals must not be accumulated in any environmental compartment.[71] It is the challenge for chemistry to develop the molecules in such a way that they have the desired effect at a minimum dose, and that they are mineralized rapidly by the environment's naturally existing catabolic potential.[72] Here, the use of renewable raw materials, such as oils and fats,[49, 73] is especially important as are starch derivatives[47] in detergents, and oils and fats for lubricants.[74]

Water-soluble functional polymers and complexing agents are components of formulations used industrially as well as in the household. The homo- and copolymers of acrylic acid (Figure 3) currently used as sequestrants and dispersants as

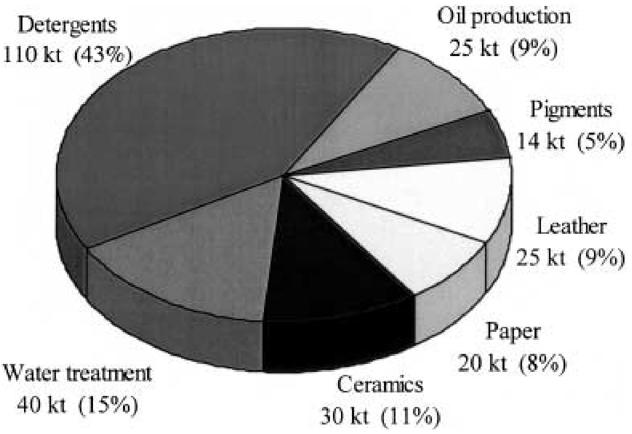


Figure 3. Areas of application of water-soluble polycarboxylates. The worldwide market volume is 265000 t/a.[16b, 75]

well as the widely used complexing agent ethylenediaminotetraacetic acid (EDTA) are biologically not sufficiently degradable and, therefore, contamination of the surface waters cannot be excluded. Products which can be substituted for the polyacrylates are the biologically degradable polyaspartic acids, produced by means of thermal polymerization.[16d] Modern, biologically degradable complexing agents of the type of aminopolycarboxylic acids as, for example, iminodisuccinic acid (IDS) are possible alternatives to persistent complexing agents.[75]

3.3. Sustainable Processing of Chemical Products

The products of the chemical industry are mostly processed by the nonchemical industry into products for the end user. Organic solvents are very often used and are emitted as volatile organic chemicals (VOCs) into the atmosphere. In Germany these emissions amounted to 1.197×10^6 t in 1988 and to 1.090×10^6 t in 1995.[76] Similar data related to industrial production can be expected for the other industrialized countries. On the one hand this is an immense waste of resources and on the other hand this is a significant cause of the tropospheric ozone formation, which contributes to the summer smog. The politically determined ozone threshold value of 110 μg m^{-3} as an environmental quality level requires that the emissions of organic compounds into the air have to decrease by 70–80% compared to the reference year (1988). For the Federal Republic of Germany this means: the total emission of VOCs including that from traffic has to be reduced from 3.241×10^6 t in 1988 to $650–950 \times 10^3$ t by the year 2007. The reductions in emission already achieved by the introduction of compulsory catalytic converters for exhaust gas, as regulated by traffic laws, now suggest that the use of solvents mainly in the processing industry makes up more than half of the total emissions. The main emissions are caused in coating, printing inks, and adhesive processing. (Figure 4). The development of chemical products which can be processed without the use and emission of VOCs in areas including those mentioned in Figure 4 is by no means trivial, but is a great challenge to chemistry. More success in this field would mean an important contribution to sustainable development. This contribution would be even more vital if these products from renewable raw materials could be produced ecologically benign and could be disposed of without problems.[77] In a case where a solvent is absolutely necessary, fluid or supercritical CO_2 may be a substantial tool for the solution of environmental problems.[78]

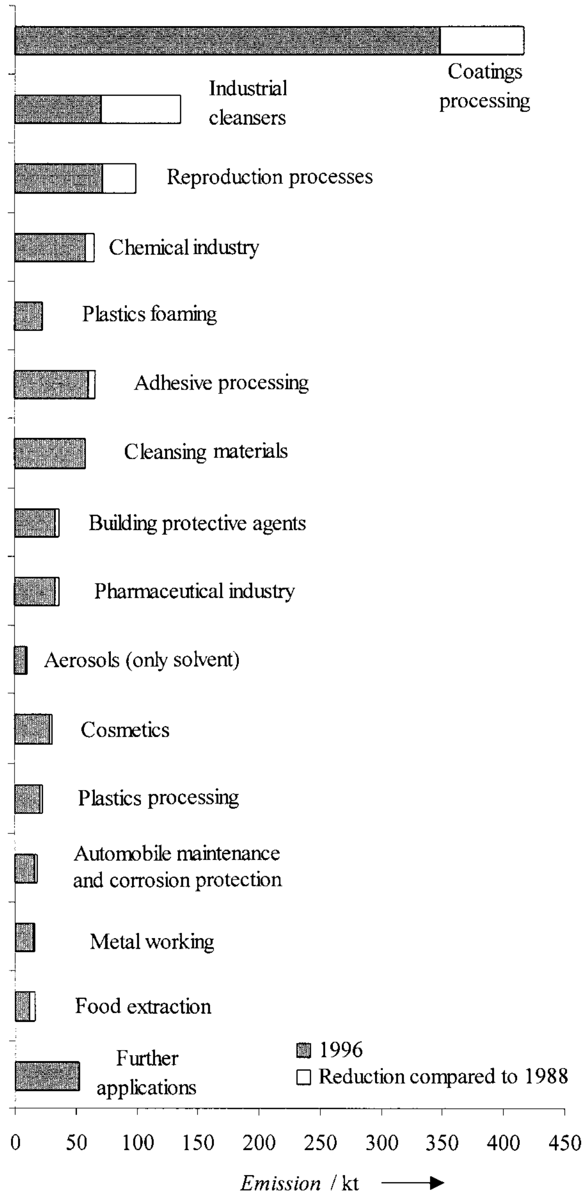


Figure 4. Emission of VOCs in Germany from the use of solvents in different industry segments (1988: 1.197×10^6 t/a; 1995: 1.09×10^6 t/a). The VOC emissions have to be reduced to 650 kt/a by the year 2007.[76]

The following steps are currently taken for the reduction of the VOC emissions in the development of new coating systems:[79, 80]

a) binders are used with an essentially higher content of solid matter dissolved in organic solvents (high-solid coatings);
b) water-diluted coatings that have a remaining content of organic solvents are used;
c) powder coatings are used without solvents but frequently with organic cleavage products formed during the curing process;

d) radiation-hardening coating systems are used which to a large extent are free from solvents and even during the hardening do not develop any organic cleavage products.

Binders based on oils and fats seem to be very promising for the development of solvent-free coatings.[81]

4. Assessment of the Contribution of Chemical Process and Product Innovations to a Sustainable Development

Agenda 21 calls for "criteria and methodologies for the assessment of environmental impacts and resource requirements throughout the full life cycle of products and processes" (Chapter 4.20), and in numerous chapters it formulates the aims and measures necessary for chemistry to make an important contribution. These aims and measures have to be considered for an assessment of chemical processes and products in regard to their contribution to a sustainable development. There are three dimensions that generally need to be considered in an integrated way:

- an economic dimension
- a social dimension
- an ecological dimension

If the state of the operationalization is to be considered in regard to the economic and social dimension, then they are still at the very beginning.[9] The economic dimension is normally equated with the microeconomic success of the firms in question, the macroeconomic sustainability criteria are only formulated in single cases. For the social dimension, there are single indicator sets; however, they are only consistent to a certain extent. In contrast, the ecological dimension is extensively operationally defined.

4.1. The Ecological Dimension

The ecological dimension of chemistry's contribution to sustainable development and its assessment has two sides:

1. The stress on the environment and consequently on the population by chemical production and its emissions as well as by chemical substances that are emitted into the environment for useful purposes but which also have negative effects.[82]
2. The more efficient exploitation of the resources by new chemical processes and new products in order to create conditions so that nine billion people can live in human dignity on earth.

4.1.1. Environmentally Friendly Handling of Chemicals

Chapter 19 of Agenda 21 takes up the chemistry discussion of the last 30 years and comes to a final conclusion. However, many details need to be clarified. It contains detailed orders for action pertaining to the sustainable handling of toxic, that is, dangerous, chemicals and calls for a worldwide harmonization of classification and labeling of chemicals by the year 2000. Its implementation by state regulations will bring about on a national, European, and international level a complete set of compound records, safety guidelines, safety data sheets, and poison characteristics of all chemicals used. The implementation of Chapter 19 was summarized by Hildebrandt and Schlottmann.[10] The program areas outlined in Chapter 19 refer to single-compound assessments. With regard to human toxicity, however, toxicological data of preparations and formulations ought to be recorded as well. This process would help to decide whether a single-compound treatment in the mixture represents a sufficient basis for a sustainable health protection or whether specific combinatory effects have to be considered as well.[83] The leading principles concerning this subject in the Responsible Care Initiative are as follows: "to provide chemicals that can be manufactured, transported, used and disposed of safely."[11]

4.1.2. Approaches to the Assessment of the Sustainability of Chemical Processes

The process parameters of established processes are (internally) known and can be used for the quantification of the use of resources, gross energy requirements (GER), waste, emissions, and related costs per product unit. A number of metrics have been developed which are used for assessment in the chemical industry.[84] As an example, the GER was compared for the two propylene oxide processes currently performed. Surprisingly, it was about the same for both processes at 104 $\mathrm{GJ\,t^{-1}}$ of propylene oxide.[23c] Further criteria such as waste, investments, expected profit, and social acceptance need to be included to enable a sound decision to be made. After consideration of all aspects, the oxirane process with styrene as a coupled product has clearly succeeded in taking over the top rank when it comes to new investments, relative to the chlorohydrin process. In Europe, the social discussion on "chlorine chemistry" was most probably decisive for this outcome.

The GER is accessible for a number of processes carried out at present to produce important organic base chemicals and intermediates (Figure 5); for example, it is approximately 40 $\mathrm{GJ\,t^{-1}}$ for acetaldehyde, 80 $\mathrm{GJ\,t^{-1}}$ for adipic acid, and 104 $\mathrm{GJ\,t^{-1}}$ for propylene oxide;[23a,b] Vegetable oils such as rape seed oil and linseed oil require a GER of approximately 20 $\mathrm{GJ\,t^{-1}}$.[23a,b, 85] Here, the differences in the resource consumption are so high that it can be assumed that products based on vegetable oils could clearly be more environmentally benign than petrochemical products. Significantly different values for the GER is also evident in important bulk plastics (Figure 6). For example, the GER for one ton of epoxy resin is 107 $\mathrm{GJ\,t^{-1}}$, which is almost twice as high as it is for alkyd resins at 64 $\mathrm{GJ\,t^{-1}}$ because the latter contains a portion of renewable raw materials. Remarkably, PVC has the lowest GER of 53 $\mathrm{GJ\,t^{-1}}$, which is clearly lower than that for polyethylene at 65 $\mathrm{GJ\,t^{-1}}$. However, the process energy for PVC at 32 $\mathrm{GJ\,t^{-1}}$ is 50% higher than for polyethylene at 21 $\mathrm{GJ\,t^{-1}}$. The chemical energy accumulated in PVC at 20 $\mathrm{GJ\,t^{-1}}$, however, is less than half that of polyethylene (43 $\mathrm{GJ\,t^{-1}}$) because of the high chlorine content in the former. The GER, in relation to the process energy and the chemical

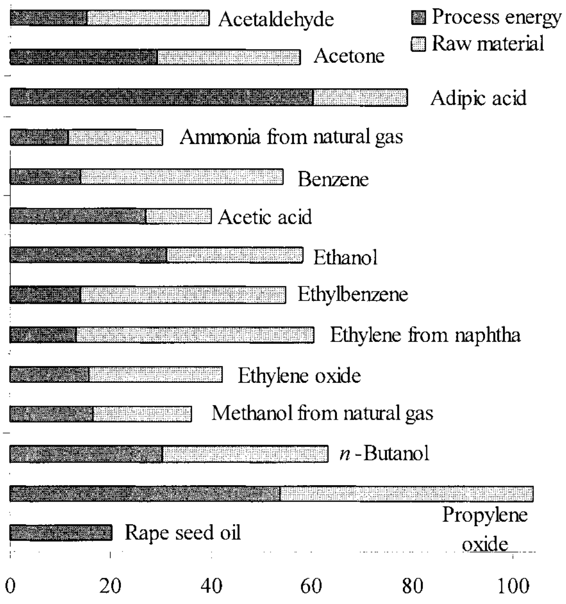


Figure 5. Gross energy requirements (GER) for important base chemicals.[22, 23c]

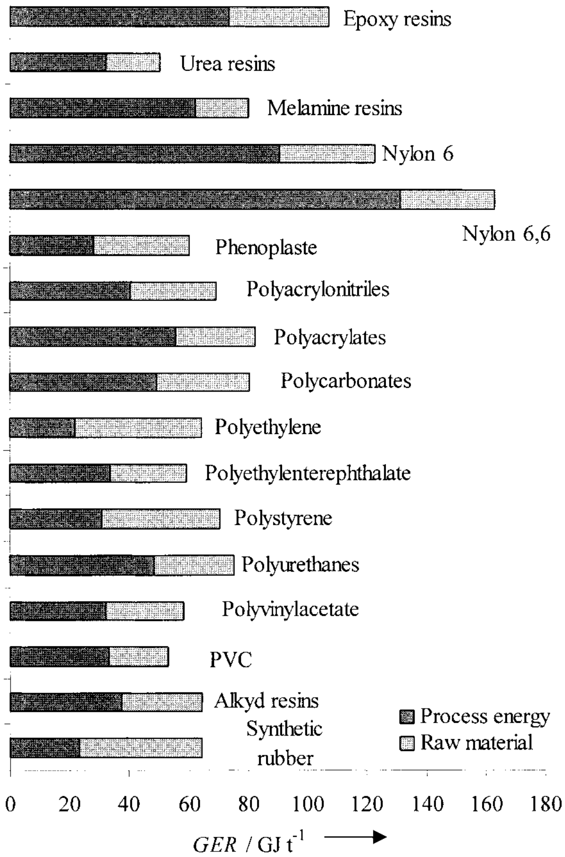


Figure 6. Gross energy requirements (GER) for important bulk plastics.[22, 23c]

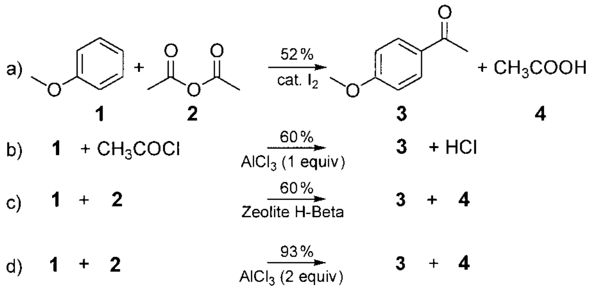
energy accumulated in the product, is a useful measure for the assessment of bulk products.

A simple method for a quantitative comparison of the use of resources and environmental impact in syntheses of fine chemicals and pharmaceuticals at the earliest possible stage of process design,[86a] preferably already at the laboratory stage,[86b] is essential for the precise development of sustainable processes. Some approaches have been presented during the last few years.[87] We mainly follow Sheldon's proposal[88] which weights the environmental factor E (mass of waste, that is all compounds used which are not incorporated in the product, per mass unit of product) of a process with substance-specific weighting factors Q_{output}.[89] In this way, an environmental index[87a] EI_out of the waste is obtained for a process, the value of which reflects the potential environmental impact based on the mass of the product (PEI kg^{-1}).[87f] Correspondingly, the mass index S^{-1} is weighted with Q_{input} to obtain the environmental index EI_in, which quantifies the potential environmental impact by the raw materials used (substrates, solvents, catalysts, auxiliary materials for the reaction and work-up procedure; Table 1). The weighting factor Q_{input} considers the resources used, as well as the aspects of occupational safety and health, while Q_{output} essentially considers the human toxicity and ecotoxicity.[89b] As an example, these metrics were determined both fast and simply for four different laboratory syntheses of 4-methoxyacetophenone (Scheme 6) by using the software "EATOS" (Environmental Assessment Tool for Organic Syntheses[89a] (Figure 7). The zeolite-catalyzed Friedel–Crafts acylation requires the lowest material input, and therefore has the lowest mass index S^{-1} and correspondingly the lowest environmental factor E. The environmental indices EI_in and EI_out are also about one order of magnitude lower than in the other syntheses. Clearly, this synthesis of 4-methoxyacetophenone

Table 1. Metrics applied to chemical syntheses for the assessment of resource requirement and potential environmental impact.

Metrics	Unit
mass index $S^{-1} = \dfrac{\sum \text{raw materials [kg]}}{\text{product [kg]}}$	[kg per kg]
environmental factor $E = \dfrac{\sum \text{waste [kg]}}{\text{product [kg]}}$	[kg per kg]
substance-specific potential environmental impact Q_{input}[d] and Q_{output}[d]	[PEI per kg][a,b]
environmental index EI_in $= Q_{\text{input}} S^{-1}$	[PEI per kg][a,c]
environmental index EI_out $= Q_{\text{output}} E$	[PEI per kg][a,c]

[a] PEI = potential environmental impact.[87f] [b] Refers to one kilogram of substance. [c] Refers to one kilogram of product. [d] $1 \leq Q \leq 10$.



Scheme 6. Different syntheses of 4-methoxyacetophenone from the same substrate with different acylation agents, solvents, and catalysts.

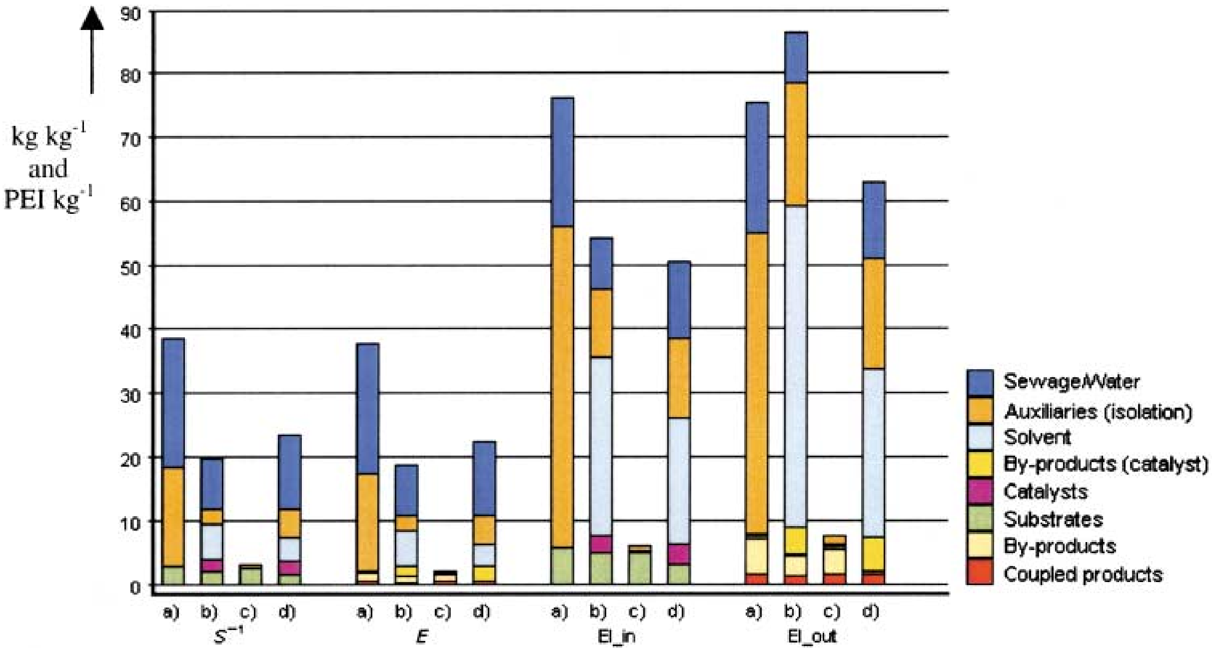


Figure 7. Assessment of syntheses of 4-methoxyacetophenone (Scheme 6) by means of the software EATOS: mass index S^{-1}, environmental factor E, environmental indices for input EI_in and output EI_out (see Table 1).

stresses the environment the least and should, therefore, be the preferred one. It is remarkable that the yield, the chemist's most often used value for estimating the synthesis quality, is clearly lower for synthesis c) than for synthesis d) and comparable to syntheses a) and b) (Scheme 6). Analysis by EATOS permits a detailed balancing of the reaction, a balancing that includes solvents, catalysts, by-products as well as auxiliary materials used during the work-up procedure. From this, it can clearly be seen, that reaction a) requires a costly work-up procedure while reactions b) and d) require solvents during reaction and work-up procedure that contribute decisively to the high resource requirements and the high potential environmental impact.

A system of building blocks with modules for the most important process chains that allows both the resource requirements and environmental impact on production of base chemicals, intermediates, and end products to be covered quantitatively by means of metrics that refer to a consistent basis data set would be extremely useful for an assessment of syntheses or processes, but unfortunately it is not yet available.

4.1.3. Life-Cycle Assessment (LCA)

A life-cycle assessment[90] of a product is drawn from the "cradle to the grave", that is, from the extraction of raw materials to waste disposal or recycling. A life-cycle assessment consists of the goal and scope definition, inventory analysis, impact assessment, and interpretation. These proceedings are described in the ISO EN DIN 14040-43.[91] Azapagic and Clift have written an overview on the application of the LCA method for process optimization.[92] Life-cycle assessments were thus set up for bulk plastics.[93]

Leading surfactant and detergent producers compared the production of fat alcohol sulfate on the basis of renewable raw materials with the petrochemical production in a life-cycle assessment.[87e, 94] There, it was stated that resource and energy consumption and emissions for the surfactant based on palm oil were clearly more favorable than for the one being produced from fossil feedstock. The comparison of UV-curable coatings, with linseed oil epoxide as a binder, to a binder produced on a petrochemical basis has shown clear advantages for the renewable raw material linseed oil. The gross energy requirements as well as the CO_2 and NO_x emissions are almost one order of magnitude smaller when linseed oil epoxide was used. It is remarkable that during the production of the petrochemically derived binder, propylene oxide contributes more than half of the environmental impact (Figure 8).[85]

Life-cycle assessments were also set up for some biotechnological processes.[57] It is remarkable that bio-ethanol (world production 1991: 15.1×10^6 t/a) has clear ecological advantages over synthetic ethanol (2.5×10^6 t/a). The demand for fossil primary energy for the latter amounts to 62.3 MJ kg^{-1}, but only to 4.8 MJ kg^{-1} for ethanol derived from sugar cane and 19.1 MJ kg^{-1} for ethanol from sugar beet. The CO_2 emissions for synthetic ethanol amount to 1.88 kg kg^{-1}, while the CO_2 emissions are credited for bioethanol.

4.2. Measuring Economic-Ecological Efficiency

Economic-ecological parameters result from the microeconomic imperative on efficiency to achieve either a predefined environmental relief with as little financial effort as possible or a maximum environmental relief with a fixed financial sum. Therefore, simple measurements of economic-ecological efficiency link concrete single-environmental relief measures to microeconomic parameters:[92, 95] examples are the amount of reduction of SO_2 per investment volume in

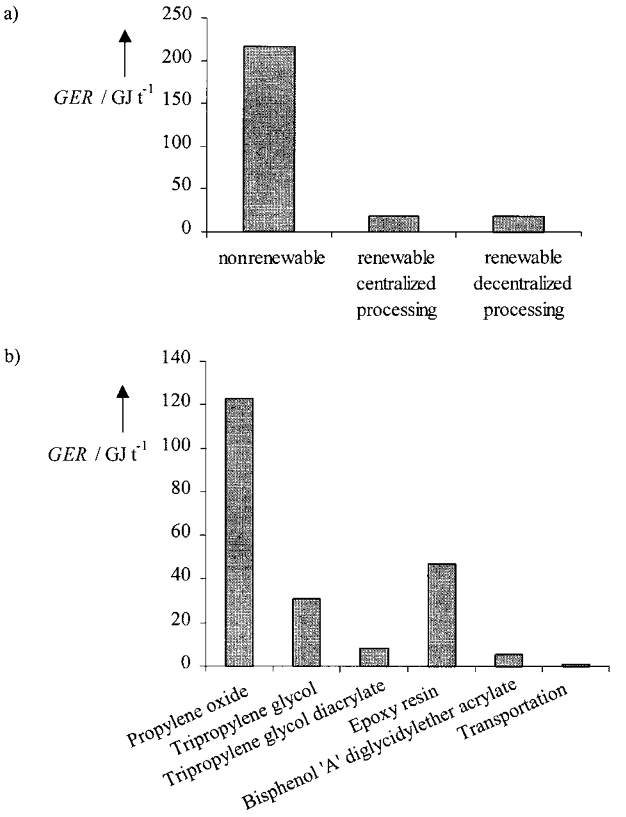


Figure 8. Comparison of the gross energy requirements (GER) for the production of a) a petrochemical (tripropyleneglycol diacrylate/bisphenol A diglycidether acrylate 1/1) and of a renewable binder (linseed expoxide, centralized and decentralized processing of linseed); b) the compounds of the petrochemical binder. Similar relationships exist for CO_2 and NO_x emissions.[85]

filters, costs per reduced kilogram of waste material, and turnover in Euro per energy consumption in kWh. Today, such environmental metrics parameters have largely been implemented in chemical firms, since they are also readily applicable.[95b] Evaluation is more difficult if product performance or even the total enterprise performance is to be assessed by means of an economic-ecological measure of efficiency. If, for example, three product alternatives (for example, for a dye) have to be estimated from the perspective of economic-ecological efficiency, the development expenditure or the increased production costs have to be contrasted with the total ecological relief. This is the point at which the aggregation problem which is well-known from the life-cycle assessment (for example, the trade-off between lower production of waste materials and higher energy consumption) comes in. In 1991, Schaltegger and Sturm presented the first comprehensive approach for such an aggregated ecological efficiency evaluation.[96] They based their report on the Swiss eco-point system and they chose the net contribution of product variants as a means of evaluation. In this way, they were able to calculate an aggregated economic-ecological efficiency value.

This economic-ecological efficiency evaluation has been slow to win recognition in Germany, mainly because the underlying eco-point aggregation methodology has not reached any consensus. Only recently have efforts been undertaken by firms to take up the concept introduced by Schaltegger and Sturm, for example, the eco-efficiency analysis by BASF and the eco-check “Product excellence” by Bayer.[97]

4.3. Concepts Incorporating Sociopolitical Assessment Dimensions

Against the background of the sustainability postulate, the sociopolitical evaluation of innovative chemical processes and products has to orientate itself by criteria aimed at achieving a long-term social acceptability of the planned innovations. This comprises measures such as the reduction of risk potentials, health protection, the number and quality of jobs which are raised or lowered in the process, increased intra-generational and inter-generational social justice, broad acceptance, and compatibility with democracy. Naturally, balancing these criteria with the other dimensions of sustainability, which represent ecological and economic demands, is an endeavor that is not free from conflicting interests; a redefinition is required for every single case.

Therefore, concepts that evaluate chemical-political innovations for their social compatibility also have to consider the other dimensions of sustainability as early as possible in their initial stages so as to avoid developments in the wrong direction. This approach calls for evaluation concepts which, as the Enquete Commission of the German Bundestag on “Schutz der Umwelt und des Menschen” stated in its final report, cannot be decreed, but must be worked out by considering the various interests arising in a discursive process that includes a high number of participants.[9b] In this way, the sustainability postulate will, although it claims to be normative, become a concept of social orientation aimed at cooperation and the balance of interests.

Since the meaningfulness of cost-benefit analyses and risk analyses is only limited in regard to an estimation of the social consequences of the sustainability of chemical innovations, scenario analyses would probably provide the most suitable basis for evaluation since they display alternative development paths based on a collection and integrated processing of data. The most prominent advantage of the scenario analysis is that it presents future fields and their scopes for complex design, thus allowing an identification of synergies and potential conflicts. They might—perhaps in a discursive process—be suitable for an evaluation by means of ecological, economical, and social indicators.[92] The interests of the different parties involved might be considered in its formulation and moreover, the political options, which can be rated enforceable, could be shown more clearly. Such concepts have been successfully applied in a number of studies dealing with the complex consequences of social innovations.[98]

The first attempts have been made to create feasible operational systems which balance potential actions. There are two major examples of this: the concept “Who needs it”,[99] developed in the cooperation of Dow Chemical with the London Sustainability Agency “Sustainability” which covers those fields in which chemical products are used and determines to what extent the needs arising in these fields can be generalized. The concept does not qualitatively asses single products, but allows firms to identify suitable or critical fields of need in a fairly early stage and to adapt decisions on the product portfolio to sustainable development requirements. The instrument PROSA[100] developed in a cooperation between the Öko-Institut, (eco-institute) and Hoechst AG is heading for a similar direction. By means of this tool different product alternatives are evaluated for sustainability (in the pilot project, for example, roof material made from plastics and preserving agents were used), not only by applying various individual ecological parameters, but also in the context of their application fields (Germany versus China).

5. Organization and Innovation

Process and product innovations are the results of the creative thinking and actions of humans within organizations. This also applies to ecological innovations. However, businesses and chemical sub-branches widely differ with respect to their innovation potential.[101] Research on organizations has shown that a number of factors have an impact on the development of process and product innovations. These factors are summarized under the term of "innovation system"[102] (Figure 9). In addition to political and legal frame conditions (Section 6) as well as societal concepts and values, the term also comprises the marketing conditions (customer demand for ecologically optimized products and competitive pressure arising from the ecological product innovations of competitors) and internal company factors. Empirical studies have shown that the majority of chemical innovations were basically generated by committed key personalities within companies.[103] The following section focuses on internal factors that can be influenced by companies. Such factors have so far been treated in papers on innovation management in the chemical industry, on corporate environmental innovation in general, as well as on environmental innovation in the chemical industry in particular. This section focuses on the latter subject area. However, only a limited number of empirical studies on this topic have so far been published.[104] Hence, transfers from the two other subject areas also need to be considered for statements regarding the conditions for promoting ecological innovation in the chemical industry.

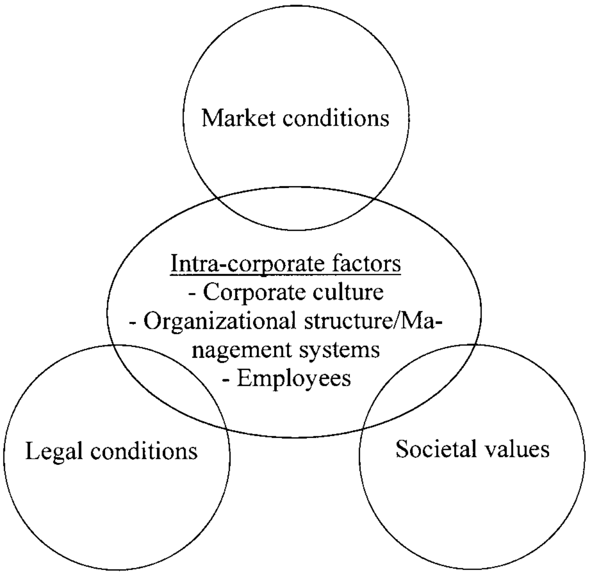


Figure 9. Factors that influence the innovation performance of companies.

Research and development (R&D) processes are characterized by high risks and enormous capital needs. They also require interdisciplinary cooperation, particularly at the interfaces.[105] As a consequence, the number of company cooperations aimed at incorporating external knowledge into R&D processes rises. This not only applies to company cooperations between customers and suppliers, but also between competitors in the framework of R&D alliances, as well as—to a rising degree—to cooperations between external interest groups (for example, environmental protection groups). It is precisely these groups that have turned out to be the driving force behind the promotion of sustainable process and product innovation.[106] At the same time, a trend towards company mergers and a concomitant orientation towards specialized product areas has been observed, particularly in research-intensive sections of the chemical industry.[103]

It is revealing to link these general features of innovations to research on corporate environmental innovation. In this way it becomes clear how the general conditions of the market and of companies affect the environmental innovation behavior of companies (Table 2).[107]

Table 2. Factors determining corporate environmental innovations. The major variables established in an empirical study by Lee are shown.[107]

Market/company characteristics	Influence on the innovation activities
size of company	higher formalization of innovation processes in big companies, no better innovation results
type of industry	no significant differences between producers of consumer and industrial goods
growth rate	positive correlation with risky innovation, no correlation with environmental innovation
intensity of competition	price competition influences innovations in the direction of cost savings
attractiveness of markets (size and growth rate)	attractive markets only foster innovation activities in general

Accordingly, the branch concentrations (that is, the relatively increased importance of major companies in this sector)[108] which have been observed in the chemical industry and which were among other things triggered by R&D dynamics[108] do not necessarily lead to a greater success in environmentally related innovation. Although environmental protection is more formalized in bigger companies, this does not automatically correlate with successful environmental process and product innovations. The highly intense competition that has been observed in many chemical sub-branches promotes cost-saving innovations.[109] This opens up opportunities for innovations in environmental processes that are accompanied by cost savings in the production process (low-energy consumption or low amounts of waste, higher yields, etc.). In rapidly growing markets (for example, pharmaceuticals, specific areas of specialized chemistry), the general conditions for successful product innovation are also improving, however, not necessarily towards environmental innovations.

Studies on chemical innovations and on corporate environmental innovations clearly show that the emergence of innovations in environmental processes and products cannot only be attributed to external factors, but was promoted considerably by company-specific factors,[110] namely factors such as the company culture, company management,[111] and the respective R&D policies pursued. This finding corresponds to the results of the few relevant empirical data available so far on the environmental innovation behavior in the chemical industry.[104,112] In his studies of the chemical industry Kreikebaum, for example, identified "long-term planning horizons, capable and motivated staff, interdisciplinary R&D working groups,[113] unhindered communication within the company, involvement of external people in new product developments, and an ecologically oriented R&D management" as company-specific factors that promote successful environmental innovations.

Studies on the correlations between stock and environmental performance in the chemical industry stress the importance of an orientation towards sustainability for ecologically and economically successful innovations.[114] More recent studies have revealed the importance of "soft" factors, of cooperations,[115] and of a supply-chain management that is supported by suitable cost-accounting systems[116] for successful environmental innovations.

A promising strategy that can be pursued with respect to basic innovations is to break up central concern structures in favor of cooperations with small innovative companies: Empirical studies on the plastics industry have shown that basic innovations are frequently generated by "outsiders", namely, by individuals or companies which only play a marginal role in a branch. By contrast, major companies are more predestined to organize incremental innovations efficiently.[117] It is essential to also consider these findings in environment-oriented process and product innovations, for example, by closely cooperating with innovative biotech start-up companies in the field of ecologically oriented process improvements,[118] by involving researchers with unconventional ways of working and thinking in development processes, and by an open communication climate.

"Soft" factors for innovations cannot be controlled directly, but organizational conditions can be created under which they can develop easily. In this context, industrial models and visions (such as those realized particularly in the US chemical industry[13] but which are also part of the Responsible Care Program[11]) as well as company-specific visions (such as the zero-waste philosophies of many US companies, for example, Monsanto and DuPont) play a major role. At the management level, such models are needed to focus strategic programs on specific goals. An illustrative example of this is the "Verbund" vision of BASF AG[119] which promotes thinking in terms of integrated synergies not only with respect to production processes (efficient use of raw materials, energy, and intermediates, re-use by-products and residual materials, minimization of transportation of substances, etc.), but also promotes relationships between BASF and its suppliers, customers, and interest groups by following a common model.

5.1. Cooperations

Cooperations have become a key factor of environmental innovation in the chemical industry. They not only play a crucial role in the innovation process itself, which should include as much external knowledge as possible (see Section 5), but also in the implementation of innovations in value-added chains: It has become clear that many technically and economically impressive product innovations which, by ecological and economic standards, were marketed successfully by the various pioneer companies are slow to win recognition in the entire application branch.[120]

Most companies only have a limited innovation potential and a high level of persistency. In general, the innovation-readiness of the persons involved is overestimated. The limited innovation potential not only shows itself through key personalities in companies but also by suppliers and the institutes counseling the companies. In particular, innovations are rejected for being too risky if a company is in a difficult economic situation. The same is true for companies working to capacity, who fear that changes in processes will jeopardize the smooth flow of production.[121] The time at which a substitution can be made always seems to be wrong.

The proportion of innovative and flexible companies which are ready to implement environmental innovation is rather small in the branches. Lissner's[122] estimate of their share ranges from 1–20 %, depending on the branch. It is crucial for the diffusion of more sustainable chemicals that companies operate successfully in this field. If this success turns out to be lasting, this will get around, thus encouraging follow-up companies to make substitutions. Nonetheless, the pioneer companies take great risks (for example, because plant and machine makers disclaim liability if new, environmentally friendly tools/operational procedures are applied). The importance of interorganizational cooperation for a sustainable development also arises from other considerations: Most chemical products are incorporated in product systems, that is, are not used in an isolated manner. The use of plastics in automobile production to reduce weight is a good example of this (such as for the development of the "3-liter car" which uses 3 liters of fuel to travel 100 km). Substitution of the currently used material with plastics can only be achieved through a close cooperation between producers and customers and, possibly, standardization panels to ensure that the substitute not only has the appropriate properties (for example, shock resistance, durability) but also meets all legal norms and quality standards beyond this level.

6. An Innovation-Promoting Political Pattern for Sustainable Development

As a result of the 1992 Rio Declaration[1] and Agenda 21[7] the international and political efforts aimed at promoting a sustainable development in chemistry have been considerably increased. Major requirements of Agenda 21 that need to be met by the chemical industry and political institutions center around an internationally agreed assessment of chemical risks, a harmonization of classification and labeling of chemicals, the exchange of information, the implementation of risk-reduction programs, and the creation of favorable conditions for an efficient management of hazardous material, particularly in Third-World countries. These requirements were to be met by establishing a number of international forums (Intergovernmental Forum on Chemical Safety, IFCS), programs (for example, International Program on Chemical Safety, IPCS), conventions (Prior Informed Consent, PIC), and by holding various follow-up conferences. These efforts gave rise to a wide international discussion on the safe management of chemicals. Significant progress has been made, at least as far as the assessment of risks involved and regulations to be introduced are concerned.[10]

In parallel with this development, the Responsible Care Program of the chemical industry[11] launched by Canada (1984) and the USA has in the meantime induced companies worldwide to voluntarily commit themselves to constantly upgrade and implement standards in the areas of safety, health care, and environmental protection, regardless of legal requirements. This has also been documented in reports issued by the chemical industry.[123] The chemical industry, particularly in the USA, has closely interlinked their efforts with governmental programs such as the "Green Chemistry Challenge". This federal program now also includes standards from the Responsible Care Program. The Research Ministry in Germany has stated that it intends to point the way by allocating research assignments on "Sustainable Chemistry".[124] The Responsible Care Program is currently being extended by social and economic elements of entrepreneurial responsibility, thus making it a self-obligation for the chemical industry to focus on sustainability in the steps they take.[14,125a]

If the chemical industry is to make a substantial contribution to a worldwide sustainable development it needs to go beyond the current level of safety regulations and risk reduction that exist in this sector. On the one hand, the quantities of chemicals used must be reduced in order to save resources and energy, and on the other hand, the search for lower risk substances must be pushed ahead in order to make it possible to avoid the use of high-risk chemicals outside of chemical production processes. This can be achieved by making sure as early as possible in the development of base chemicals and in the product design[17] that sustainability requirements are met when the substances are further processed. One of the demands made by Agenda 21 to governments to meet this goal was to coordinate their efforts with international organizations in charge and to "adopt policies and regulatory and non-regulatory measures to identify, and minimize exposure to, toxic chemicals by replacing them with less toxic substitutes and ultimately phasing out the chemicals that pose unreasonable and otherwise unmanageable risk to human health and the environment and those that are toxic, persistent and bio-accumulative and whose use cannot be adequately controlled" (Agenda 21, chapter 19.49c).[7] Measures that are considered effective in this context are: advancing environmentally friendly products and technologies, giving financial incentives, improving product labeling, and strengthening restrictions and prohibitions.

Numerous political concepts have been developed in recent years at the national, European, and international level to improve the political conditions for innovations. All the concepts have one feature in common: the realization that governmental control systems (command and control) need to be complemented by context-oriented bottom-up approaches which give more importance to procedural regulations, economic incentives, self-control, and the participation of social participants.

The most recent White Paper of the European Commission entitled "Strategy for a future Chemicals Policy", a preliminary version of a new integrated Chemicals Guideline, includes some elements of these political goals. In view of the precautionary principles and the EU guideline guaranteeing a high level of protection to human health and the environment, the "creation of incentives for substituting hazardous with less hazardous substances, where alternatives are available", is considered the overall objective to be achieved.[126] Experience has shown that the notification system currently in place impaired innovations in the development of new and safer substances. Instead, a strengthened liability law and a facilitated access to information on chemicals for consumers and the public could advance innovation in this field. Extending responsibility for the safety, disposal, and recycling of a product to suppliers is another possibility of boosting innovation. Changes in testing procedures which existing chemicals now also have to undergo may considerably boost the demand for substitute substances. With respect to these procedures, the Commission suggests to "raise the current threshold values for the notification and testing of new substances, to extend the conditions of deviations in research and development assignments and to allow a more flexible use and provision of test data".[126] Priorities in research need to be set at the national as well as at the EU level.[127]

Although the chemical industry in Europe agreed in principle to the basic objectives of the White Paper, it sharply criticized the practical measures which need to be taken as being too bureaucratic and counterproductive: "Of particular concern is the introduction of an 'Authorization' process that is based on the intrinsic properties of chemicals rather than on the real risks that they may pose. As a result decisions may be taken that increase the number of chemicals that are restricted or banned arbitrarily."[128] The output and mode of usage and not the intrinsic properties of chemicals should provide the basis for an assessment of risks. A compromise between the two controversial positions will probably be established during the process of bargaining on the directives which guarantees the necessary economic incentives for the substitution of hazardous substances, while taking into account the reservations about using too elaborate testing procedures on substances which are processed on a small scale.

The "Green Book on Integrated Product Policy"[129] published in March 2001 by the European Commission was written to open up the markets for environmentally friendly products. In addition to this, it suggests that economic incentives should be offered and transparency created. An integrated product policy needs to center around decisive environmentally relevant stages in the life cycle of a product, that is, ecological design in which the "pollutant-pays-first" principle in establishing the product prices and enabling consumers to make an informed decision are considered. A mixture of instruments has been suggested to bring about the change: differentiated taxation, an extension of producer responsibility by EU legal regulations, introducing privileges in the public procurement system, extended product information, and developing standards for ecologically friendly design. In particular, however, the Green Book is expected to stimulate a public discussion of product policy and thus to generate a European strategy for product-related ecopolitical measures.

The discussion of chemicals legislation in the USA is also dominated by the heavy legal restrictions that are in place. These are the result of strict standards for cost-consumer trade-offs and of a stricter interpretation of the term "risk". The American policy pursued in this field is also changing and now includes new innovation-oriented elements which give more importance to negotiation and coordination processes and which favor "softer" instruments that are based on willingness and mutuality. Accordingly, the procedure for licensing new substances in the USA comprises more flexible tests which vary according to the risks involved; by contrast, the block test procedures applied in the European Union are rather inflexible. These different licensing procedures has meant that companies in the USA had on average 425 new substances registered annually compared to 143 in the EU.[130] In general it can be stated that the environmental policy pursued by the US government in consensus with industry is more closely linked to a management approach in order to promote alternative substances.[131] In 1998 the US government, represented by the Environmental Defense Fund (EDF), reached an agreement with the Chemical Manufacturers Association (CMA) which states that within a 6-year period 2800 common chemicals with a high output (more than 500 t/a year) will be tested for their toxicity. According to CMA this ambitious program can only be completed if it is supported by chemical companies from all OECD member states.[132]

6.1. The Search for a Political Pattern Promoting Innovation

The new control policy pursued worldwide is aimed at reaching agreements at the negotiating table through consensus-building strategies and through revised decision-making principles that result from increased informative transparency. The rationality of these strategies is supported by the experience gained in the use of a political pattern that focused on bans and substance restriction. Only rarely are substitution processes generated as a result of bans on substances that are hazardous to health or to the environment. Such processes can only be sustained for an extended period of time through major political efforts. The most recent example of this is the convention on banning the 12 most-persistent organic pollutants (POPs) that was reached on 23 May 2001.[133] However, this most important convention has not been ratified by the most important industrialized countries up until now. However, there are other bans, restrictions of use, and instructive and qualifying regulations which are widely opposed. Many practicioners prefer eluding existing regulations to searching for less-hazardous substitute substances.

A successful example, such as the International CFC Regime that resulted from the Montreal protocols of 1987, which stipulates a gradual strengthening of regulations shows how "the diffusion of new procedures can be achieved through minimal political cost if the achievement of objectives set by the state is supported by graded and flexible instrumentation which increases the obligation to adjust in a calculable way and only provides for mandatory restraints as a last resort."[134] It appears that new forms of political regulation are required to promote sustainable innovations. To achieve this, a complex political pattern needs to be implemented in which state and nonstate participants unite their efforts (as has been called for in Agenda 21, chapter 23). Not only the course of the decision-making process and the individual measures taken are important in this context, but also the political style chosen, as well as the configuration of participants involved and the political-institutional context in which this process passes must be considered.

The international comparative environmental innovation research has in recent years developed determinants which make it possible to pursue a policy of sustainability on the basis of politically determined conditions. These determinants include: rapid circulation of environmental information, notification of new regulations or their strengthening in conjunction with graded and flexible instrumentation ("threat and control"), and a cooperative political style.[135] An innovation-promoting policy pattern needs to be pursued which meets the following requirements:

- innovation-friendly instruments which are based on strategic environmental planning and objectives need to be combined, economic incentives must be offered, and efforts to implement innovations need to be promoted in all stages.
- an innovation-friendly political style which is dialogic, consensus-oriented, calculable, ambitious, flexible, and management-oriented.
- a configuration of participants which promotes the political integration and networking of many stakeholders and institutions involved, leads to close ties between regulators and those regulated, involves major stakeholders in the dialogue, and interlinks those targeted by the policy.[136]

The international debate on sustainability in the chemical sector which started after the 1992 Rio summit has had two major consequences: Firstly, it generated a number of institutional provisions by which the risks involved in the handling of toxic chemicals were reduced and secondly this debate pushed the search for a political pattern by which a sustainable development in the chemical sector can be achieved through the interaction between central (supra)national and nonstate participants. Political networks have emerged during the process which seek to reach a consensus on the objectives to be pursued and on the ways in which suitable political instruments can be combined; some success has already been achieved. It is anticipated that the substitution of unsustainable substances and mixtures is facilitated if "the ecological motivation and the provision of potential innovators with information is improved and above all if their investment risk is reduced by calculable provisions".[137]

The first signs of such cooperation relationships emerged some years ago in some countries. In Germany, for example, the so-called "Chemiedialog", in which representatives of the chemical industry, of the chemistry union, of environmental associations, and state officials participated, has helped to promote a cooperative political style which has paved the way for an innovation-friendly political climate despite existing conflicts of interests.[138] A political pattern that is most suitable for monitoring and promoting processes of innovation not only comprises regulatory measures and incentives from the state but also self-regulatory efforts undertaken by the chemical industry as well as a dialogue between the three participants involved, namely, the state, the chemical industry, and the general public, on the objectives to be achieved.

The responsibilities incumbent upon the state are: strategic environmental planning by drawing up national environmental plans including quantitative objectives to be achieved, institutionalized success control, and pursuing a differentiated target-group policy, which has already been implemented with considerable success, for example, in Sweden, Denmark, The Netherlands, and South Korea. EU regulations for the public sector nowadays allow for opening up the public procurement system to environmentally friendly products.[129b] It is also necessary to develop criteria for the allocation of funds to research in the sensitive area of product development and procedures applied. Application of these criteria makes it possible to assess if a research project promotes sustainability.

In addition to this, measures taken to improve the availability of information and to increase product transparency are gaining in importance: labeling requirements which also include life-cycle assessments (according to ISO 14021), awarding of environmental quality marks, and warnings issued by the state provide the consumer with practicable guidelines. The EU Green Book on an Integrated Product Policy suggests, in following the "new approach",[17] that influence on the product design be exerted at an early stage. Manufacturers are expected to implement "harmonized norms" which are currently developed (by order of the EU commission) by standardization authorities that also take environmentally relevant features into account and ensure citizen participation in the procedure. If manufacturers applied these norms they could choose the way in which they prove that basic requirements were met and their products could be distributed freely within the European Single Market because they meet the relevant legal regulations.[129c]

Some self-regulatory measures have already been put to the test in the chemical industry. Voluntary branch agreements which have stimulated continued improvements of some technologies are already in place, such as the reduction of health-hazardous emissions. Positive experience has been gained in Denmark by setting up so-called "product panels" which are composed of manufacturers of a specific product group who agreed to reduce the use of hazardous substances.[129d] It is well known in industry that self-obligations with respect to the reduction of ecologically harmful discharges within limited time periods already exist, however, permanent state control and sanctioning measures are needed to ensure that these obligations are met. Although environmental management systems which also include environmental screening (pursuant to EMAS II or ISO 14001) are not primarily aimed at products but at implementing controlled operational procedures and their continual improvement with respect to environmental sustainability, they nevertheless are of great importance in the gathering of data on the environmental impact of the respective production process. A political pattern in which state interference only increases gradually, would give industry the chance to release its self-regulatory powers, to get ready for the transition over an extended period of time, and to implement the transformation under economically justifiable conditions.

7. Summary and Outlook

The principles given in the 1992 Rio Declaration on Environment and Development and in Agenda 21 should provide the basis for the development of concepts on the contribution of chemistry to a sustainable development. Our review has been aimed at identifying the goals that need to be met by chemistry in fundamental as well as in applied research and we have given examples of chemical processes and products, particularly for organic chemistry. We have exemplified the outstanding role of catalysis—heterogeneous, homogeneous, enzymatic—with direct oxidations with oxygen, and we have pointed to the possibility of using renewable raw materials in the chemical industry. Furthermore we stressed the importance of optimizing separation operations to reduce energy consumption, with reactive rectification as an example. Polyolefins are an example of the challenge of obtaining the manifold and diverse product properties of the mass products of the chemical industry by using as few chemical elements as possible. The new metallocene catalysts open up an enormous range of possibilities to tailor the structure of polymers and hence to widely vary the material properties. Moreover the use of only a few base chemicals not only enables an effective, large-scale recovery, it is also reasonable in economic terms. The numerous fine and special chemicals must achieve the desired effect with significantly lower amounts of substance and the possibility of bioaccumulation must be excluded by molecule design as early as possible in the planning stage of the synthesis. After all, it must be possible to process the products of the chemical industry by applying environmentally friendly procedures, namely without VOC emissions.

Chemical process and product innovations per se don't contribute positively to a sustainable development. To achieve this an understanding of product and process innovations and their economic implications, their potential for political and social control, and their ecological effects is required, as is a comparative evaluation. The first signs of this have emerged and have been described. The ongoing discussion of the Green Book of the EU Commission on integrated product policies shows the importance of such an integrated view. The issue of a "product responsibility" in the chemical sector can only be treated if the chemical properties of products and their application patterns are analyzed together with the possibilities of political control over individual product classes.

A critical stocktaking of the implementation of Agenda 21 needs to be done prior to the 2002 Rio + 10 Conference in Johannesburg. Some of the urgent questions raised in Agenda 21 have been addressed by chemistry as well as in science and industry, but so far no definite answers have been given. Hence, it is imperative to address these questions and to scientifically tackle those aspects that can be treated by chemistry in interdisciplinary cooperation. The five-level model used in the present review may serve as an example of this. A concept such as this should also be applied to teaching and become part of the chemistry curricula in school and universities.

Rio Declaration—Selected Principles

Principle 1: Human beings are at the center of concerns for sustainable development. They are entitled to a healthy and productive life in harmony with nature.

Principle 2: States have, in accordance with the Charter of the United Nations and the principles of international law, the sovereign right to exploit their own resources pursuant to their own environmental and developmental policies, and the responsibility to ensure that activities within their jurisdiction or control do not cause damage to the environment of other States or of areas beyond the limits of national jurisdiction.

Principle 3: The right to development must be fulfilled so as to equitably meet developmental and environmental needs of present and future generations.

Principle 4: In order to achieve sustainable development, environmental protection shall constitute an integral part of the development process and cannot be considered in isolation from it.

Principle 5: All States and all people shall cooperate in the essential task of eradicating poverty as an indispensable requirement for sustainable development, in order to decrease the disparities in standards of living and better meet the needs of the majority of the people of the world.

Principle 6: The special situation and needs of developing countries, particularly the least developed and those most environmentally vulnerable, shall be given special priority. International actions in the field of environment and development should also address the interests and needs of all countries.

Principle 7: States shall cooperate in a spirit of global partnership to conserve, protect, and restore the health and integrity of the Earth's ecosystem. In view of the different contributions to global environmental degradation, States have common but differentiated responsibilities. The developed countries acknowledge the responsibility that they bear in the international pursuit of sustainable development in view of the pressures their societies place on the global environment and of the technologies and financial resources they command.

Principle 8: To achieve sustainable development and a higher quality of life for all people, States should reduce and eliminate unsustainable patterns of production and consumption and promote appropriate demographic policies.

Principle 9: States should cooperate to strengthen endogenous capacity building for sustainable development by improving scientific understanding through exchanges of scientific and technological knowledge, and by enhancing the development, adaptation, diffusion, and transfer of technologies, including new and innovative technologies.

Principle 11: States shall enact effective environmental legislation. Environmental standards, management objectives, and priorities should reflect the environmental and developmental context to which they apply. Standards applied by some countries may be inappropriate and of unwarranted economic and social cost to other countries, in particular developing countries.

Principle 14: States should effectively cooperate to discourage or prevent the relocation and transfer to other States of any activities and substances that cause severe environmental degradation or are found to be harmful to human health.

Principle 15: In order to protect the environment, the precautionary approach shall be widely applied by States according to their capabilities. Where there are threats of serious or irreversible damage, lack of full scientific certainty shall not be used as a reason for postponing cost-effective measures to prevent environmental degradation.

Principle 16: National authorities should endeavour to promote the internalization of environmental costs and the use of economic instruments, taking into account the approach that the polluter should, in principle, bear the cost of pollution, with due regard to the public interest and without distorting international trade and investment.

Principle 17: Environmental impact assessment, as a national instrument, shall be undertaken for proposed activities that are likely to have a significant adverse impact on the environment and are subject to a decision of a competent national authority.

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Glossary

Base chemicals: Products of the chemical industry, manufactured globally at a scale of more than 1×10^6 tons per year.

Chemical biotechnology: Application of biotechnology to produce chemicals.

Economic-ecological efficiency: Ratio of ecological improvement to economic input variable (for example, cost, profit reduction/reduction of the marginal return).

End of the pipe environmental protection: A term used to describe environmental measures taken after the occurrence of emissions in the widest sense (exhaust air, waste water, waste, noise, etc.).

Gross energy requirements (GER): GER indicate the total **primary energy** consumption of the entire process chain to manufacture a chemical product. The GER includes energetic consumption, which in chemical processes is largely the process energy, and nonenergetic consumption, namely the direct, material use of fossil energy sources such as crude oil.

Innovation system: The term comprises external influencing factors (such as, framework conditions set by the state, market conditions, customer behavior) and internal company influencing factors which impact the innovation behavior of companies.

Integrated environmental protection: A term used for pollution-control measures which help to avoid ecologically harmful effects by selecting environmentally friendly substances, procedures, and technologies (production-integrated environmental protection) and for products which are developed in an effort to keep the burden on the environment as small as possible during their life cycle (product-integrated environmental protection).

Integrated product policy: The concept of an integrated product policy is aimed at reducing the burden that products place on the environment during their life cycles—from the depletion of resources to waste disposal.

Life-cycle assessment (LCA): In life-cycle assessments the entire life cycle (product line) of a product (extraction and processing of raw materials, production, distribution and transport, use, consumption, and disposal) as well as the potential ecological effects are analyzed, and the material and energy conversions occurring in the life cycle and the resulting burden on the environment are assessed.

Metrics: Metrics such as mass index, environmental factor, and environmental indices are ratios which can be used as benchmarks for assessing phenomena such as chemical syntheses.

Political pattern: Contrary to another approach which only considers the question of instruments used, this term comprises the totality of the factors dominating the political decision-making process: the political-institutional context of action, the political style, the instruments used, and the relationship between the state and the target groups.

Preventive environmental protection: The term comprises all those measures which directly or indirectly help to avoid environmental damage or burdens (for example, product and production-integrated environmental protection, technology assessment).

Primary energy: A term used for energy sources, for example, crude oil, mineral coal, natural gas, and uranium, in the state they are mined, namely, prior to conversion.

Product panels: Groups of companies, which join their efforts to determine how environmental goals can be achieved for their product group and how arising obstacles can be overcome.

Resources: In a narrower sense the term is used for natural capital, raw materials, energy sources, and environmental media, whereby a distinction can be made between (partly) renewable and nonrenewable resources.

Responsible care: Binding obligation of the chemical industry to self-responsibility in the areas of health, safety, and environment. The self-obligations are established in basic guidelines and are implemented by the national chemical associations.

Sustainable development: A term used to describe an environmental and development concept, which was formulated together with other papers in the Brundtland Report; at the 1992 UN Conference on Environment and Development in Rio de Janeiro the 27 principles of sustainable development were adopted and put in concrete terms in the working program of Agenda 21.

Verbund: Interplay between production processes and production plants as well as a close cooperation between businesses and customers, suppliers, and interest groups to achieve economic and ecological advantages.

VOCs (volatile organic chemicals): A large variety of substances which under intense solar radiation promote the formation of tropospheric ozone and hence of summer smog.

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