SUSTAINABLE DEVELOPMENT AND CHEMISTRY

1. Introduction

The United Nations Conference on Environment and Development (UNCED), held in Rio de Janeiro in 1992, provided the fundamental principles (Rio Declaration) and the program of action (Agenda 21) for achieving sustainable development (1). Sustainable chemistry is understood as the contribution of chemistry to the implementation of the Rio Declaration and Agenda 21 including its ongoing advancements, such as the Johannesburg Declaration of the World Summit of Sustainable Development that was held in the year 2002 (2,3). Principle 1 of the Rio declaration proclaims: that human beings are at the center of concerns for sustainable development. They are entitled to a healthy and productive life in harmony with Nature. 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 United States considers a population number of 9 billion to be most likely (4). The population 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 living in the developing countries has to grow and adapt to the standard of the industrial countries, which must not drop if Principle 3 of the Rio Declaration of a sustainable development has to be met. Principle 3 stated that 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 (5): “Sustainable development is development that meets the needs of the present without compromising the ability of future generations to meet their own needs.” 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 4 and more. Resources will have to be used much more efficiently than today, ie, 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 4 will not be sufficient since the existing fossil resources will be increasingly difficult to access (6,7). 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. The global proved oil reserves were estimated at end 2001 to last for 40.3 years (8). 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 twenty-first century which was adopted by > 170 governments (1). Agenda 21 addresses the pressing problems of today and also aims at preparing the world for the challenges of the next century. In Section I, Chapters 2–8, the social and economic dimensions of sustainable development are outlined with the most important aim of integrating environment and development in decision making. The conservation and management of resources for development are the main focus of interest of Section II, Chapters 9–22. Strengthening the role of major social groups is described in Section III, Chapters 23–32 such as the role of business and industry. Finally, Section IV, Chapters 33–40, gives the means of implementation. The sciences have to make a considerable contribution if the 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 understood as an essential component in the search for feasible pathways toward sustainable development by integrating physical, economic, and social sciences in order to better understand the impacts of economic and social behavior on the environment and of environmental degradation on local and global economies. The World Summit on Sustainable Development held in 2002 in Johannesburg strongly reaffirmed the commitment to the Rio principles, the full implementation of Agenda 21 and the program for the further implementation of Agenda 21 (1,2).

During the last 10 years, essential aspects of the Rio Declaration and Agenda 21 have been tackled. The safety of chemicals, which in Agenda 21 is addressed in the separate Chapter 19, has been improved significantly by international agreements (9), to which the worldwide voluntary initiative "Responsible Care" of the chemical industry contributes considerably. These findings are acknowledged in Chapter 30.10 (10). In their future programs, the chemical industries of Europe, Japan, and the United States have explicitly accepted the contribution of chemistry to sustainable development (11–14). In general, it must be said that the chemical companies are attempting to understand the implications of sustainable development for them (15) (see Fig. 1).

The principles of production and product-integrated environmental protection are increasingly accepted and implemented by numerous enterprises of the chemical industry (16–18). Basic concepts for an environment-oriented design of chemical products and processes have been developed (19,20). "Green Chemistry" was proposed as an orientation for chemical industry as well as applied and basic research in chemistry (21).

Since base chemicals, namely, chemicals that are each produced worldwide in >1 million tons/ year (t/year), are produced in large quantities and important product lines are synthesized from them, their resource-saving and environmental benign production is hence especially important for sustainable development (see Fig. 1, level 2a). This calls for the development of new processes for certain base chemicals or even completely new base chemicals. The base chemicals directly affect the chemical products that are produced from them in one or several steps. The chemical products are then processed in fields of industry that frequently do not belong to the chemical industry and 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.

2. Conservation and Management of Resources

2.1. Pollution Prevention. As stated in agenda 21 Chapter 18 the protection of water resources, water quality, and aquatic ecosystems is of highest priority for sustainable development. The International Year of Freshwater 2003 was declared by the United Nations to raise awareness of the worsening state of the world's water resources that currently forces >1 billion to drink from sources contaminated with human waste, and leaves countless millions more with insufficient supplies to water their crops, or to spur industrial development. The water crisis is real. If action is not taken, millions of people will be condemned to a premature death (22).

Marine environmental protection is another important topic. Land-based sources contribute 70% of marine pollution, while maritime transport and dumping-at-sea activities contribute 10% each. Many of the polluting substances originating from land-based sources are of particular concern to the marine environment since they exhibit at the same time toxicity, persistence, and bioaccumulation in the food chain. There is currently no global scheme to address marine pollution from land-based sources (23).

Chemical compounds, which as a result of their product characteristics can enter the aquatic environment, should not endanger this environment and need to be biologically degradable, ie, product development needs to make use of biodegradable materials (24) in product design. Persistent and semipersistent chemicals must not be accumulated in any environmental compartment (25) because they can be found even in remote areas of the world (26).

Air pollution is a major concern. Thus, regulations aimed at reducing tropospheric ozone concentrations have a great impact. As a result, the total anthropogenic Volatile Organic Compounds (VOCs) emissions are decreasing slowly in United States (27). The politically determined ozone threshold value of 110 $\mu g/m^3$ as an environmental quality level in European Union requires that the emissions of organic compounds into the air have to decrease by 70–80% compared to the reference year (1990). For Germany, this means that the total emission of VOCs including that from traffic has to be reduced to 650×10^3 t by the year 2010. 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, which makes up more than one-half of the total emissions in Germany, may be reduced by technological means (28).

2.2. Energy. Reducing the amount of energy and materials used per unit in the production of goods and services can contribute both to the alleviation of environmental stress and to greater economic and industrial productivity and competitiveness (29). The energy and environmental profile of the chemical industry in the United States has been investigated and recently described in detail (30,31). In 1997, the chemical industry used 6650 PJ (Peta $= 10^{15}$) of energy, which represents ~7% of all domestic energy used and 25% of the energy consumed in all manufacturing processes. Remarkably, this amounts to ~1.8% of global energy consumption of approximately 350,000 PJ. Approximately 51% of the total was used as feedstock for chemical products (nonenergy consumption) and 49% as process energy for carrying out the processes (energy consumption). The main energy consumption at 2640 PJ is invested in the production of the organic base chemicals (Fig. 2).

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 ~30%. Analysis of the production output of the chemical industry from 1974 to 1997 shows, however, that the energy consumption per unit of emission declined by > 39% between 1974 and 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%. The conclusion is 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 twentieth century (12,13) can be realized, this will be an important contribution to sustainable development (see Fig. 1, level 2a). 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.

An estimation of the material, energy, and CO_2 flows for the chemical industry in Germany in 1995 showed there was a primary energy demand of ~1700 PJ, of which 830 PJ was used in the generation of synthetic organic products (32,33). 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 $\sim 57 \times 10^6$ t, which is ~20% of all manufacturing and 6% of the total emissions. The potential reduction by the year 2005 was estimated at 16×10^6 t (33). 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 (34).

The ratio of the primary energy input in the United States and in Germany corresponds quite well with the ratio of the chemistry turnover in both countries of $\$419 \times 10^9$ ($\$448 \times 10^9$) and $\$105 \times 10^9$ ($\$120 \times 10^9$), respectively, in the year 1998 (2001) (35). 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 with the actual consumption of energy. Basic innovations for the production of the necessary goods combined with a significantly lower need of resources, approximately one-tenth, are necessary (7). Energy consumption and carbon dioxide release are closely connected. The implications of the carbon management for R&D in the chemical sciences were recently discussed (36).

New and Renewable Sources of Energy. Agenda 21 aims at encouraging the environmentally sound use of new and renewable sources of energy (37). On the way to a renewable energy supply, research and development of fuel cells and electrolyzers will play a significant role (38). In this context, efficiencies of photovoltaic technology (39) will have to be increased, whereas cost of their production will have to be brought down (40). Besides inorganic solar cells, organic ones represent an important scientific challenge (41). Dye-sensitized nanocrystalline injection solar cells are regarded to be promising candidates to directly produce high energetic chemicals from sunlight by the energy that could be chemically stored (42). With regard to high distances and the deficient electricity network, photovoltaic home systems appear to be the most viable alternative source of electricity in developing countries (43). To revert to renewable energies is in compliance with the Agenda 21 which states that most of the commercial and noncommercial energy produced today is used in and for human settlements, and a substantial percentage of it is used by the household sector. Developing countries are at present faced with the need to increase their energy production to accelerate development and raise the living standards of their populations, while at the same time reducing energy production costs and energy-related pollution. Increasing the efficiency of energy use to reduce its polluting effects and to promote the use of renewable energies must be a priority in any action taken to protect the urban environment (44).

3. Materials and Processes

3.1. Materials. The products of the chemical industry display a great chemical diversity. Agenda 21 assumes there are ~100,000 chemical substances on the market worldwide. Approximately 1500 compounds make up ~95% of the total world production (45). 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.

The vision of a product life cycle management is a scheme of reuse and control of chemical substances in a material cycle concept (46). An effective and large-scale recycling that is an aim of Agenda 21 ought to be feasible and economic with only a few base products. The numerous fine and special chemicals have to become more effective, ie, 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.

Renewable Raw Materials. The encouragement of environmentally sound and the sustainable use of renewable natural resources (47) and biotechnology (48) is one aim of Agenda 21. At present, the share of renewable raw materials in the feedstock consumption of the chemical industry in the United States (Table 1) and in Germany (3) runs to ~5 and 8%, respectively. It is assumed that this percentage will increase notably. 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 (50) (see Fig. 1; level 2**e**).

Approximately 51% of the renewable raw materials used at present in Germany are fats and oils. Carbohydrates constitute the second largest portion at 43%, whereas, a further 6% is made up of other renewables such as proteins and protein surfactants (3). When renewables are used as base chemicals for organic synthesis, Nature's synthetic input has to be used to obtain in one or only a very few chemical reaction steps those complex molecules that 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 renewables (51,52). Many highly oxidized industrial chemical products based on starch are available and are further developed (53,54). Alkyl polyglucosides are a good example; they are produced as skin-compatible, environmentally benign tensides on a scale of 70,000 t/year (55). Only recently, reviews of new syntheses with oils and fats (56,57) and with carbohydrates (58) as renewable raw materials for the chemical industry were presented. The transition-metal catalyzed metathesis of unsaturated fatty acids produces ω-alkenoic acids; eg, 9-decenoic acid is obtained from oleic acid and 12-tridecenoic acid is obtained from erucic acid (59,60). The catalytic oxidative cleavage of unsaturated fatty acids yields dicarboxylic acids such as azelaic acid (61,62). All these chemical compounds are potential base chemicals. The epoxidation of unsaturated fatty compounds leads to epoxides of fats that can be used as coating binders, and once ring opened by water as polyol components for polyurethanes (63). 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 (64). The conversion of corn into plastic via a newly opened polylactic acid plant was set into commercial production by Cargill Dow (65). This initiative earned them one of the 2002 Presidential Green Chemistry Challenge Awards.

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. A signal is given by the Biomass Research and Development Act of 2000 on the basis of the recommendations of the National Research Council of the United States on the estimated development of renewable feedstocks up until 2090 (66,67). In 2030, 25% of the production of organic chemical products is expected to come from renewable feedstocks (Table 1).

In Europe, biomass already contributes ~5% of the European Union (EU) energy supply and 65% of the total primary renewable energy production, predominantly for heat and power applications. In the long term, the contribution of biomass to the EU energy supply is thought to have the potential to increase to 20%. Of the renewable energy sources technologies, only biomass produces solid or liquid fuels that could be used as, or transformed into, fuels for heating and transport applications. The main research and technology development priority is the development of cost—effective integrated approaches from biomass sustainable procurement to fuel production and use. However, research and technology development for the chemical transformation of biomass to useful biobased products is being totally neglected at present in the European Union as well as in Germany (68).

The competition of the cultivation of food and of renewable raw materials on the limited available agricultural area (69) could make problems, because food demand and consumption will also increase dramatically. For that reason, the United Nations program to combat desertification (1) is most important. As stated in Chapter 12.4b of agenda 21 the realization of this program has to be greatly intensified, on the one hand to stop desertification, on the other hand to regenerate agricultural areas by combating land degradation through, inter alia, intensified soil conservation, afforestation, and reforestation activities. The sciences, and especially chemistry, can make enormous contributions to that program, which may contribute as well to stabilize a favorable global climate.

Polymers and Plastics. 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 (70) very difficult. Moreover, there are a number of monomers, eg, isocyanates, ethylene and propylene glycol, and acrylates, used for the synthesis of bulk plastics that rank comparably highly in the value-adding chain. Thus, the gross energy requirement for the production of important bulk plastics differs by a factor of 2 and more (Fig. 3). The future program Vision 2020 of the chemical industry in the United States (12,13) aims at methods of synthesis and catalysis to convert product molecules and polymers back to useful starting materials (see Fig. 1, level 2d). 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 fibers, would be an important contribution to sustainable development (72) (see Fig. 1, levels 2b–d).

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 $\sim$44% of the total production of plastics, and is rising sharply. In 1990, production 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 (73). Moreover, they make a detailed understanding of the mechanism and the stereochemistry of the polymerization of olefins possible (74–77). 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 (78).

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 poly(vinyl chloride) (PVC) which is increasingly being queried socially, since it is produced from a toxic monomer and contains a large amount of plasticizers that can be washed out. Toxic waste is produced during its production and its disposal causes problems since hydrogen chloride is produced during combustion. PVC is now gradually being substituted by polyolefins. This is also the case with other special plastics, eg, polycarbonates, polyaziridines, and polyimides, since their production requires a high amount of material and energy (73). New advances in catalysis are upgrading common polymers into materials offering uncommon performance (12,13).

Solvents and Solvent-Free Processing. 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 in processing and are emitted as VOCs into the atmosphere. Of the total VOC emissions in United States 5.3×10^6 t were emitted from solvent utilization in 1992 and 4.4×10^6 t in 1999. That is 28 and 27% of total emissions, respectively. Not only is this a significant cause of the tropospheric ozone formation (see Fig. 1, level 3), which contributes to the summer smog, but it is also an immense waste of resources (see Fig. 1, level 2c). In Germany, emissions from solvent utilization amounted to 1.160×10^6 t in 1990 (total VOCs: 3.221×10^6 t) and 1×10^6 t in 2000 (total VOCs: 1.6 x10^6 t) (79).

The main emissions from solvents in the processing industry are caused in coating, color printing, and adhesive processing. The development of chemical products that can be processed without the use and emission of VOCs in areas mentioned 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 could be produced from renewable raw materials ecologically benign and could be disposed of without problems (80). In a case where a solvent is absolutely necessary, the use of fluid or supercritical CO_2 should be considered (81,82). To emphasis the importance of developing alternatives to common solvents Joseph M. DeSimone earned the Academic Award in 1997 of the Presidential Green Chemistry Challenge for the development of technologies for the design and applications on surfactants for CO_2 so as to advance the solubility performance characteristics of CO_2 systems (83).

The following steps are currently taken for the reduction of the VOC emissions in the development of new coating systems. (1) Binders are used with an essentially higher content of solid matter dissolved in organic solvents (high solid coatings). (2) Water-diluted coatings have a remaining content of organic solvents. (3) Powder coatings are used without solvents, but frequently with organic cleavage products formed during the curing process. (4) Radiation-hardening coating systems are used that 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 (84). The benefits of VOC reduction among other issues are reflected in the eco-efficiency analysis. For example, a comparative assessment of four alternative metallic topcoats at Akzo Nobel gave information enough to activate marketing and the production department to prepare the promising candidate for market introduction (85). BASF introduced ultraviolet (uv)-curing water-based coatings that showed high ecoefficiency compared to usual coatings (86). For eco-efficiency and eco-innovation (see also section 4.2).

Biodegradable Materials. It is the challenge for chemistry to develop molecules that have the desired effect at a minimum dose and that are mineralized rapidly by the naturally existing ecosystem (87). Here, the use of renewable raw materials, such as oils and fats, (56,88,89), is especially important as are starch derivatives (53) in detergents, and oils and fats for lubricants (90).

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 (Fig. 4) currently used as sequestrants and dispersants as well as the widely used complexing agent ethylenediaminotetraacetic acid (EDTA) are not sufficiently biologically degradable and, therefore, contamination of the surface waters cannot be excluded. Products that can be substituted for the polyacrylates are the biologically degradable polyaspartic acids, produced by means of thermal polymerization (18). Modern, biologically degradable complexing agents of the type of aminopolycarboxylic acids as, eg, iminodisuccinic acid (IDS) are possible alternatives to persistent complexing agents. Bayer earned the 2001 Alternative Synthetic Pathways Award of the Presidential Green Chemistry Challenge for the introduction of IDS.

3.2. Syntheses

Catalytic Direct Oxidations. Oxidation is one of the most important reactions in organic chemistry. However, it causes the strongest stress on the environment. It is remarkable how poorly direct oxidation with oxygen is understood and controlled (91–93). Here, as shown by the example of propylene oxide, a breakthrough would be a substantial contribution of chemistry in the field of 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 United States, $\sim 1 \times 10^6$ t were produced in Germany, and $\sim 4 \times 10^6$ t were produced worldwide. In the United States, and this distribution is typical for the world market, 65–70% is reacted via polyether polyols to form polyurethane foams and 22% to form propylene glycol.

Chlorohydrin processes and oxirane processes with isobutane or ethylbenzene are the industrial processes used. Both are indirect processes and the first one in particular is extremely polluting. Remarkably, both processes show very similar GER of ~ 104 GJ/t of propylene oxide (Fig. 5). The oxirane process is a more indirect process for the synthesis of *tert*-butyl alcohol and styrene; it can be done economically, only if these coupled products can be sold. At present, this is the case with styrene, but this is no longer the case with *tert*-butyl alcohol since *tert*-butyl methyl ether (MTBA) will no longer be 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.

During the last few years, the epoxidation of propylene with titanium silicalite (TS-1)/hydrogen peroxide (yield $> 90\%$) has been developed (eq. 1). This process requires hydrogen peroxide (H_2O_2), 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 *in situ* process, whereby water is generally the only by-product and yields of propylene oxide of up to 57% have been obtained so far (94). Quite recently, it has been shown that carbon dioxide is an excellent solvent for the formation of propylene oxide from hydrogen, oxygen, and propene over a Pd/TS-1 catalyst (95).

(1)

A new investment cycle for the existing propylene oxide plants has begun recently. Most of the chlorohydrin plants will be closed down. New plants using the oxirane procedure with styrene as the coupled product are being built in the United States as well as in Europe and Asia. A Sumitomo Chemical propylene oxide plant that was set to open in Japan in 2003 is based on the use of cumene in the oxirane process. The dimethylbenzyl alcohol coproduct is to dehydrated and hydrogenated back to cumene (96). Degussa and Krupp, however, developed a large-scale catalytic oxidation of propylene with hydrogen peroxide (97). BASF and Solvay expect to start building a 250,000 metric-ton propylene oxide plant based on hydrogen peroxide (98).

It has become very clear that the process direct oxidation of propylene or, even better, of propane with oxygen from the air has to be developed for the next investment cycle (eq. 2). An interesting attempt carried out with oxygen is the oxidation of propylene to propylene oxide with gold catalyst on a titanium oxide support (99). A disadvantage of this procedure is the need to add hydrogen to the reaction of the second oxygen atom and that more than stoichiometric amounts of water are formed, and hence, the catalyst also catalyzes the oxyhydrogen gas reaction. Other catalysts, eg, bimetallic M/Ti-silicates (M = Pd, Pd−Pt, Au) have also been described (100,101). So far, no attempt has been made to achieve the direct oxidation of propane to propylene oxide with oxygen from the air, a process that 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.

(2)

Caprolactam (world capacity ~4.4×10^6 t/year) is another important base chemical produced by oxidation that has a high demand in resources. The C_6 route from cyclohexanone oxime by Beckmann rearrangement forms 2 or 3 mol of ammonium sulfate. The synthetic process should be improved to be environmentally more benign. However, a comparison of 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 (102).

Adipic acid (world production ~2.3×10^6 t/year in 1995), 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 (see Fig. 5). The existing process was improved by use of the coupled product for energy production (18), and for the oxidation of benzene to phenol (102). 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 (103). Progress has also been made in the catalytic oxidations of cyclohexane(104) and cyclohexene (105) to adipic acid. The advantages of the catalytic process compared to the classical process have been discussed by Thomas and co-workers (106). A recent review reports on new by-product free synthesis routes (107).

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 (50). An excellent overview on the relevance of catalysis for carbon management has recently been published (92).

Biotechnology. Properties of genetically modified plants such as resistibility against pests, enhanced productivity of healthy ingredients (eg, vitamins), tolerance of soil salinity, etc, have high potential to improve or even ensure the world nutrition situation. Therefore, the Agenda 21 prompts to develop plant cultivars tolerant and/or resistant to stress from factors such as pests and diseases and from abiotic causes (108).

However, despite of these social benefits these modifications are scrutinized intensely against the background of the precautionary principle because of the potential gene transfer through outcrossing and other hazards (109–112). As indicated in Agenda 21, these impacts should be carefully identified in the earliest phases of the development of biotechnology in order to enable appropriate management of the consequences of transferring biotechnology (113). Nevertheless, the better understanding of code, especially in the course of the human genome project, leads to a variety of technology platforms. According to the future program Vision 2020 fully automated sequencing of very large genes will have to be complemented by information systems that offer easy access to the data obtained (12,13). "Designer drugs" (114–116) may alleviate suffering caused by various diseases. Agenda 21 prompts international and regional organizations, academic and scientific institutions, and the pharmaceutical industry to take into account appropriate safety and ethical considerations. They must establish and enforce screening, systematic sampling and evaluation procedures for drugs and medical technologies, with a view to barring the use of those that are unsafe for the purposes of experimentation; ensure that drugs and technologies relating to reproductive health are safe and effective and take into account ethical considerations (117). Quantitative Structure–Activity Relationship (QSAR) may help in the understanding of the chemical reactivity and biological activity of the toxic molecular configurations anticipated (118,119).

Chem-Bioinformatic Tools. The development of new computational techniques to guide synthesis by theory and molecular modeling is claimed in the future program Vision 2020 of the chemical industry in the United States (12,13). The culture of the chemical industry's research community needs to shift away from empirical design toward computational design. The consideration of those chem-bioinformatic tools is envisaged by the Agenda 21 as using the tools provided by modern biotechnology, develop, inter alia, improved diagnostics, new drugs and improved treatments and delivery systems (120). Natural products, eg, such as hybrid systems (121) that are constructs of different molecular entities, natural or unnatural, are regarded to be an appropriate basis. The development, improvement, and more effective utilization of medicinal plants and other related sources are claimed (122).

Chemical Biotechnology. The Agenda 21 claims to "develop processes to increase the availability of materials derived from biotechnology, for use in improving human health (123). Chemical biotechnology is the quickly spreading application of biotechnology in chemical production as expressed in the Vision 2020 of the U.S. chemical industry (124). Biotechnological procedures are mainly employed for the production of fine chemicals and pharmaceuticals (125,126). The use of biocatalysis for the industrial synthesis of fine chemicals is increasing rapidly (127). Here, the driving force is certainly not sustainability, but the fact that a nonbiocatalytic process is impossible 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 2001: 24 million tons (28)], and citric acid, only the lipase-catalyzed hydrolysis of acrylonitrile to acrylamide by the Nitto Chemical Company with 30,000 t/year has been achieved. The production of bio-ethanol will first increase considerably in the United States from the present 6.3×10^6 t in 2002 to 10.5×10^6 t in 2004 by the substitution of MTBA as a gasoline additive (129). It is remarkable that the addition of ethanol to gasoline as an anti-knock compound was already known in 1917 and that in 1923 General Motors, DuPont, and Standard Oil pushed for the use of tetraethyllead despite its long-known toxicity for patent reasons (130,131). 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 United States alone would have been prevented. The amount is increasing still further since tetraethyllead is still produced and sold to Third World countries. This is an impressive example that shows clearly how important it is to steer toward the aims of sustainable development, especially in the highly developed countries, as defined in the Rio Declaration and Agenda 21.

3.3. 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 (132). 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. Integration of reactor and separation systems such as reactive distillation or extraction, membrane reactors, and supercritical fluid systems is part of the Vision 2020 of the chemical industry in the United States (12,13,132).

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 (133). The heterogeneously catalyzed reactive rectification, eg, of methyl acetate is especially advantageous, since here the separation of the catalyst does not apply (134). For all other separation methods, eg, 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 (132).

4. Assessment

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 (135). In numerous chapters, Agenda 21 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 economic, social, and ecologic dimensions that generally need to be considered in an integrated way.

According to Agenda 21 Chapter 35.7c appropriate tools are mandatory for sustainable development: ‘Develop, apply, and institute the necessary tools for sustainable development, with regard to:

1. Quality-of-life indicators covering, eg, health, education, social welfare, state of the environment, and the economy.
2. Economic approaches to environmentally sound development and new and improved incentive structures for better resource management.
3. Long-term environmental policy formulation, risk management and environmentally sound technology assessment.

Tools are especially important in the early stage of design. Companies engaged in these processing fields (ie, in the sustainable manufacturing of chemicals, materials, and bio-products) face increasing societal demands to reduce their environmental footprint and are beginning to adopt these new paradigms, as well as advanced integrated environmental, health and safety (EHS) practices, to support their commitment to sustainable development. In order to drive these changes throughout their organizations, industry needs an expanded “tool-kit” for practitioners to apply during the early development phase of a manufacturing process (136).

Tools for comparative analysis of alternatives are shown in Figure 6. Life cycle assessment (LCA), benefit cost analysis (BCA), comparative risk analysis of alternatives (CRAoA), risk tradeoff analysis (RTA), and programmatic comparative risk assessment (PCRA) cover a more or less expanded part within the two dimensions level of analysis and dimensions of analysis. None of these tools alone is enough to match all risks quoted in Table 2. Following the principles for tool specific decision making (Table 3) decision makers are aided in the priority setting process. The selection of tools can be guided by corresponding questions related to Table 2, Table 3, and Figure 6 (138). The impact of changes can be of incremental or more of a fundamental nature depending on the level of analysis (micro, meso, or macro). Whereas optimization of processes become possible eg, by means of life cycle assessment, integrated product policy (IPP) (139–141) and even more eco-innovation markets may turn (142,143) toward a desired direction (see Fig. 1, levels 2b–d, 3).

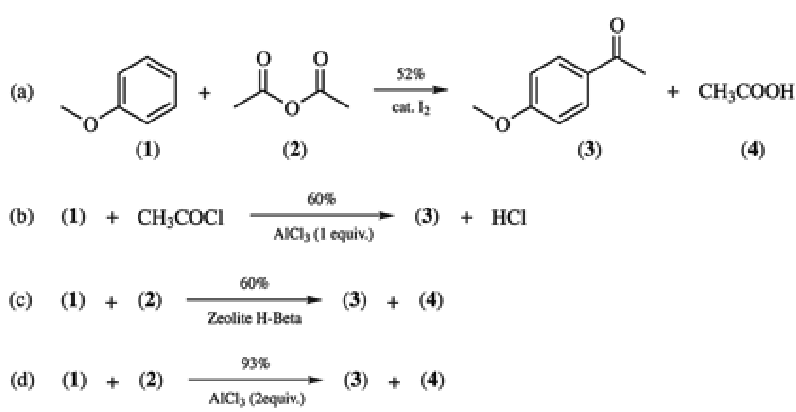
4.1. Metrics for Assessment of Sustainability. The process parameters of established processes are (internally) known and can be used for the quantification of the use of resources, gross energy requirements (GER), waste, emissions, and related costs per product unit. A number of metrics have been developed that are used for assessment in the chemical industry (144–147). Some of them were examined with regard to their significance as green chemistry metrics (148). As an example, the GER was compared for the two propylene oxide processes (chlorohydrin vs. oxirane process) currently performed. Surprisingly, it was about the same for both processes at 104 GJ/t of propylene oxide (72). 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.

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

The GER is accessible for a number of important organic base chemicals (Fig. 5); eg, it is ~40 GJ/t for acetaldehyde, 80 GJ/t for adipic acid, and 104 GJ/t for propylene oxide(149); vegetable oils such as rape seed oil and linseed oil require a GER of ~20 GJ/t (013,149). 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 are also evident in important bulk plastics (Fig. 3). For example, the GER for 1 ton of epoxy resin is 107 GJ/t, which is almost twice as high as it is for alkyd resins at 64 GJ/t, because the latter contains a portion of renewable raw materials. Remarkably, PVC has the lowest GER of 53 GJ/t, which is clearly lower than that for polyethylene at 65 GJ/t. However, the process energy for PVC at 32 GJ/t is 50% higher than for polyethylene at 21 GJ/t. The chemical energy accumulated in PVC at 20 GJ/t, however, is less than one-half that of polyethylene (43 GJ/t) because of the high chlorine content in the former. The GER, in relation to the process energy and the chemical energy accumulated in the product, is a useful measure for the assessment of bulk products.

Environmental Assessment of Syntheses. 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 (150), preferably already at the laboratory stage (151), is essential for the precise development of sustainable processes (see Fig. 1, level 2a). Some approaches have been presented during the last few years (152–157). Sheldon's proposal (158) weights the environmental factor E (mass of waste, ie, all compounds used that are not incorporated in the product, per mass unit of product) of a process with substance-specific weighting factors Q_{output}. That proposal was developed to an "Environmental Assessment Tool for Organic Synthesis" (159–161). In this way, an environmental index (152) 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) (157). 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 4).

The weighting factor Q_{input} considers the resources used, as well as the aspects of occupational safety and health, the parameter Q_{output} essentially considers the human toxicity and eco-toxicity (161) (see Fig. 1; level 3). As an example, these metrics were determined both fast and simply for four different laboratory syntheses of 4-methoxyacetophenone (eq. 3) by using the software EATOS (Environmental Assessment Tool for Organic Syntheses, (159,160)) (Fig. 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 $E\text{I}_{\text{in}}$ and $E\text{I}_{\text{out}}$ are also about one order of magnitude lower than in the other syntheses. Clearly, this synthesis of 4-methoxyacetophenone 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) (eq. 3).



(3)

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 whereas reactions (b) and (d) require solvents during reaction and a work-up procedure that contribute decisively to the high resource requirements and the high potential environmental impact.

The advantage of such a tool is that it can rapidly be applied to keep the overview of mass balances and problematic substances in complex competing chemical routes. Discussions on economic, safety, and waste treatment aspects with corresponding experts would be stimulated at the earliest stage of process design, the most sensitive phase in process development with regard to environmental compatibility, economic performance, and occupational health. Weak points become obvious and scenarios can be played in theory or by means of new synthetic results.

According to the future program Vision 2020 (12,13), eg, solid acid and base catalysts should replace the toxic and corrosive mineral acids and bases for organic syntheses. In the end, a full mass balance becomes necessary to evaluate the progress that is achieved by the new development (162). By means of a mass balance, alternatives appearing unfavorable at first glance, eg, because of lower yield or enantiomeric ratio, could reveal advantages at a later point in time and should, therefore, always be included into the investigations. Thus, synthetic protocols and routes quasi represent competing reference values for each other in an onward assessment, optimization, and decision process.

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. Unfortunately it is not yet available.

4.2. Life-Cycle Assessment. In life-cycle assessments (LCA) 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.

A life-cycle assessment (163) of a product is drawn from the “cradle to the grave” (see Fig. 1, level 2d), ie, 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 (164) and represent the basis for the eco-efficiency concept (see eg, Ref. 165). Azapagic and Clift have written an overview on the application of the LCA method for process optimization (166). Life-cycle assessments were thus set up for bulk plastics (167). 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 (156,168). 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 GER as well as the CO_2 and NO_x emissions are almost one order of magnitude smaller when linseed oil epoxide was used (categories such as toxicity, eutrophication, acidification were not examined). It is remarkable that during the production of the petrochemically derived binder, propylene oxide contributes more than one-half of the environmental impact (Fig. 8). Patel compared results from LCA studies for the commercially most important bio-based polymeric materials with equivalent products made from petrochemical polymers. The body of work analyzed indicates overwhelmingly that bio-based polymers offer important environmental benefits not only for today but also for the future (169).

Life-cycle assessments were also set up for some biotechnological processes (125). It is remarkable that bio-ethanol (world production (127) 2001: 22.4×10^6 t/year see Ref. 108) has clear ecological advantages over synthetic ethanol (2001: 2.2×10^6 t/year). The demand for fossil primary energy for the latter amounts to 62.3 MJ/kg, but only to 4.8 MJ/kg for ethanol derived from sugar cane and 19.1 MJ/kg for ethanol from sugar beet. The CO_2 emissions for synthetic ethanol amount to 1.88 kg/kg, the CO_2 emissions are credited for bioethanol.

4.3. Safety, Hazard Analysis, and Risk Assessment. Spectacular accidents like the Bhophal disaster (170,171) and Seveso debacle (172) attracted public and legislators' attention, and the Agenda 21 accentuated: that the overall objective is to minimize hazards and maintain the environment to a degree that human health and safety is not impaired or endangered and yet encourage development to proceed (173). The aim is that injuries because of industrial activity will be avoided by developing, in accordance with national plans, strategies in all sectors (industry, traffic and others) consistent with the WHO safe cities and safe communities programs, to reduce the frequency and severity of injury (174).

In the meantime the number of possible risks and probably also their potentially hazardous effects have even further increased. But, the objective to reduce occupational accidents, injuries, and diseases according to recognized statistical reporting procedures (175) seems to be approximated or even achieved, because the number of accidents per unit of activity has tended to decrease slightly and the overall potential risks associated with chemical process plants seems to have decreased (176). This tendency is encouraging; nevertheless, runaway reactions, eg, and the resulting decomposition (177) and secondary events (release of toxic or explosive material, etc) still occur. Accidents in Europe (172) and Asia (178–180) are described in the literature. Following a number of accidents in the United States, eg, the EPA promoted a case study based on a lethal accident in a plant producing resin in Columbus in 1997, to reduce the dangers of runaway reactions (181). Risk analysis in chemical process industries relies on a variety (182) of techniques and methodologies; risks should be identified as early as possible (183–186). Past mistakes should not reoccur and have to result into a learning process (187,188) in order to develop improved safety measures (189): “Emphasize preventive strategies to reduce occupationally derived diseases and diseases caused by environmental and occupational toxins to enhance worker safety” (190). The teaching (191) of safety issues is very important: to increase the provision of workers' education, training and retraining, particularly in the area of occupational health and safety and environment, (192). In particular the agenda states that workers and their representatives should have access to adequate training to augment environmental awareness, ensure their safety and health, and improve their economic and social welfare. Such training should ensure that the necessary skills are available to promote sustainable livelihoods and improve the working environment. Trade unions, employers, governments, and international agencies should cooperate in assessing training needs within their respective spheres of activity. Workers and their representatives should be involved in the design and implementation of worker training programes conducted by employers and governments (193).

Training efforts must not be limited to the worker in industry. They should be related to all levels, including the management: Comprehensive national strategies should be designed to overcome the lack of qualified human resources, which is a major impediment to progress in dealing with environmental health hazards. Training should include environmental and health officials at all levels from managers to inspectors. More emphasis needs to be placed on including the subject of environmental health in the curricula of secondary schools and universities and on educating the public (194). The indifferent attitude of management toward safety is one of the primary reasons for disasters such as the Bhopal tragedy (195,196), which is independent of the level of development in a country. Therefore, not only developing countries, whose safety standards are sometimes regarded to be lower compared to those of industrialized countries, but each country should develop the knowledge and practical skills to foresee and identify environmental health hazards, and the capacity to reduce the risks (197).

Management and Risk Assessment of Toxic Chemicals. Chapter 19 of Agenda 21 involved environmentally sound management of toxic chemicals, including prevention of illegal international traffic in toxic and dangerous products and takes up the chemistry discussion of the last 30 years, and comes to a final conclusion. It states: that a substantial use of chemicals is essential to meet the social and economic goals of the world community and today's best practice demonstrates that they can be used widely in a cost-effective manner and with a high degree of safety. However, a great deal remains to be done to ensure the environmentally sound management of toxic chemicals, within the principles of sustainable development and improved quality of life for humankind. Two of the major problems, particularly in developing countries, are lack of sufficient scientific information for the assessment of risks entailed by the use of a great number of chemicals, and lack of resources for assessment of chemicals for which data are at hand. Chapter 19.1 of agenda 21 contains detailed orders for action pertaining to the sustainable handling of toxic, ie, dangerous, chemicals and calls for a worldwide harmonization of classification and labeling of chemicals by the year 2000.

Six program areas are proposed.

1. Expanding and accelerating international assessment of chemical risks.
2. Harmonization of classification and labelling of chemicals.
3. Information exchange on toxic chemicals and chemical risks.

4. Establishment of risk reduction program.
5. Strengthening of national capabilities and capacities for management of chemicals.
6. Prevention of illegal international traffic in toxic and dangerous products.

Implementation by state regulations will bring about on a national, and international level, a complete set of compound records, safety guidelines, safety data sheets, and poison characteristics of all chemicals used. These requirements were to be met by establishing a number of international forums (Intergovernmental Forum on Chemical Safety, IFCS), programs (eg, 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. As reported by Hildebrandt and Schlottmann (9), significant progress has been made, at least as far as the assessment of risks involved and regulations to be introduced were addressed.

The "Plan of Implementation" of the World Summit of Sustainable Development held in 2002 in Johannesburg renewed in Chapter 23 the commitment, as advanced in Agenda 21, to sound management of chemicals throughout their life cycle and of hazardous wastes for sustainable development as well as for the protection of human health and the environment, inter alia, aiming to achieve by 2020 that chemicals are used and produced in ways that lead to the minimization of significant adverse effects on human health and the environment, using transparent science-based risk assessment procedures and science-based risk management procedures, taking into account the precautionary approach, as set out in principle 15 of the Rio Declaration, and support developing countries in strengthening their capacity for the sound management of chemicals and hazardous wastes by providing technical and financial assistance (1,2).

Chapter 19.11 of Agenda 21 states that assessing the risks to human health and the environment hazards that a chemical may cause is a prerequisite to planning for its safe and beneficial use. Among the $\sim$100,000 chemical substances in commerce and the thousands of substances of natural origin with which human beings come into contact, many appear as pollutants and contaminants in food, commercial products, and the various environmental media. Fortunately, exposure to most chemicals (some 1500 cover $>$95% of total world production) is rather limited, as most are used in very small amounts. However, a serious problem is that even for a great number of chemicals characterized by high volume production, crucial data for risk assessment are often lacking. Within the framework of the OECD chemicals program such data are now being generated for a number of chemicals. Risk assessment is resource-intensive. It could be made cost-effective by strengthening international cooperation and better coordination, thereby making the best use of available resources and avoiding unnecessary duplication of effort (198). The testing of several hundred high production volume (HPV) chemicals (ie, chemicals produced in at least one OECD member country at a rate of $>$ 1000 tons/ year) was proposed by the year 2000. The testing of a total of some 2800 HPVs is to be conducted by 2004 by the U.S. HPV Challenge Program, including the 1000 substances taken on by the

International Chemical Council Association (ICCA). A status report has been published in 2003 (199). The OECD list comprehends, however, > 5200 HPV chemicals and the remaining should be tested within a reasonable period of time.

The many other chemicals that are produced and traded at a rate of < 1000 t/year are a problem. The present system for general industrial chemicals distinguishes between existing substances, ie, all chemicals declared to be on the market in August 1980 (USA) and September 1981 (EU), and new substances ie, those placed on the market since that date. The respective regulations in the United States, in the European Union and in Japan including a comparison of the European and the U.S. system (200) have been described in detail. Different priorities in regulations' content and structure have been identified in the hazardous substance legislation in Australia, Germany, the United Kingdom and the United States (201). According to this comparison the Australian Hazardous Substance Regulation was designated to be the basis for the harmonization process because of its comprehensive approach of identification, assessment, and control.

There are some thousands of new substances being tested. In contrast, existing substances amount to $> 90\%$ of the total volume of all substances on the market, and are not subject to the same testing requirements. The number of existing substances reported in 1981 in the European Union was 100,106. The current number of existing substances marketed in volumes > 1 ton is estimated at 30,000. This problem will be tackled by the European Union in area to protect human health and promote a nontoxic environment (202).

Nevertheless, the remaining problem will be that only those hazards will be identified one is testing for, negative consequences can befall the unaware person because of unknown hazards. History has shown that early warnings often are not noticed or even ignored deliberately when they have become "loud" (203). One can distinguish between three risk areas: normal, transition (or intermediate), and prohibited (or intolerable) (Fig. 9) (204). Management strategies have to act according to the extent of damage and of the probability that both can be low, high, or uncertain (Table 5) (205–207).

The history of chemistry has created examples typically belonging to the Pandora risk class requiring the precautionary approach. Persistent organic pollutants (POPs), chlorofluorocarbon (CFCs), are allocated to the Pandora class because of high ubiquity, persistence, and irreversibility. Implementing the precautionary principle in those cases is in compliance with principle 15 of the Rio Declaration which states that 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. In fact, there are different perceptions in the United States and Europe of when and how to apply the precautionary principle, but it seems that the application on either side predominantly does not show much difference below the line (208).

Ubiquity, persistence, and irreversibility are important catchwords for the assessment of new developments such as chemicals. The example of the nontoxic chlorofluorocarbons shows that the examination of known criteria at a given time (eg, toxicity) is not sufficient. The unknown hazard of ozone layer destruction became evident at a later date. Therefore, it appears to be irrelevant whether hazards can be identified or not. If it is not possible to recover a chemical released, management strategies have to be adjusted. Concerning chemicals, the main criteria are persistence and spatial range, which are judged by their environmental threat (209–211). Not until it can be shown that a substance and its metabolites that are going to be used without control mechanisms are comparatively well degradable in every environmental compartment examination of lower ranking criteria such as toxicity need not be started. According to Table 5, substitutes will have to be developed.

Even if degradability has been proven, a responsible care attitude includes close monitoring of the chemicals' fate in nature because transferability of test results into its behavior in nature is not necessarily given.

4.4. Economic-Ecological Efficiency. At the ecological dimension, sustainable development of the chemical industry should address two major concerns:

1. The stress on the environment and the population caused by emissions of chemical products including substances that are emitted into the environment for useful purposes, but also have negative effects (212).
2. Efficient exploitation of resources so as to create conditions, that will enable 9 billion people to live in human dignity on earth.

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 (165,213,214). Examples are the amount of reduction of SO_2 per investment volume in filters, costs per reduced kilogram of waste material, and turnover in dollar per energy consumption in kilowatt hours (kWh). Today, such environmental metric parameters have largely been implemented in chemical firms, since they are also readily applicable (214). 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, eg, three product alternatives 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 that is well known from the life-cycle assessment (eg, 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 (215). They based their report on the Swiss eco-point system and they chose the net contribution of product variants as a means of evaluation. Thus, they were able to calculate an aggregated economic-ecological efficiency value.

Only recently have efforts been undertaken by firms to take up the concept introduced by Schaltegger and Sturm, eg, the eco-efficiency analysis by BASF (216,217) and the eco-check Product excellence by Bayer (218). An interesting example of economic importance is the eco-efficiency analysis of BASF concluding that, contrary to its image, strawboard with polymeric methylene diisocyanate resins (PMDI) is more expensive and less ecoefficient than traditional particleboards based on wood and urea–formaldehyde or PMDI (219). Generally, the eco-efficiency concept can practically be applied to improve or even to develop more radically new eco-efficient products. Experiences are described, eg, from Akzo Nobel (85).

4.5. Sociopolitical 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 that are raised or lowered in the process, increased intragenerational and intergenerational 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 that must be worked out by considering the various interests arising in a discursive process that includes a high number of participants. 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 (220).

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 (166). 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.

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” (122), developed in the cooperation of Dow Chemical with the London Sustainability Agency; and “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 assess 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. BASF is going to integrate social factors into the BASF–eco-efficiency analysis. J. F. Strube pointed out: “All our activities concentrate on integrating the three dimensions of sustainability. Only the equilibrium between the economy, the environment and society guarantees the stability that is necessary to our success. This applies equally to processes within the company and to our relationships with other stakeholders" (222).

By integrating economic, environmental, and social success factors in their strategies and operations, sustainability driven companies position themselves for the future. Dow Jones Sustainability Indexes try to cover the three dimensions of sustainability using the following selected criteria:

- *Economic*: Corporate governance; strategic planning; intellectual capital management; product focus on sustainability trends; alliances/ partnerships.
- *Environmental*: Environmental performance; environmental management systems; sustainability reporting; eco-design of products; genetic engineering; animal testing.
- *Social*: Employee relations; stakeholder involvement; human rights policies; social guidelines for suppliers (223).

Apparently, the consideration of ecological and social concerns pays off in favor of the economic situation. At least according to the stock market, companies that rated highest for a set of sustainability criteria performed within a time frame of 3.5 years $>$ 60% better than the worst-rated companies (Fig. 10).

5. Organizational and Political Initiatives

Inventions and innovations of more sustainable chemical processes and products have to be realized in order to achieve sustainable development. These could be achieved relatively shortly by linking their development with development of appropriate management tools as well as with efficient environmental–political control procedures (3). Agenda 21, Chapter 30, assigns business and industry an important role in innovations for a sustainable development. The improvement of production systems through technologies and processes that utilize resources more efficiently and at the same time produce less wastes achieving more with less is an important pathway toward sustainability for business and industry (see Fig. 1; level 2). Similarly, facilitating and encouraging inventiveness, competitiveness, and voluntary initiatives are necessary for stimulating more varied, efficient and effective options (225).

For their part, governments should identify and implement an appropriate mix of economic instruments and normative measures such as laws, legislations, and standards. Business and industry will then promote the implementation of more sustainable processes and products. In particular, a systematic risk assessment of chemical products is of increasing importance (226). Development and implementation of concepts and methodologies for the internalization of environmental costs into accounting and pricing mechanisms should be emphasized (227).

One of the demands made by Agenda 21 to governments is to coordinate their efforts with international organizations and to adopt policies and regulatory and nonregulatory 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 (228). 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.

Various concepts have been developed in recent years 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 that give more importance to procedural regulations, economic incentives, self-control, and the participation of social parties.

5.1. Initiatives

The Responsible Care Program. The Responsible Care Program of the chemical industry (10) launched by Canada (1984) and the United States 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 (see Fig. 1; levels 2a, 3). This findings has also been documented in reports issued by the chemical industry. 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 (15).

BioInitiative. The Biomass Research and Development Initiative (BioInitiative) was created as a multiagency effort to coordinate and accelerate all Federal biobased fuels, power, and products research and development. The goals for the Initiative set forth by the Act include

- Improved strategic security and balance of payments.
- Healthier rural economies.
- Improved environmental quality.
- Near-zero net greenhouse gas emissions.
- Technology export.
- Sustainable resource supply.

The agencies that comprise the BioInitiative are conducting, fully or partially funding, >500 active research and development projects in the biofuels, biopower, and bioproducts areas (229). The Biomass Technical Advisory Committee presented the "Vision for Bioenergy and Biobased Products in the United States" (66).

Industrial Initiatives. Soft factors for innovations cannot be controlled directly, but organizational conditions can be created under which they can be developed more easily. In this context, industrial models and visions of many

U.S. companies, eg, 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 (230), which promotes thinking in terms of integrated synergies not only with respect to production processes (efficient use of raw materials, energy, and intermediates, reuse by-products and residual materials, minimization of transportation of substances, etc (see Fig. 1; level 2)), but also promotes relationships between BASF and its suppliers, customers, and interest groups by following a common model.

5.2. The White Paper of the European Commission. A most important example is the recent White Paper of the European Commission entitled "Strategy for a Future Chemicals Policy", it is a preliminary version of a new integrated Chemicals Guideline, that 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 (231). Experience has shown that the notification system currently in place in Europe (226) 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. The European Commission proposed that in the future existing and new substances, following the phasing in of existing substances until 2012, should be subjected to the same procedure under a *single system*. The current system for new substances should be revised to become more effective and efficient and the revised obligations should be extended to existing substances. The proposed system is called REACH, for the *R*egistration, *E*valuation and *A*uthorization of *CH*emicals. The requirements, including the testing requirements, of the REACH-system depend on the proven or suspected hazardous properties, uses, exposure, and volumes of chemicals produced or imported. All chemicals produced in >1 t/year should be registered in a central database. At higher tonnage, special attention should be given to long-term and chronic effects.

The EU Commission proposed to implement a step-by-step process to address the burden of the past and develop adequate knowledge for existing substances that industry wants to continue marketing. Given the vast number of existing substances on the market, the Commission proposes that first priority is given to substances that lead to a high exposure or cause concern by their known or suspected dangerous physical, chemical, toxicological, or ecotoxicological properties. All such substances should be tested within 5 years and subsequently be properly assessed for their impact on human health and the environment. The other existing substances should be registered at the latest by end of 2012. Responsibility to generate knowledge about chemicals should be placed on industry. Industry should also ensure that only chemicals that are safe for the intended uses are produced and/or placed on the market. The EU Commission proposes to shift responsibility to enterprises, for generating and assessing data and assessing the risks of the use of the substances (see Fig. 1; level 3). The enterprises should also provide adequate information to downstream users. Downstream users, as well as manufacturers and importers, of chemicals should be responsible for all the aspects of the safety of their products and should provide information on use and exposure for the assessments of chemicals. Producers of preparations and other downstream users will be obliged to assess the safety of their products for the part of the life cycle to which they contribute, including disposal and waste management. Substances with certain hazardous properties that give rise to very high concern will have to be given use-specific permission before they can be employed in particular uses. Evidence demonstrating that the specific use presents only a negligible risk or, in other cases, that the use is acceptable taking into account socioeconomic benefits, lack of safer chemicals for the same task and measures minimizing the exposure of consumers, workers, the general public and the environment, will be considered before granting an authorization. Uses that do not give rise to concern may be subject to general exemptions from the authorization procedure. Another important objective is to encourage the *substitution* of dangerous by less dangerous substances where suitable alternatives are available. The increased accountability of downstream users and better public information will create a strong demand for substitute chemicals that have been sufficiently tested and that are safe for the envisaged use.

The European chemical industry supports the political objectives of the White Paper, aimed at ensuring the protection of human health and the environment, as well as the competitiveness of the industry. It stresses the need to create a workable system to focus on science-based risk assessment, which is in line with the conclusions of the World Summit on Sustainable Development in Johannesburg. Sound scientific risk assessment of chemicals, a fundamental principle that has long governed chemicals regulation, must be maintained and targeted to deliver real results on areas of most concern in the shortest possible time. As the European chemical industry is a genuine success story that contributes significantly to the economy, technological innovation, and welfare of society, it needs a legislative framework that still enables it to remain competitive on the global stage (232).

The implementation of this initiative will have significant impacts that need to be taken into consideration. According to a study published by the Federation of German Industries (BDI), drastic consequences are said to be expected for employment. Depending on the scenario, between 150,000 and 2.3 million jobs could cease to exist in Germany alone due to the production loss of 1.4–20.2% (233). One problem is that not only final products are to be controlled, but also intermediates in multistage syntheses. “[The] concept would be that a producer would have to register the chemicals at every stage: all the intermediates, even if they are not the final products.” (234). This has a crucial impact on the competitiveness of European companies. If a United States or Japanese producer makes the same molecule, that producer would have to register only the final product being imported. There are substantial implications for investment (234). The costs for testing alone have been estimated between \$1.4 billion and nearly \$7 billion (235).

6. Appendix

6.1. 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.

6.2. Glossary

Base chemicals: Products of the chemical industry, manufactured globally at a scale of $>1\times10^6$ tons/year.

Chemical biotechnology: Application of biotechnology to produce chemicals.

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

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.

Integrated environmental protection: A term used for pollution-control measures that help to avoid ecologically harmful effects by selecting environmentally friendly substances, procedures, and technologies (production-integrated environmental protection) and for products that 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 indexes are ratios that can be used as benchmarks for assessing phenomena such as chemical syntheses.

Political pattern: Contrary to another approach that 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.

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

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 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 Compounds)**:** A large variety of substances that under intense solar radiation promote the formation of tropospheric ozone and hence of summer smog.

BIBLIOGRAPHY

CITED PUBLICATIONS

1. Report of the United Nations Conference on Environment and Development, Rio de Janeiro, 1992 (Rio Declaration and Agenda 21).
2. Johannesburg Declaration and Johannesburg Plan of Implementation, 2002, `http://www.un.org/esa/sustdev`
3. M. Eissen, J. O. Metzger, E. Schmidt and U. Schneidewind, *Angew. Chem.* **114**, 402 (2002); *Angew. Chem. Int. Ed. Engl.* **41**, 414 (2002).
4. J. Bongaarts and R. A. Bulatao, eds., Beyond Six Billion: Forecasting the World's Population, Panel on Population Projections, Committee on Population, National Research Council, Washington, D.C., 2000, `http://www.nationalacademies.org`
5. G. Brundtland, *Our Common Future*, Oxford University Press, Oxford, 1987.
6. E. U. von Weizäcker, A. B. Lovins, and L. Hunter Lovins, *Factor four: Doubling Wealth—Halving Resource Use*, Earthscan, London, 1997.
7. F. Schmidt-Bleek, Das MIPS-Konzept, Weniger Naturverbrauch- mehr Lebensqualität durch Faktor 10, Munich, 1998.
8. R. Bentley, `http://www.oildepletion.org/roger/about/about.htm`; BP statistical review of world energy, 2001 in review, June 2002, `http://www.bp.com/centres/energy 2002/`
9. B. U. Hildebrandt and U. Schlottmann, *Angew. Chem.* **110**, 1382 (1998); *Angew. Chem. Int. Ed. Engl.* **37**, 1316 (1998).
10. Chemical Manufacturers Association, ed., *Responsible Care: A Public Commitment*, Washington, D.C., 1998, `http://www.cmahq.com`
11. Chemistry - Europe and the future, `http://www.cefic.be/allcheme`
12. Technology Vision 2020, The U.S. Chemical Industry, 1996, `http://www.ccrhq.org/vision/index.html`
13. M. Reisch, *Chem. Eng. News* **79**(9), 10 (2001).
14. Chemical Innovation Institute, Japan—Towards a New Platform for Chemical Science and Technology, Basic Concept for Advancement of Innovation in Chemical Science and Technology in Japan, `http://www.jcii.or.jp./report/report1.htm`
15. M. S. Reisch, *Chem. Eng. News* **79**(36), 17 (2001).
16. C. Christ, ed., *Production-Integrated Environmental Protection and Waste Management in the Chemical Industry*, Wiley-VCH, Weinheim, 1999.
17. J. Wiesner and co-workers, "Production-Integrated Environmental Protection," in *Ullmann's Encyclopedia of Industrial Chemistry*, Wiley-VCH, on-line ed., 2002.
18. H. Hugl and C. Gürtler, *Chemosphere* **43**, 17 (2001).
19. K. Hungerbühler, J. Ranke, and T. Mettier, *Chemische Produkte und Prozesse, Grundkonzepte zum umweltorientierten Design*, Springer, Berlin, 1998.
20. M. Frei, Öko-effektive Produktgestaltung, Betriebswirtschaftlicher Verlag Dr. Th. Gabler GmbH, Wiesbaden, 1999.
21. P. T. Anastas and J. C. Warner, *Green Chemistry: Theory and Practice*, Oxford University Press, Oxford, 1998, p. 11.
22. P. Aldhous, *Nature (London)* **422**, 251 (2003).
23. Ref. 1, Chapt. 17.18.
24. Ref. 1, Chapt. 16.23.
25. K. Ballschmiter, *Pure Appl. Chem.* **68**, 1771 (1996).

26. K. Ballschmiter, R. Hackenberg, W. M. Jarman, and R. Looser, *Environ. Sci. Poll. Res.* **9**, 274 (2002).
27. U. S. Environmental Protection Agency, National Air Quality and Emissions Trends Report, 1999; EPA 454/R-01-004, http://www.epa.gov/air/agtrnd99
28. E. C. Moretti, *Chem. Eng. Prog.* **98**, 30 (2002).
29. Ref. , Chapt. 4.18.
30. L. Sousa, ed., *Energy and Environmental Profile of the U.S. Chemical Industry*, Office of Industrial Technologies, U.S. Department of Energy Washington D.C., 2000.
31. J. Johnson, *Chem. Eng. News* **78**(30), 31 (2000).
32. M. Patel, *Closing carbon cycles*, Proefschrift Universiteit Utrecht, 1999. http://www.library.uu.nl/digiarchief/dip/diss/1894529/inhoud.htm
33. M. Patel, E. Jochem, F. Marscheider-Weidemann, P. Radgen, and N. von Thienen, *C-Ströme: Abschätzung der Material-, Energie- und CO_2-Ströme für Modellsysteme im Zusammenhang mit dem nichtenergetischen Verbrauch, orientiert am Lebensweg – Stand und Szenarienbetrachtung, Band I: Abschätzungen für das Gesamtsystem*, Fraunhofer-Institut für Systemtechnik und Innovationsforschung, Karlsruhe, 1999.
34. Agreement on Climate Protection between the Government of the Federal Republic of Germany and German Business, 9.11., 2000. http://www.bmu.de/english/topics/climateprotection/agreement.php
35. Facts & Figures for the Chemical Industry, *Chem. Eng. News* **80**(25), 42 (2002).
36. Carbon Management: Implications for R&D in the Chemical Sciences and Technology, A Workshop Report to the Chemical Sciences Worktable, National Academy Press, Washington, D.C., 2001.
37. Ref. 1, Chapt. 4.18d.
38. J. A. Turner, *Science* **285**, 687 (1999).
39. A. Shah, P. Torres, R. Tscharner, N. Wyrsch, and H. Keppner, *Science* **285**, 692 (1999).
40. M. I. Hoffert, K. Caldeira, G. Benford, D. R. Criswell, C. Green, H. Herzog, A. K. Jain, H. S. Kheshgi, K. S. Lackner, J. S. Lewis, H. D. Lightfoot, W. Manheimer, J. C. Mankins, M. E. Mauel, L. J. Perkins, M. E. Schlesinger, T. Volk and T. M. L. Wigley, *Science* **298**, 981 (2002).
41. J. Nelson, *Science* **293**, 1059 (2001).
42. A. Hagfeldt and M. Gratzel, *Acc. Chem. Res.* **33**, 269 (2000).
43. H. Othieno, *Discov. Innovat.* **14**, 70 (2002).
44. Ref. 1, Chapt. 7.46.
45. Ref. 1, Chapt. 19.11.
46. S. Sakai, *Environ. Sci. Pollut. Res.* **7**, 225 (2000).
47. Ref. 1, Chapt. 4.18, 16.1a.
48. Ref. 1, Chapt. 16.
49. Biomass Research and Development Technical Advisory Comitee,Vision for Bioenergy & Biobased Products in The United States, 2002, http://www.bioproducts-bioenergy.gov/pdfs/BioVision_03_Web.pdf.; Biomass Research and Development Technical Advisory Comitee, *Roadmap for Biomass technologies in the United States*, 2002, http://www.bioproducts-bioenergy.gov/pdfs/FinalBiomassRoadmap.pdf
50. B. Cornils and W. A. Herrmann, eds., *Catalysis from A to Z, A Concise Encyclopedia*, Wiley-VCH, Weinheim, 2000.
51. M. Eggersdorfer, S. Warwel, and G. Wulff, eds., *Nachwachsende Rohstoffe, Perspektiven für die Chemie*, VCH, Weinheim, 1993.
52. H. Eierdanz, ed., *Perspektiven nachwachsender Rohstoffe in der Chemie*, VCH, Weinheim, 1996.

53. H. Koch, R. Beck, and H. Röper, *Starch / Stärke* **45**, 2 (1993).
54. H. Koch and H. Röper, *Starch / Stärke* **40**, 121 (1998).
55. W. von Rybinski and K. Hill, *Angew. Chem.* **100**, 1394 (1998); *Angew. Chem. Int. Ed. Engl.* **37**, 1328 (1998).
56. U. Biermann, W. Friedt, S. Lang, W. Lühs, G. Machmüller, J. O. Metzger, M. Rüsch gen. Klaas, H. J. Schäfer, and M. P. Schneider, *Angew. Chem.* **112**, 2292 (2000); *Angew. Chem. Int. Ed. Engl.* **39**, 2206 (2000).
57. U. Biermann, S. Fürmeier, and J. O. Metzger, in F. D. Gunstone and R. J. Hamilton, eds., *Oleochemical Manufacture and Applications*, Sheffield Academic Press and CRC Press, 2001, pp. 2, 266–299.
58. F. W. Lichtenthaler, *Acc. Chem. Res.* **35**, 728 (2002).
59. A. Herrmann, W. Wagner, U. N. Flessner, U. Volkhardt, and H. Komter, *Angew. Chem.* **103**, 1704 (1991); *Angew. Chem. Int. Ed. Engl.* **30**, 1641 (1991).
60. S. Warwel, P. Bavaj, M. Rüsch gen. Klaas, and B. Wolff, H. Eierdanz in Ref. 52, pp. 119–135.
61. Germ. Offen DE-A 3,902,357 A1 (Aug. 2, 1990), W. A. Herrmann, D. Marz, J. G. Kuchler, G. Weichselbaumer, and R. W. Fischer (to Hoechst AG) [*Chem. Abstr.* **114**, 143714 (1991)].
62. S. Warwel, M. Rüsch gen. Klaas, and M. Sojka, *Chem. Commun.* 1578 (1991).
63. A. Heidbreder, R. Höfer, R. Grützmacher, A. Westfechtel, and C. W. Blewett, *Fett/ Lipid* **101** (1999).
64. K. M. Draths and J. W. Frost, in P. T. Anastas and T. C. Williamson, *Green Chemistry, Designing Chemistry for the Environment*, American Chemical Society, Washington, D.C., 1996, pp. 150–177.
65. P. R. Gruber, *Commodity Polymers from Renewable Resources: Polylactic Acid*, in Ref. 36, pp. 166–184.
66. National Research Council, ed., *Biobased Industrial Products; Priorities for Research and Commercialisation* Washington, D.C., 2000.
67. A. Thayer, *Chem. Eng. News* **78**(22), 40 (2000); European estimations are given in: *European Climate Change Programme*- Long report, Brussels (2001). `http://europa.eu.int/comm/environment/climat/eccp_longreport_0106.pdf`
68. *EU-Commission*, Thematic Priority No. 6, Sustainable development, global change and ecosystems, Sustainable energy systems, Research activities having an impact in the medium to longer term, Work Program, *Version 9.September 2002, p. 11*, `europa.eu.int/comm/research`)
69. M. Wackernagel, N. B. Schulz, D. Deumling, A. C. Linares, M. Jenkins, V. Kapos, C. Monfreda, J. Loh, N. Myers, R. Norgaard, and J. Randers, *Proc. Nat. Acad. Sci. U.S.A.* **99**, 9266 (2002).
70. J.-P. Lange, *Green Chem.* **4**, 546 (2002).
71. Ref. 33, pp. 109–113.
72. H.-J. Warnecke, in U.-H. Felcht, ed., Chemie: eine reife Industrie oder weiterhin Innovationsmotor? Verlag der Universitätsbuchhandlung Blazek und Bergmann seit 1891, Frankfurt, 2000, pp. 123–151.
73. W. Kaminsky, *Chemosphere* **43**, 33 (2001).
74. J. Scheirs and W. Kaminsky, ed., *Metallocene-based polyolefins-preparation, properties and technology*, Wiley, Chichester, 2000.
75. G. Erker, *Acc. Chem. Res.* **34**, 309 (2001).
76. G. W. Coates and R. M. Waymouth, *Science* **267**, 217 (1995).
77. H. H. Brintzinger, D. Fischer, R. Mülhaupt, B. Rieger, and R. M. Waymouth, *Angew. Chem.* **107**, 1255 (1995); *Angew. Chem. Int. Ed. Engl.* **34**, 1143 (1995).
78. W. Kaminsky, *Macromol. Chem. Phys.* **197**, 3907 (1996).

79. Umweltbundesamt, VOC Emissions in Germany, http://www.umweltbundesamt.de/luft/emissionen/bericht/aktuelle-daten/schadstoffe/nmvoc/index.htm
80. J. O. Metzger, *Chemosphere* **43**, 83 (2001).
81. S. L. Wells and J. M. DeSimone, *Angew. Chem.* **113**, 534 (2001); *Angew. Chem. Int. Ed. Engl.* **40**, 518 (2001).
82. E. J. Beckman, *Environ. Sci. Technol.* **36**, 347A (2002).
83. http://www.epa.gov/greenchemistry/docs/award entries and recipients1997.pdf
84. J. V. Crivello and R. Narayan, *Chem. Mater.* **4**, 692 (1992).
85. J. Cramer and H. v. Lochem, *J. Sustainable Product Design* **1**, 171 (2001).
86. BASF, http://www.basf.de/en/corporate/sustainability/oekoeffizienz/oea_projekte/moebelklar.htm
87. P.-G. Rieger, H. M. Meier, M. Gerle, U. Vogt, T. Groth, and H.-J. Knackmuss, *J. Biotechnol.* **94**, 101 (2002).
88. S. G. Wildes, *Chem. Innov.* 23 (2001).
89. S. T. Giolando, R. A. Rapaport, R. J. Larson, T. W. Federle, M. Stalmans, and P. Masscheleyn, *Chemosphere* **30**, 1067 (1995).
90. A. Willing, *Chemosphere* **43**, 89 (2001).
91. W. Adam, *Peroxide Chemistry: Mechanistic and Preparative Aspects of Oxygen Transfer*, Wiley-VCH und DFG, Weinheim, 2000.
92. H. Arakawa, M. Aresta, J. N. Armor, M. A. Barteau, E. J. Beckman, A. T. Bell, J. E. Bercaw, C. Creutz, E. Dinjus, D. A. Dixon, K. Domen, D. L. DuBois, J. Eckert, E. Fujita, D. H. Gibson, W. A. Goddard, D. W. Goodman, J. Keller, G. J. Kubas, H. H. Kung, J. E. Lyons, L. E. Manzer, T. J. Marks, K. Morokuma, K. M. Nicholas, R. Periana, L. Que, J. Rostrup-Nielson, W. M. H. Sachtler, L. D. Schmidt, A. Sen, G. A. Somorjai, P. C. Stair, B. R. Stults, and W. Tumas, *Chem. Rev.* **101**, 953 (2001).
93. T. J. Collins, *Acc. Chem. Res.* **27**, 279 (1997).
94. M. G. Clerici and P. Ingallina, in Ref. 64, pp. 59–68.
95. T. Danciu, E. J. Beckman, D. Hancu, R. N. Cochran, R. Grey, D. M. Hajnik, and J. Jewson, *Angew. Chem.* **115**, 1172 (2003); *Angew. Chem. Int. Ed. Engl.* **42**, 1140 (2003) and references cited therein.
96. M. McCoy, *Chem. Eng. News* **79**(43), 19 (2001).
97. Anon., Firm's goal: styrene-free propylene oxide route, *Chem. Eng. News* **79**(3), 14 (2001).
98. Anon., Solvay, BASF team up on propylene oxide, *Chem. Eng. News* **80**(31), 19 (2002).
99. M. Haruta, *Catal. Today* **36**, 153 (1997).
100. Ger. Offen. DE 44,25,672 A1 (Jan. 25, 1996), U. Müller, P. Lingelbach, P. Bassler, W. Harder, E. Karsten, V. Kohl, J. Dembowski, N. Reiber, and M. Fischer (to BASF) [*Chem. Abstr.* **124**, 205,575 (1996)].
101. R. Meiers, U. Dingerdissen, and W. Hölderlich, *J. Catal.* **176**, 376 (1998).
102. W. F. Hoelderich and G. Dahlhoff, *Chem. Innov.* 29 (2001); M. Mc Coy, *Chem. Eng. News* **78**(40), 32 (2000).
103. R. Raja, G. Sankar, and J. M. Thomas, *Angew. Chem.* **112**, 2403 (2000); *Angew. Chem. Int. Ed. Engl.* **39**, 2313 (2000).
104. M. Dugal, G. Sankar, R. Raja, and J. M. Thomas, *Angew. Chem.* **112**, 2399 (2000); *Angew. Chem. Int. Ed. Engl.* **39**, 2310 (2000).
105. K. Sato, M. Aoki, and R. Noyori, *Science* **281**, 1646 (1998).
106. J. M. Thomas, R. Raja, G. Sankar, B. F. G. Johnson, and D. W. Lewis, *Chem. Eur. J.* **7**, 2973 (2001).
107. G. Dahlhoff, J. P. M. Niederer, and W. F. Hoelderich, *Catal. Rev.* **43**, 381 (2001).

108. Ref. 1, Chapt. 16.5c.
109. A. McMeekin and K. Green, *New Genet. Soc.* **21**, 101 (2002).
110. F. Berkhout, *New Genet. Soc.* **21**, 131 (2002).
111. A. M. Shelton, J. Z. Zhao, and R. T. Roush, *Annu. Rev. Entomol.* **47**, 845 (2002).
112. P. J. Dale, B. Clarke, and E. M. G. Fontes, *Nat. Biotechnol.* **20**, 567 (2002).
113. Ref. 1, Chapt. 16.38.
114. I. Gozes and S. Furman, *Curr. Pharm. Design* **9**, 483 (2003).
115. B. J. Stockman and C. Dalvit, *Prog. Nucl. Mag. Res. Sp.* **41**, 187 (2002).
116. S. Kamphausen, N. Holtge, F. Wirsching, C. Morys-Wortmann, D. Riester, R. Goetz, M. Thurk, and A. Schwienhorst, *J. Comput. Aid. Mol. Design* **16**, 551 (2002).
117. Ref. 1, Chapt. 16.13c.
118. C. Hansch, D. Hoekman, A. Leo, D. Weininger, and C. D. Selassie, *Chem. Rev.* **102**, 783 (2002).
119. J. V. de Julian-Ortiz, *Comb. Chem. High Throughput Scr.* **4**, 295 (2001).
120. Ref. 1, Chapt. 16.23h.
121. G. Mehta and V. Singh, *Chem. Soc. Rev.* **31**, 324 (2002).
122. Ref. 1, Chapt. 16.23i.
123. Ref. 1, Chapt. 16.23j.
124. W. H. Scouten and G. Petersen, New Biocatalysts, Essential Tools for a Sustainable 21st Century Chemical Industry, CCR Vision 2020 Bioprocessing/Biotechnology Work group, 1999, `http://www.ccrhq/vision.org/index.html`
125. OECD, Biotechnology for Clean Industrial Products and Processes, Paris, 1998, pp. 91–122.
126. OECD, The Application of Biotechnology to Industrial Sustainability, Paris Cedex, 2001, Report No. 52185, 2001.
127. A. Schmid, J. S. Dordick, B. Hauer, A. Kiener, M. Wubbolts, and B. Witholt, *Nature (London)* **409**, 258 (2001).
128. C. Berg, World ethanol production (2001), `http://www.distill.com/world_ethanol_production.html`
129. Renewable Fuels Association, Press Release, June 15 (2001); `http://www.ethanolrfa.org/pr010615.html`
130. L. L. Kitman, The secret history of lead, *The Nation*, March 20 (2000), `http://www.thenation.com`
131. B. Hileman, *Chem. Eng. News* **78**(16), 29 (2000).
132. *Separations Roadmap Summary*, `http:www.oit.doe.gov/chemicals/separations_ roadmap.shtml`
133. G. E. Keller II and P. F. Bryan, *Chem. Eng. Prog.* **96**, 41 (2000).
134. T. Pöpken, S. Steinigeweg, and J. Gmehling, *Ind. Eng. Chem. Res.* **40**, 1566 (2001).
135. Ref. 1, Chapt. 4.20.
136. S. Adler, S. Robinson, and J. Rogers, Sustainable Manufacturing Roadmap, in Center for Waste Reduction Technologies of the AIChE, 2002; `http://www.aiche.org/cwrt/pdf/smroadmap.pdf`
137. P. Hofstetter, J. C. Bare, J. K. Hammitt, P. A. Murphy, and G. E. Rice, *Risk Anal.* **22**, 833 (2002).
138. Ref. 137, Chapt. 5.
139. Commission of the European Community, Green Paper on Integrated Product Policy, Com. (2001).
140. F. Rubik and G. Scholl, *J. Clean. Prod.* **10**, 507 (2002).
141. R. Nuij, *J. Sustainable Product Design* **1**, 49 (2001).
142. E. Jones, D. Harrison, and J. McLaren, *J. Sustainable Product Design* **1**, 27 (2001).
143. A. Tukker, P. Eder, M. Charter, E. Haag, A. Vercalsteren, and T. Wiedmann, *J. Sustainable Product Design* **1**, 147 (2001).

144. Commitee on Industrial Environmental Performance Metrics, ed., Industrial environmental performance metrics: challenges and opportunities, National Academy of Engineering, National Research Council, National Academy Press, Washington, D.C., pp. 85–105 (1999).
145. J. A. Cano-Ruiz and G. J. McRae, *Ann. Rev. Energy Environ.* **23**, 499 (1998).
146. A. Azapagic and S. Perdan, *Trans IChemE* **78**(B), 243 (2000).
147. A. D. Curzons, D. J. C. Constable, D. N. Mortimer, and V. L. Cunningham, *Green Chem.* **3**, 1 (2001).
148. D. J. C. Constable, A. D. Curzons, and V. L. Cunningham, *Green Chem.* **4**, 521 (2002).
149. Ref. 33, pp. VIII–IX.
150. E. Heinzle and K. Hungerbühler, *Chimia* **51**, 176 (1997).
151. M. Misono, *C. R. Acad. Sci. Paris, Série IIc, Chim./Chem.* **3**, 471 (2000).
152. G. Koller, U. Fischer, and K. Hungerbühler, *Ind. Eng. Chem. Res.* **37**, 960 (2000).
153. D. Young; R. Scharp, and H. Cabezas, *Waste Management* **20**(8), 605 (2000).
154. A. A. Linninger, E. Stephanopoulos, S. A. Ali, C. Han, and G. Stephanopoulos, *Comput. Chem. Eng.* **19**, S7 (1995).
155. A. Steinbach, and R. Winkenbach, *Chem. Eng.* **4**, 94 (2000).
156. P. Lepper, D. Keller, M. Herrchen, U. Wahnschaffe, and I. Mangelsdorf, *Chemosphere* **35**(11), 2603 (1997).
157. D. M. Young and H. Cabezas, *Comput. Chem. Eng.* **23**, 1477 (1999).
158. R. A. Sheldon, *CHEMTECH* **3**, 38 (1994).
159. M. Eissen and J. O. Metzger, *Chem. Eur. J.* **8**, 3580 (2000).
160. M. Eissen and J. O. Metzger, EATOS—Environmental Assessment Tool for Organic Syntheses; the software is free available: `http://www.chemie.uni-oldenburg.de/oc/metzger`
161. M. Eissen, *Bewertung der Umweltverträglichkeit organisch-chemischer Synthesen*, Ph.D. thesis, Universität Oldenburg (2001): `http://docserver.bis.uni-oldenburg.de/publikationen/bisverlag/2002/eisbew01/eisbew01.html`
162. M. Eissen, S. Dirks, J. O. Metzger, and K. Hungerbühler, *Green Chem.* **5**(2), G25 (2003).
163. P. Frankl and F. Rubik, *Life cycle assessment in industry and business: adoption patterns, applications and implications*, Springer Verlag, Berlin, Heidelberg, 2000.
164. DIN EN ISO 14040: Environmental management, Life Cycle Assessment, Principles and Framework, DIN (Deutsches Institut für Normung), Berlin, (1997); DIN EN ISO 14041: Environmental management, Life Cycle Assessment, Inventory Analysis (draft) (1998); DIN EN ISO 14042: Environmental management, Life Cycle Assessment, Impact Assessment (draft) (1998); DIN EN ISO 14043: Environmental management, Life Cycle Assessment, Improvement Assessment (draft) (1999).
165. J. Cramer and H. v. Lochem, *J. Sustainable Product Design* **1**, 171 (2001).
166. A. Azapagic and R. Clift, *Comput. Chem. Eng.* **23**, 1509 (1999).
167. I. Boustead, Eco-profiles of the European Plastics Industry, Reports for the European Centre for Plastics in the Environment, 1993-1996, `http://Lca.apme.org/`
168. M. Stalmans, H. Berenbold, J. L. Berna, L. Cavalli, A. Dillarstone, M. Franke, F. Hirsinger, D. Janzen, K. Kosswig, D. Postlethwaite, Th. Rappert, C. Renta, D. Scharer, K.-P. Schick, W. Schul, H. Thomas, and R. Van Sloten, *Tenside Surfact. Det.* **32**, 84 (1995).
169. M. Patel, C. Bastioli, L. Marini, and E. Würdinger, in A. Steinbüchel, ed., *Biopolymers*, Vol. 10, Wiley-VCH, Germany, 2003.
170. B. Allen, *Green Chem.* **2**, G56 (2000).
171. R. Kilger, *Nachr. Chem. Tech. Lab.* **33**, 590 (1985).

172. E. Homberger, G. Reggiani, J. Sambeth, and H. K. Wipf, *Ann. Occup. Hyg.* **22**, 327 (1979).
173. Ref. 1, Chapt. 6.40.
174. Ref. 1, Chapt. 6.41.
175. Ref. 1, Chapt. 29.3d.
176. C. Kirchsteiger, *J. Loss Prevent. Proc.* **12**, 7 (1999).
177. T. Grewer and R. L. Rogers, *Thermochim. Acta* **225**, 289 (1993).
178. T. C. Ho, Y. S. Duh, and J. R. Chen, *Process Saf. Prog.* **17**, 259 (1998).
179. M. Wakakura and Y. Iiduka, *J. Loss Prevent. Proc.* **12**, 79 (1999).
180. S. J. Kang, *J. Loss Prevent. Proc.* **12**, 75 (1999).
181. Anon., *Chem. Eng. News* **77**(36), 24 (1999).
182. F. I. Khan and S. A. Abbasi, *J. Loss Prevent. Proc.* **11**, 261 (1998).
183. T. Grewer, D. J. Frurip, and B. K. Harrison, *J. Loss Prevent. Proc.* **12**, 391 (1999).
184. G. Koller, U. Fischer, and K. Hungerbühler, *Trans IChemE* **79**, 157 (2001).
185. D. W. Mosley, A. I. Ness, and D. C. Hendershot, *Chem. Eng. Prog.* **96**(11), 51 (2000).
186. G. Koller, U. Fischer, and K. Hungerbuhler, *Ind. Eng. Chem. Res.* **39**, 960 (2000).
187. T. Kletz, *An engineer's view of human error*, 3rd ed., IChemE (2001).
188. T. A. Kletz, *Process Saf. Environ.* **80**, 3 (2002).
189. R. C. Wedlich, *Chem. Eng. Prog.* **97**, 60 (2001).
190. Ref. 1, Chapt. 6.41k iii.
191. M. Eissen, A. Zogg, and K. Hungerbühler, *J. Loss Prevent. Proc.* **16**, 289 (2003).
192. Ref. 1, Chapt. 29.3e.
193. Ref. 1, Chapt. 29.12.
194. Ref. 1, Chapt. 6.45.
195. J. P. Gupta, *J. Loss Prevent. Proc.* **15**, 1 (2002).
196. R. B. Ward, *Process Saf. Environ.* **80**, 47 (2002).
197. Ref. 1, Chapt. 6.46.
198. Ref. 1, Chapt. 19.12.
199. R. A. Denison and K. Florini, Facing the Challenge, A STATUS REPORT ON THE U.S. HPV CHALLENGE PROGRAM, Environmental Defense 2003, `http://www.environmentaldefense.org/article.cfm?ContentID=2686`
200. J.-M. Devos, L. Krämer, G. H. Williamson, P. Kromarek, T. T. Smith, and M. Itoda, "Legal Aspects," *Ullmann's Encyclopedia of Industrial Chemistry*, Wiley-VCH, On line Ed., 2002.
201. G. Malich, M. Braun, P. Loullis, and C. Winder, *J. Hazard. Mater.* **62**, 143 (1998).
202. See Chapt. 5, Organizational and Political Initiatives.
203. OPOCE (Office for official publications of the european communities), Late lessons from early warnings: the precautionary principle 1896-2000, Copenhagen, 2002; `http://reports.eea.eu.int/environmental_issue_report_2001_22/en/tab_abstract_RLR`
204. German Advisory Council on Global Change (WBGU), World in Transition Strategies for Managing Global Environmental Risks Strategies for Managing Global Environmental Risks, Springer-Verlag, Berlin, 1999, p. 9; `http://www.wbgu.de/wbgu_jg1998_engl.pdf`
205. A. Klinke and O. Renn, *J. Risk Res.* **4**, 159 (2001).
206. A. Klinke and O. Renn, *Risk Anal.* **22**, 1071 (2002).
207. A. Klinke and O. Renn, *Z. Angew. Umweltforsch.* 138 (1999).
208. B. Hileman, *Chem. Eng. News* **80**(16), 24 (2002).
209. M. Scheringer and M. Berg, *Fres. Environm. Bull.* **3**, 493 (1994).
210. M. Scheringer, *Persistence and Spatial Range of Environmental Chemicals*, Wiley-VCH, Weinheim, 2002.
211. S. Böschen, D. Lenoir, and M. Scheringer, *Naturwissenschaften* **90**, 93 (2003).

212. J. Thornton, *Pandora's Poison: Chlorine, Health, and a New Environmental Strategy*, MIT Press, Cambridge, 2000.
213. Bundesumweltministerium, Umweltbundesamt, eds., *Handbuch Umweltcontrolling*, 2nd ed., Verlag Vahlen, München, 2001, pp. 597–623.
214. Ref. 213, pp. 617–619.
215. S. Schaltegger, A. Sturm, Ökologieorientierte Entscheidungen in Unternehmen: Ökologisches Rechnungswesen statt Ökobilanzierung: Notwendigkeit, Kriterien, Konzepte, 2., aktualisierte und erw. Auflage, Verlag Paul Haupt Bern Stuttgart Wien, 1994; http://www.uni-lueneburg.de/umanagement/pdf-dateien/Schaltegger-Sturm.pdf. Examples are cited in the book.
216. P. Saling, A. Kicherer, B. Dittrich-Krämer, R. Wittlinger, W. Zombik, I. Schmidt, and W. Schrott, *Int. J. Life Cycle Ass.* **7**, 203 (2002).
217. R. Landsiedel and P. Saling, *Int. J. Life Cycle Ass.* **7**, 261 (2002).
218. E. Gärtner, *Nachr. Chem.* **48**, 1357 (2000).
219. M. McCoy, *Chem. Engn. News* **79**(14), 36 (2001).
220. Ref. 1, Chapt. 23.
221. SustainAbility, Who needs it? Market Implications for Sustainable Lifestyles, London (1995).
222. BASF, Social Responsibility 2001 report, http://www.basf.de/en/corporate/sustainability/sb01/?id=-X2K-nP**bsf200
223. C. le Duc, Dow Jones Sustainability Indexes Corporate Sustainability Assessment, Methodology and Review 2002, http://www.sustainability-index.com
224. A. J. B. Zehnder and H. Wulff, *Nat. Biotechnol.* **17**, BV25 (1999).
225. Ref. 1, Chapt. 30.4.
226. Technical Guidance Document in support of Commission Directive 93/67/EEC on Risk Assessment for new notified substances, Commission Regulation (EC) No 1488/94 on Risk Assessment for existing substances and Directive 98/8/EC of the European Parliament and of the Council concerning the placing of biocidal products on the market; http://ecb.jrc.it/cgi-bin/reframer.pl?A=ECB&B=/TGD/
227. Ref. 1, Chapt. 8.
228. Ref. 1, Chapt. 19.49c.
229. USbioinitiative, http://www.bioproductsbioenergy.gov
230. *The Verbund,* www.basf.de/corporate/verbund/
231. Commission of the European Communities, White Paper on the Strategy for a future Chemicals Policy, *COM* **88**, February 27, 2001, p. 5. http://europa.eu.int/comm/environment/chemicals/whitepaper.htm
232. CEFIC, Chemicals Policy Review (2002), http://www.chemicalspolicyreview.org; http://www.chemicalspolicyreview.org/workability.html
233. P. Short, *Chem Eng News* **80**(47), 8 (2002).
234. P. L. Short, *Chem Eng News* **79**(49), 17 (2001).
235. A. M. Thayer, *Chem Eng News* **80**(50), 17 (2002).

Marco Eissen
Konrad Hungerbühler
Jürgen O. Metzger
Eberhard Schmidt
Uwe Schneidewind
Carl von Ossietzky Universität Oldenburg
Swiss Federal Institute of Technology

Table 1. **Biomass Share of Demand for Energy, Fuels, and Organic Chemicals in the United States**[a]

	2001	2010	2020	2030
	Share of the total production in %			
BioPower	3.5	4	5	5
BioFuels	0.5	4	10	20
BioProducts	5	12	18	25

[a]Ref. 49.

Table 2. **Types of Risks Generally Considered in Comparative Analyses[a]**

Type of Risks	LCA	PCRA	CRAoA/RTA	HHA[b]	BCA	CEA[c]
direct risks	x	4	X	6	7	9
upstream risks	x	4	5		7	9
downstream risks	x	4	5		7	9
accidental risks	1	4	x		7	9
occupational health risks	2	4	10		8	
indirect risks due to off-setting behavior			sometimes		8	
risks due to changes in personal disposable income			sometimes	x		
changes in risk due to structural changes/ innovations			sometimes		8	
risks due to the depletion of natural resources	x	4			7	
risks to the manmade environment	3	4			7	

[a]Ref. 137.
[b]HHA=Health−health analysis.
[c]CEA=Cost-effectiveness analysis.

1. Includes only accidents that occur frequently enough that their emissions are included in yearly statistical compilations.
2. Only included in the north of Europe. [See (137) for Reference].
3. Suggested for inclusion by Udo de Heas and co-workers [See (137) for Reference].
4. In principle included, but usually related to total residual risk in a specified region.
5. Sometimes included in a nonsystematic way and with human health focus.
6. Although not part of HHA, it is assumed that the reduction in target risks to human health is known.
7. Included if expected damages (quantified with other tools) can be monetized.
8. In principle possible; in practice rarely done.
9. Scope usually limited to human health impacts and quantification relies on other tools.
10. Usually not considered, but see Gray and Hammitt [See (137) for Reference] for the case of pesticide regulation and Viscusi and Zeckhauser [See (137) for Reference] for an approach that relies on input−output tables.

Table 3. **Characteristics of Tools for Comparative Analysis**[a]

Tools	Units of 'costs'[b]	Units of 'benefits'[c]	Decision-making principle[d]	Distributional questions
Life Cycle Assessment (LCA)	physical impacts/ damages or "ecopoints"	equal functional unit	lowest impacts	not considered
Risk Tradeoff Analysis (RTA)/ Comparative Risk Assessment of Alternatives (CRAoA)	direct health outcomes or health metrics	differences expressed as "costs" (risks)	lowest risks	considered
Programmatic Comparative Risk Assessment (PCRA)	(ordinal) ranking	not applicable	worst thing first	sometimes considered
Cost Effectiveness Analysis (CEA)	monetary	direct health outcomes or health metrics	biggest bang for the buck	mostly not considered
Benefit Cost Analysis (BCA)	monetary	monetary	maximize net benefits	mostly not considered

[a]Ref. 137.
[b]Term means all types of adverse effects (damages, risks, or monetary costs).
[c]Term means nonmonetary and monetary use values and positive effects, such as risk reduction.
[e]Term reflects the main application originally intended when the tool was developed.

Table 4. **Metrics Applied to Chemical Syntheses for the Assessment of Resource Requirement and Potential Environmental Impact**[a]

Metrics	Unit
mass index $S^{-1} = \frac{\sum \text{raw materials (kg)}}{\text{product (kg)}}$	kg/kg
environmental factor $E = \frac{\sum \text{waste (kg)}}{\text{product (kg)}}$	kg/kg
substance specific potential environmental impact $Q_{\text{input}}{}^{e}$ and $Q_{\text{output}}{}^{e}$	PEI/kg[b,c]
environmental index $EI_{\text{in}}=Q_{\text{input}} \cdot S^{-1}$	PEI/kg[b,d]
environmental index $EI_{\text{out}}=Q_{\text{output}} \cdot E$	PEI/kg[b,d]

[a] Ref. 159.
[b] PEI_potential environmental impact.
[c] Refers to 1 kg of substance.
[d] Refers to 1 kg of product.
[e] $1 \leq Q \leq 10$.

Table 5. **Management Strategies**[a]

Management	Risk class	Damage potential	Probability	Strategies for action
risk-based	Damocles	high	low	reducing disaster potential ascertaining probability increasing resilience preventing surprises emergency management
	Cyclops	high	uncertain	
precautionary	Pythia	uncertain	uncertain	implementing precautionary principle developing substitutes improving knowledge reduction and containment emergency management
	Pandora	uncertain	uncertain	
discursive	Cassandra	high	high	consciousness building confidence building introducing substitutes improving knowledge contingency management
	Medusa	low	low	

[a]Ref. 205.

Chemistry has to contribute on three levels to sustainable development:

1. Provision of chemical products that establish and ensure social and economic wealth.
2. Conservation of resources by development of
   a. more effective chemical processes,
   b. chemical products that enhance significantly the effectiveness of production processes and products in other areas,
   c. products that allow the consumer to use resources more effectively,
   d. a product design that fits into a recycling concept, and
   e. products that base on renewable resources.
3. Management of resources and substances in a safe and in an environmentally benign manner.

Fig. 1. Chemistry contributes on three levels to sustainable development.

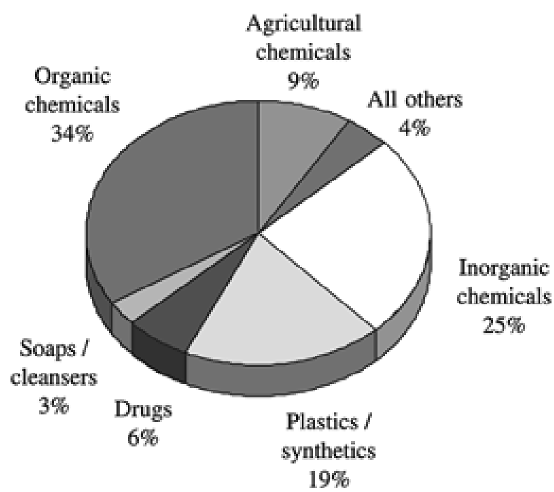


Fig. 2. Distribution of gross energy requirements (GER) of the chemical industry in the United States by product groups (30,31).

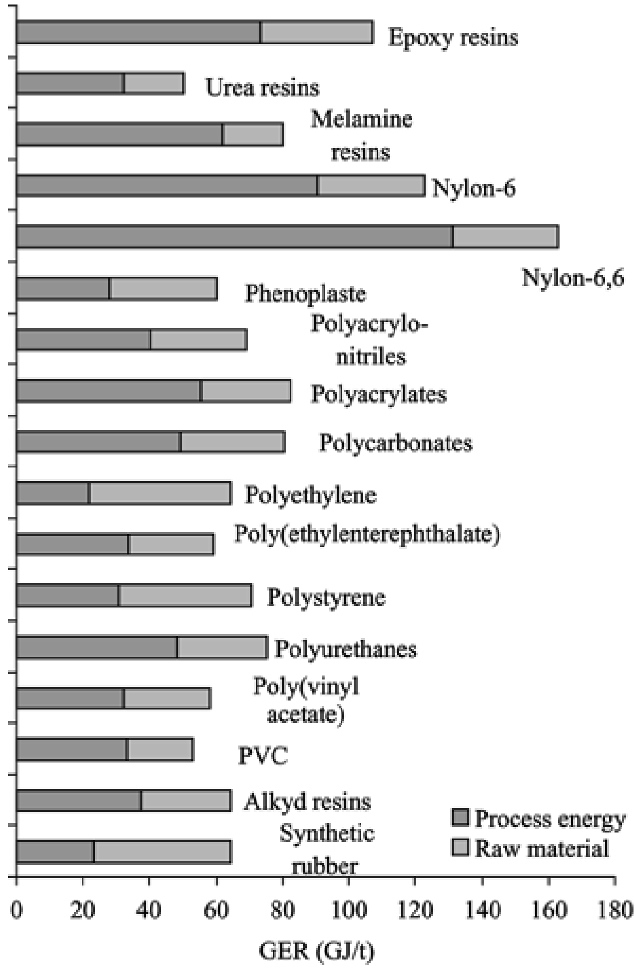


Fig. 3. Gross energy requirements for important bulk plastics (32,71).

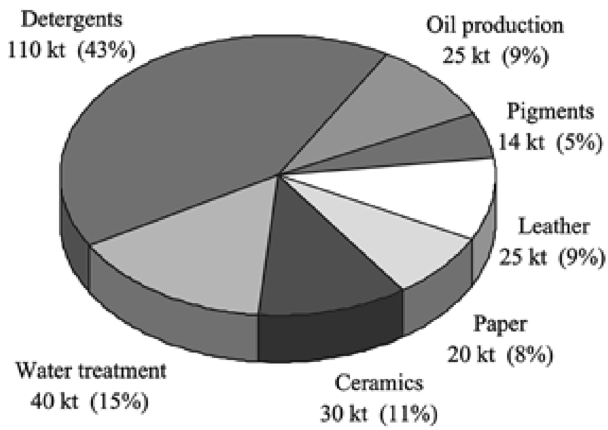


Fig. 4. Areas of application of water-soluble polycarboxylates. The worldwide market volume is 265,000 t/year (18).

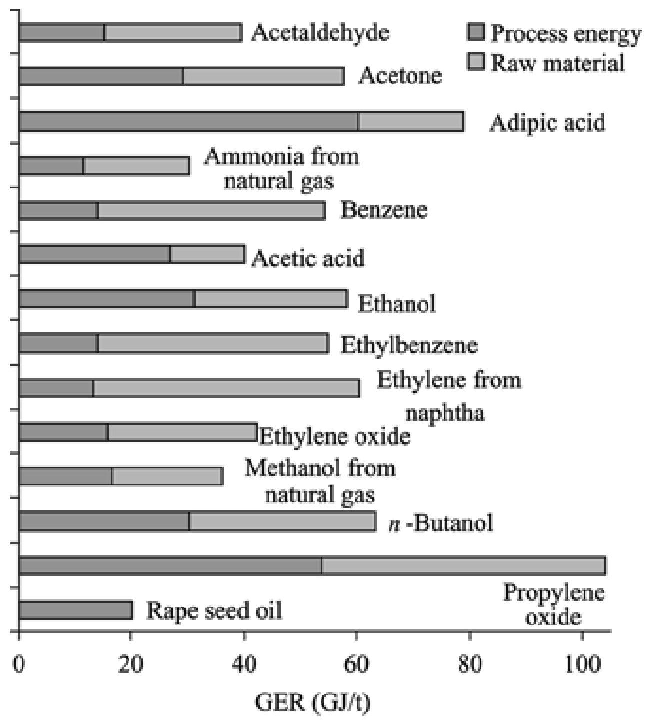


Fig. 5. Gross energy requirements for important base chemicals (32,71).

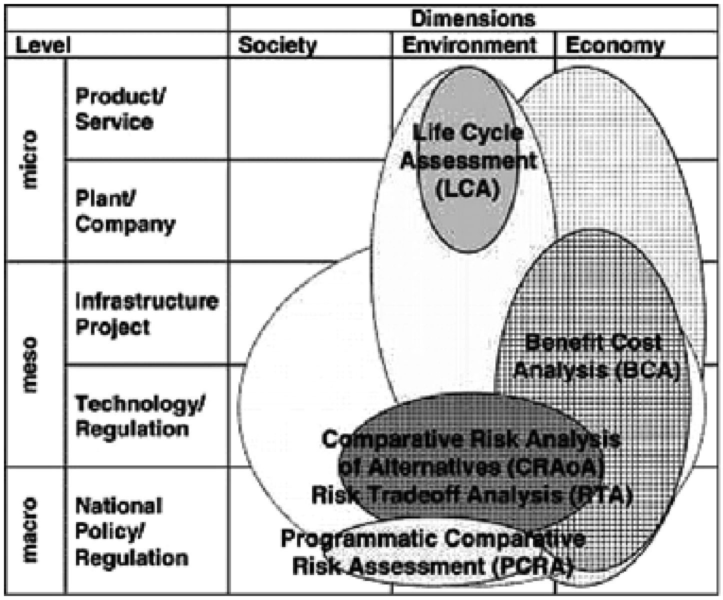


Fig. 6. Positioning of some tools for comparative analysis in the two dimensions "level of analysis" (from micro to macro) and "dimensions of analysis" (from society to economy). Black textured areas indicate the initial scope of the tools and the gray textured areas indicate more recent or potential extensions. Reproduced from Ref. 137.

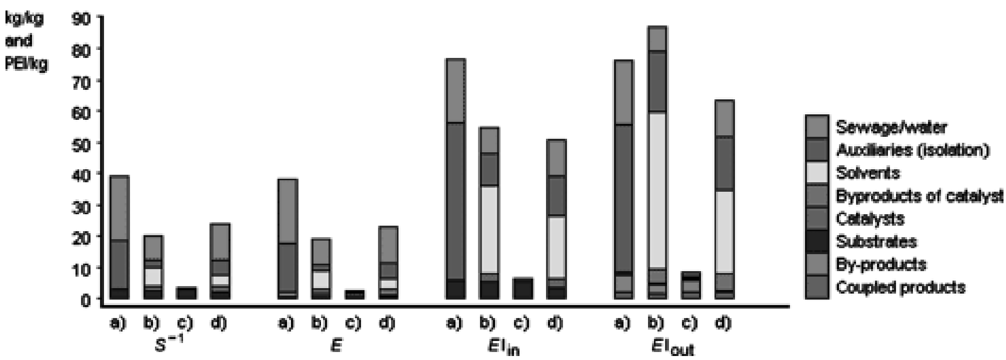


Fig. 7. Assessment of syntheses of 4-methoxyacetophenone (eq. 3) by means of the software EATOS: mass index S^{-1}, environmental factor E, environmental indices for input EI_{in} and output EI_{out} (see Table 4).

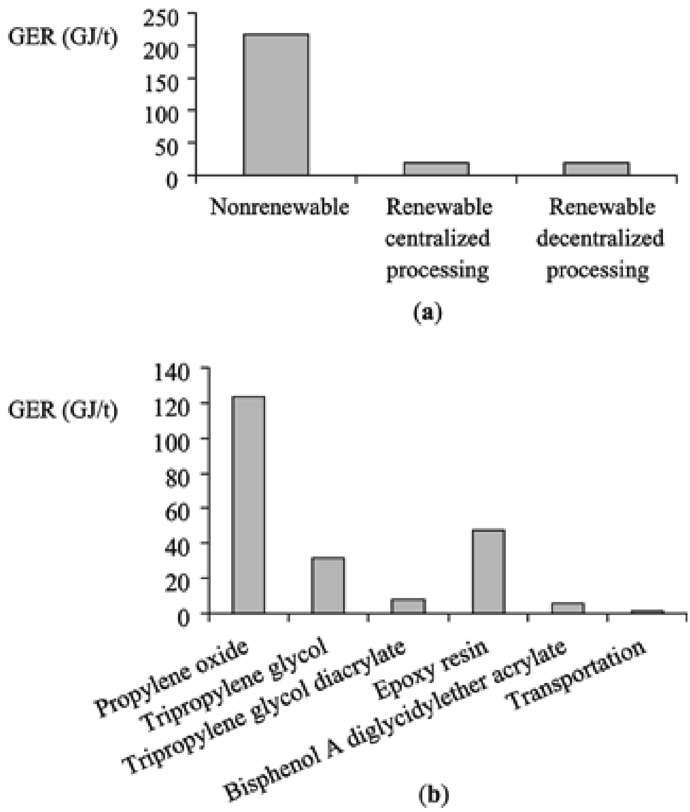


Fig. 8. Comparison of the GER for the production of (**a**) a petrochemical (tripropyleneglycol diacrylate/bisphenol A diglycidether acrylate 1:1) and of a renewable binder (linseed expoxide, centralized and decentralized processing of linseed); (**b**) the compounds of the petrochemical binder. Similar relationships exist for CO_2 and NO_x emissions (3).

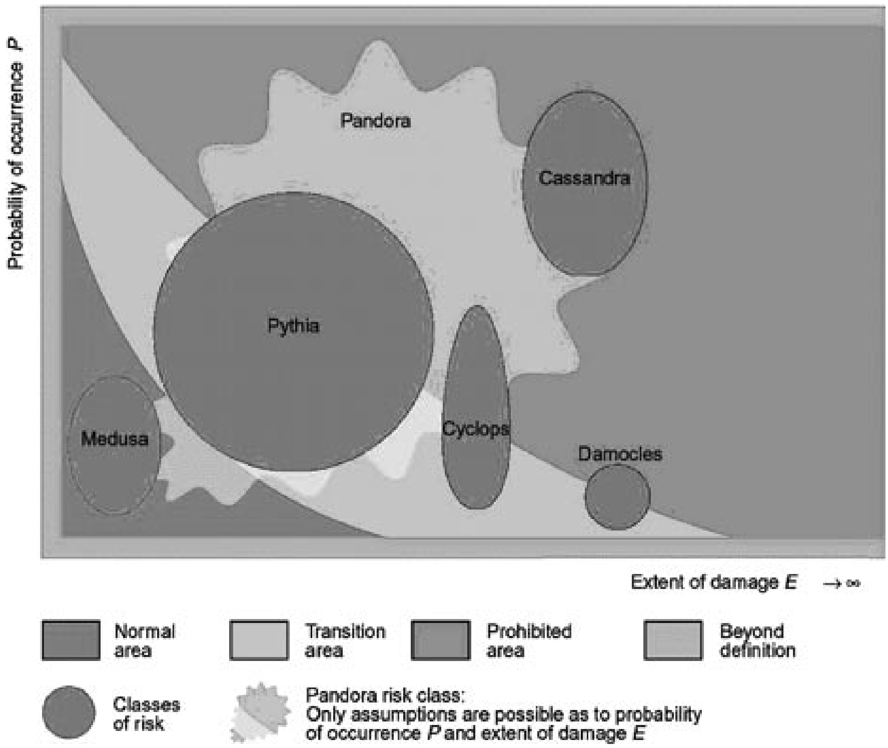


Fig. 9. Classes of risk and their location in the normal, transition, and prohibited areas. Reproduced from Ref. 204.

.

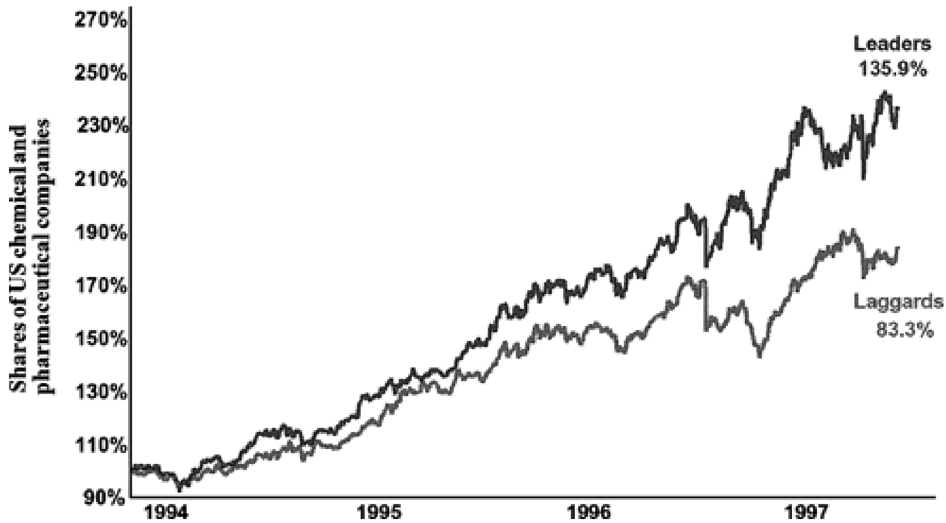


Fig. 10. Sustaining competitive advantage. Shares in the U.S. chemical and pharmaceutical companies that rated highest for a set of sustainability criteria outperformed the industry average and far outperformed the worst-rated companies. Reproduced from SAM (sustainable asset management) (224).