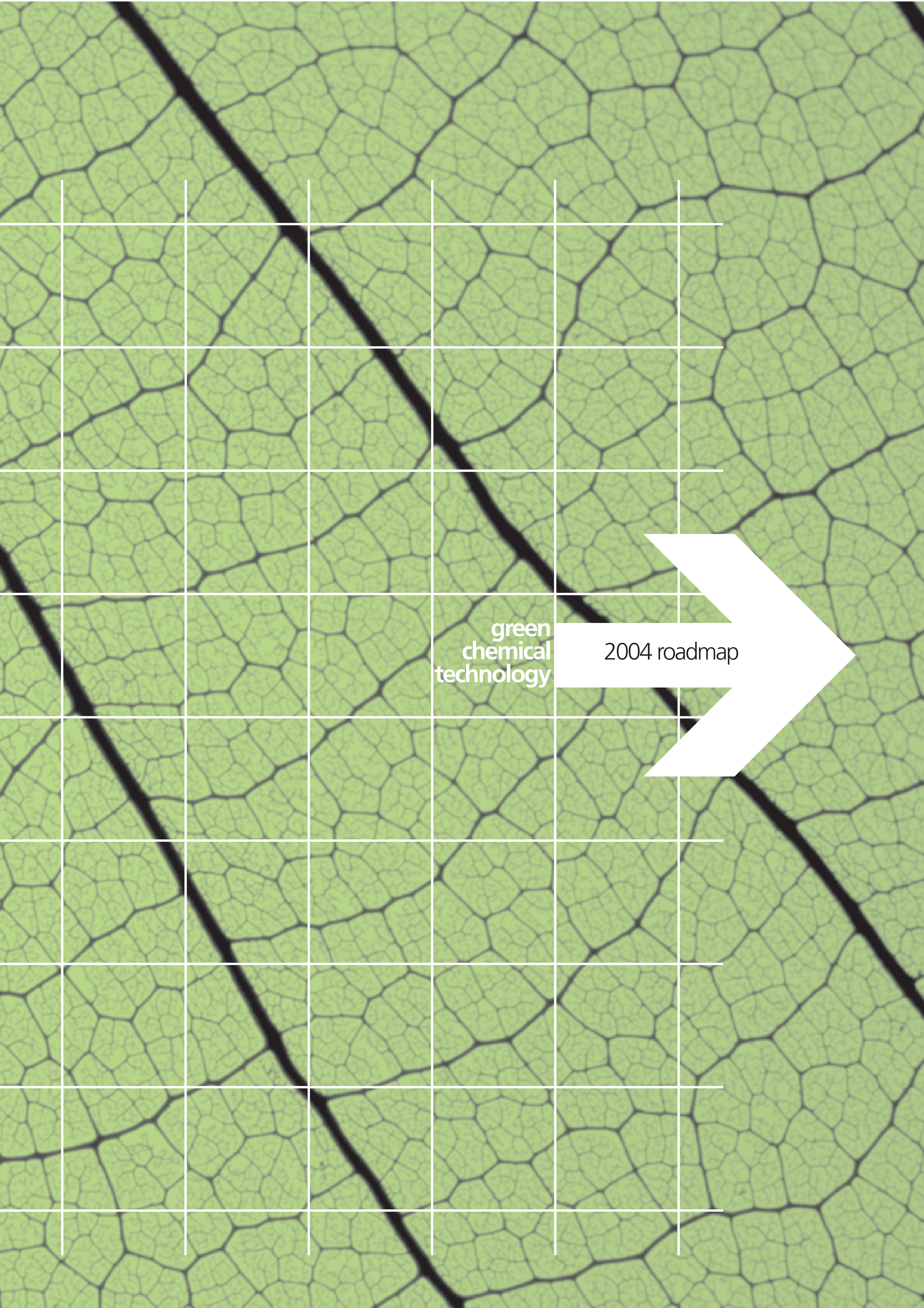


green chemical technology

2004 roadmap

The UK chemical industry is a vital part of our economy. It accounts for 2% of UK GDP and 10% of manufacturing gross value added. It is UK manufacturing's largest exporter.

Foreword

Maps are very useful things. We can try to find our way around the countryside without one, but simply following local signs may be foolhardy. For a trip from A to Z, a map is a must.

They've been around a long time. Maps started off showing just the geographical world around us – a means of sharing experience with others and remembering for ourselves. Now mapping has gone well beyond this. We map everything – including technology – without limiting ourselves to the dimensions of physical space. A technology roadmap seeks to set out how an area of technology will develop with time. We can use it to chart a way ahead. Like its geographical forebears, it helps us avoid obvious dangers and dead-ends.

Industry has already used technology roadmaps extensively to co-ordinate the activities of the whole supply chain and to provide detail in focused areas of development. This roadmap – of Green Chemical Technology – is a first edition and certainly contains errors. It will get better as more people contribute, or as those who did contribute – at the invitation of the Crystal Faraday Partnership – learn more. The fact that it exists at all is an important step for chemistry-based industries, as it lays out the current state of knowledge in a format accessible to all. Its roots are in UK experience but the contents do not recognise national boundaries, so it has global utility.

You can apply this document to your own strategic objectives and plan accordingly. Equally, the experienced Crystal team is ready to help you use it corporately or in a specific technological area. Crystal takes responsibility for the core document, but is keen to capture all the options and implications. So why not get in touch?

David Bott

Professor David Bott

The industry's products pervade our society and are critical to the quality of life currently enjoyed by the public. A thriving and sustainable chemical industry is vital to our future.

Executive summary

The UK chemical industry is a vital part of our economy. It accounts for 2% of UK GDP and 10% of manufacturing gross value added. It is UK manufacturing's largest exporter. The industry's products pervade our society and are critical to the quality of life currently enjoyed by the public. A thriving and sustainable chemical industry is vital to our future.

To secure that future the chemical industry needs to reduce its overall environmental impact. Public and political pressures plus the physical limitations of the ecosphere mean that the chemical industry must change. It cannot continue at current levels of impact.

Green chemical technology is a route to a more sustainable chemical industry. The OECD defines green chemistry as:

> "the design, manufacture, and use of environmentally benign chemical products and processes that prevent pollution, produce less hazardous waste and reduce environmental and human health risks."

Green chemical technology avoids the use of non-renewable resources, reduces energy and material use, reduces waste and lowers environmental and human health impacts.

The Crystal Faraday Partnership has been set up to be the lead organisation for the research, development, and implementation of green chemical technology and practices in the UK chemical and allied industries.

Crystal has carried out this technology roadmapping study to identify the future needs of the chemical industry for green chemical technology and to develop a strategy for their further development and implementation.

The trends and drivers affecting the chemical industry have been reviewed under five headings (the STEEP model) [see section 3]:

- **S**ocial
- **T**echnological
- **E**conomic
- **E**nvironmental
- **P**olitical

The key messages from the social trends and drivers are that the reputation of the chemical industry for environmental responsibility is low, and that consumers wish to avoid 'chemicals'. The industry must be seen to tackle these issues by developing low-risk products and low-impact manufacturing. Failure to do so could lead to the public withdrawing the industry's 'licence to operate'.

At the same time there is a growing skills gap caused by demographics and the low reputation of the industry.

Technical trends will support the move towards zero-waste and zero-impact manufacturing. Greater recycling and use of renewable raw materials will reduce unsustainable material consumption, and green product design will reduce the lifetime environmental impact and cost of products. Developments in computing capability will play an important role in creating a more sustainable chemical industry.

Economic trends are pushing the industry in highly developed countries towards added value 'effect' chemicals as bulk chemical production moves to less developed countries as part of their own industrialisation. In most sectors chemical companies will become smaller, faster and more flexible focusing on the knowledge content of products. As chemical companies are forced to account for the whole-life costs of a product, business models will change to emphasise greener products and processes, as well as product re-use, re-manufacture and recycling.

Environmental drivers will focus the industry's attention on the threat of climate change, and the need to use resources efficiently and to switch to renewable resources. The industry will need to be better at understanding the whole life-cycle impact of products, and developing routes to re-use and recycle materials.

Political trends impact the industry principally through legislation. Increasing regulation, both internationally and within the European Union, has been a powerful force for change in the chemical industry and this will continue. Green chemical technology is essential if the industry is to meet the demands of society.

There are eight areas of green chemical technology that can improve the sustainability of the chemical industry and address the issues raised by the STEEP analysis:

- Green product design – minimising environmental impact
- Feedstocks – substituting renewable for non-renewable
- Novel reactions
- Novel catalysis
- Solvents
- Process improvement
- Separation technology
- Enabling technologies

These technology areas can be used to deliver benefits in nine different areas identified as critical by the chemical industry:

- Reduce product toxicity
- Reduce environmental impact of a product
- Reduce materials needed to deliver a specific level of performance
- Reduce materials used to manufacture the product
- Reduce use of non-renewable resources
- Reduce waste and emissions during manufacture
- Reduce energy used to manufacture the product
- Reduce risk and hazard from manufacturing processes
- Reduce life-cycle cost of chemical plant

Looking at the desired benefits and the technical opportunities we can identify the key technical developments that will have the most impact on developing a sustainable chemical industry over the short to medium term [see Section 5].

The key opportunities for each technology area are summarised in the table on page 6 [see also table 5.1, page 36]. Shaded boxes are technologies ready for implementation today that need support to breakthrough to mainstream application. Unshaded boxes are technologies that need further development.

Green Product Design	**Feedstocks**	**Novel Reactions**	**Novel Catalysis**	**Solvents**	**Process Improvement**	**Separations**	**Enabling Technologies**
An integrated approach to life-cycle design	Improved routes to olefins from alkanes	Combined bio- and chemical processes	Solid supported catalysts for key reactions	Wider exploitation of closed loop systems	Exploit process synthesis	Better cost and technical data on existing membranes	Integrated approaches to modelling
Extend recycling from lubricants solvents and catalysts	Improved chemistries for recycling plastics	Which greener reagents can be implemented?	Practical enzyme reactions	Supercritical fluids	Alternative energy sources (radio frequency and microwave)	Better membranes for use in organic solvents	Fast, online chemical analysis
Develop design protocols for re-cycle and re-use	Breaking down waste streams to feedstocks	Membrane driven reactions	Chiral synthesis for key reactions	Make ionic liquids a practical tool	Spinning disc reactors	Reduce costs of affinity chromatography	Easier life-cycle analysis for comparing options
Integrate product and process design		Better ways to make small and nano-particles	Ways to develop and scale up catalytic processes	Develop solvent-free reaction schemes	Real-time measurement and control	Develop efficient bio-separations for fermentation systems	Exploiting HTE (high throughput experimentation)
Develop better understanding of downstream chemical use					New reactors – microchannel, catalytic membrane etc		Improved HTE for synthesis and performance testing Exploit small and nano-particles to reduce material intensity
Exploit small and nano-particles to reduce material intensity					Wider exploitation of process modelling		
					Higher fidelity, easier to use modelling		

As well as specific technology areas that need to be implemented or further developed, there are some general issues that need to be given priority in order to have the most impact on the sustainability of the industry. They are dealt with in Section 6.

- **Exploiting existing technologies**
  There are many technologies 'on the shelf' that we know can make a real difference to the environmental impact of the chemical industry, particularly through improving manufacturing. These technologies reduce both impact and costs and are economically self-sustaining. We need to get these off the shelf and into use.

- **Developing complete packages for industry**
  Industry needs more than a demonstration of a new technology. It needs the technology, plus the knowledge of how to implement it, plus the data to evaluate the business case. We need to create complete technology/knowledge packages for industry.

- **Demonstrating the business case**
  Green chemical technology is too often seen as a response to regulatory and public pressure, not as a better and more profitable way to operate. We need to collect, organise and communicate the evidence to industry.

- **Green product design for the chemical industry**
  The chemical industry is not as advanced as some other sectors in knowing how to design lower impact products. The industry needs to create its own capability for green product design.

From the roadmap there are some key messages for stakeholders in the development of green chemical technology and the development of a sustainable chemical industry [see Section 7].

Government
- Demonstrators are important, but we need to create complete packages for industry.
- There is a gap between universities and user industries that needs to be bridged by technology implementers/integrators.
- Be consistent and patient in funding research. This is an important process that will take time. A consistent approach is key.
- Regulation has a powerful effect on business decisions. There is a need for consistency across different regulatory regimes and for better communication of planned legislation.
- Government procurement can create market pull for environmentally superior products.

Industry
- Green chemical technology is a route to improved profitability, not just something we are forced to do.
- We must engage with the other stakeholders. Let the world know what the industry needs from green chemical technology.
- Being too conservative is a major business risk. There is real competitive advantage to be gained from green chemical technologies. It should be on the business strategy agenda.

Academia
- We need better multidisciplinary working between chemistry and chemical engineering.
- Publicise academia's capabilities. Find a showcase for technology developments.
- Industry needs to know the scope and boundaries of technology. What it can and can't do.
- Teach the workforce of thefuture about green chemical technology and how to use it.

The roadmap demonstrates that real economic, societal and environmental benefits can be obtained through greater use of existing and emerging green chemical technology. It can play an important role in developing a sustainable and thriving chemical industry in the UK.

The world changes quickly, and the technological, economic and political environment will change. This is version 1 of the roadmap, and it will be updated from time to time to reflect new developments.

1. Introduction

The Crystal Faraday Partnership has been set up to be the lead organisation for the research, development, and implementation of green chemical technology and practices in the UK chemical and allied industries.

Crystal is a knowledge transfer company for green chemical technology accessing the considerable resources of its industrial and academic participants to promote lower-cost, sustainable manufacturing, for the chemical industry. The importance of green chemical technology to the UK chemical industry was emphasised by the Foresight programme. The chemical industry is facing increasing competition and pressure on costs from environmental legislation. Crystal is helping industry to meet these challenges, and at the same time to build a research base of world-class quality in green technology.

Crystal has six key objectives:

- To be a single point of contact for green chemical technology in the UK;
- To transfer new, green technology and best practice into real application;
- To identify core research priorities matching industry's needs with innovation in universities;
- To stimulate new research or practical applications where they are needed;
- To increase awareness of best practice for sustainable products and processes;
- To train all those involved for the culture change required.

1.1 Purpose of the Roadmap

Crystal has undertaken this technology roadmapping study to develop a strategy for green chemical technology research and development based on the future needs of industry. The study has looked at the key needs of the industry out to 2025.

The technology strategy will provide key decision-makers in industry, academia and the UK government with a clear picture of the role that green chemical technology can play in developing a vibrant and sustainable chemical industry in the UK. It will identify the opportunities, the gaps and the key actions that need to be taken to make sure that the potential of green chemical technology is delivered.

The roadmap and technology strategy are living documents and will be kept constantly under review. In addition to this report a website is planned to enable all stakeholders to explore and comment on the roadmap and strategy.

1.2 The Chemical Industry

The UK chemical industry brings enormous value to the UK economy and to society at large. The products of the industry pervade all aspects of modern life, and the quality of life currently enjoyed by the public would be impossible without a thriving chemical industry.

Over many years it has provided a stream of innovations that are not only in direct use by consumers, but also underpin innovation right across the rest of industry, from engineering and electronics to food and healthcare.

The chemical industry is a large and important part of the UK manufacturing sector. Domestic production of chemicals was £34 billion in 2001. This accounts for 2% of UK GDP and 10% of manufacturing industry's gross value added. The industry is UK manufacturing's largest exporter with a trade surplus in 2001 of £5.5 billion.

In addition, the industry earned £885 million in royalty payments for exploitation of its intellectual property in other markets. Average growth rate over the period 1991-2001 was 3.1%, about the same as GDP growth and second in the manufacturing sector behind electrical and optical equipment.

Approximately 230,000 skilled people are employed in 3500 companies that range in size from fewer than 10 employees to many thousands. The industry invests £400 million per annum in training, enriching the skill base of the country, and £3.5 billion per annum on R&D activities supporting innovation of all types [1, 2].

The chemical industry was one of the first in the UK to come under the scrutiny of environmental campaigners, and has experienced progressive pressure from public opinion and government regulation.

In response it has made great strides in reducing its environmental footprint and its potential impact on human health. Waste and emissions of all types have been sharply reduced as the industry has taken steps to clean itself up.

However, despite all this good work, the chemical industry finds itself with a very poor public reputation. A recent MORI survey found that only around 20% of the public viewed the industry favourably [2]. The main reason for the low reputation was concern about the environmental and health impact of the chemical industry. A poor public reputation can have a devastating impact on an industry. It can mean:

- difficulties in raising finance;
- problems with recruiting and retaining talent;
- loss of its licence to operate – either nationally or locally;
- consumers aggressively reject the industry's products;
- a weak position in negotiations with government about the regulatory, economic and fiscal environment.

Developing a sustainable future for the UK requires the products of a strong and successful chemical industry. That industry can be in the UK or elsewhere, but it must exist. Many of the dilemmas of sustainable development can only be solved with the expertise and know-how of chemists, chemical engineers and the chemical industry. Since the chemical industry already contributes so much to the UK economy and society, it is desirable to continue to develop the chemical industry in the UK rather than simply importing our requirements from other countries.

To be able to take advantage of the economic prosperity and technical innovation of the chemical industry in the UK we need to develop and communicate a vision of a sustainable chemical industry: an industry which is valued by the public and not viewed with constant suspicion. Green chemical technology can play an important part in this transformation, continuing the work of reducing the environmental impact of the existing business, but also unleashing innovation through the application of new technologies.

For the purpose of this report the UK chemical industry is divided into four sectors each of which raises different issues of sustainability. Each will exploit green chemical technology in different ways.

- **Pharmaceuticals**

Chemicals and formulated products to prevent or treat disease conditions and to promote health. This is a large part of the UK chemical industry and dominates the total R&D investment. This is a highly innovative sector, with a constant need to find novel active ingredients and new ways to deliver drugs. There is a strong interest in reducing toxicity of actives and increasing their efficiency.

- **Consumer products**

Products sold directly to consumers, including cosmetics, cleaning products, paints and adhesives, but excluding foods and fuels. These products are sold on performance and brand. These chemical products are usually designed to be released directly into the environment, and so there is considerable interest in reducing their toxicity and overall environmental impact.

- **Specialty chemicals**

Specialty chemicals are sold on what they do, rather than what they are and what they cost. Performance is the important issue. Specialty chemicals are sold in lower volumes and at higher value than commodity chemicals. Innovation is key and the attraction for this sector is the potential of green chemical technologies to open up new areas of chemistry whilst continuing to drive down toxicity and environmental impact.

- **Commodity chemicals**

Chemicals produced in high volumes and sold on the basis of specification and price. The area of green chemical technology of most interest to this sector is improving atom efficiency by minimising resource and energy consumption, and waste.

1.3 Green Chemistry and Green Chemical Technology

The concept of Green Chemistry has been defined in a number of ways. The OECD [3] describes it as:

"the design, manufacture, and use of environmentally benign chemical products and processes that prevent pollution, produce less hazardous waste and reduce environmental and human health risks."

Green Chemistry seeks to avoid the use of depleting and non-renewable resources, reduce the matter and energy required to deliver a particular effect, reduce human health and safety issues and reduce the environmental impact of products in manufacture and use.

Some of the main themes in Green Chemistry are [4, 5]:

- atom efficiency – designing processes to maximise the amount of raw material that is converted into product;
- energy conservation – designing more energy efficient processes;
- waste minimisation – recognising that the best form of waste disposal is not to create waste in the first place;
- substitution – using safer, more environmentally benign raw materials and solvents or solvent-free processes;
- designing safer products – using molecular design and the principles of toxicity and mechanism of action to minimise the intrinsic toxicity of the product while maintaining its efficacy of function;
- developing alternative reaction conditions – designing reaction conditions that increase selectivity for the product and allow for dematerialization of the product separation process;
- use of alternative feedstocks – using feedstocks that are renewable and less toxic to human health and the environment;
- employing natural processes – using biosynthesis, biocatalysis and biotech-based chemical transformations for efficiency and selectivity.

In its activities the Crystal Faraday Partnership uses the model shown in Figure 1.1 This shows the key features and factors in green chemical technology and their interactions. This model is closely linked to the 12 Principles of Green Chemistry developed by Anastas and Warner [6] and supported by the American Chemical Society among others. The 12 Principles are:

12 Principles of Green Chemistry

❶ **Prevention –** It is better to prevent waste than to treat or clean up waste after it has been created.

❷ **Atom economy –** Synthetic methods should be designed to maximize the incorporation of all materials used in the process into the final product.

❸ **Less hazardous chemical synthesis –** Wherever practicable, synthetic methods should be designed to use and generate substances that possess little or no toxicity to human health and the environment.

❹ **Designing safer chemicals –** Chemical products should be designed to effect their desired function while minimizing their toxicity.

❺ **Safer solvents and auxiliaries –** The use of auxiliary substances (eg solvents, separation agents) should be made unnecessary wherever possible and innocuous when used.

❻ **Design for energy efficiency –** Energy requirements of chemical processes should be recognized for their environmental and economic impacts and should be minimized. If possible, synthetic methods should be conducted at ambient temperature and pressure.

❼ **Use of renewable feedstocks –** A raw material or feedstock should be renewable rather than depleting, whenever technically and economically practicable.

❽ **Reduce derivatives –** Unnecessary derivatization (use of blocking groups, protection/ deprotection, temporary modification of physical/chemical processes) should be minimized or avoided if possible, because such steps require additional reagents and can generate waste.

❾ **Catalysis –** Catalytic reagents (as selective as possible) are superior to stoichiometric reagents.

❿ **Design for degradation –** Chemical products should be designed so that at the end of their function they break down into innocuous degradation products and do not persist in the environment.

⓫ **Real-time analysis for pollution prevention –** Analytical methodologies need to be further developed to allow for real-time, in-process monitoring and control prior to the formation of hazardous substances.

⓬ **Inherently safer chemistry for accident prevention –** Substances and the form of a substance used in a chemical process should be chosen to minimize the potential for chemical accidents, including releases, explosions, and fires.

Each of the topics in the Crystal model that links to one of the 12 principles is marked with the number of the relevant principle.

Crystal has also defined key technology areas in green chemical technology:

1. Green product design

Designing products to minimise environmental impact. Including use of life-cycle analysis in the design process and design for re-cycling and re-use.

2. Feedstocks

Use of unconventional feedstocks to substitute for non-renewable or hazardous materials.

3. Novel reactions

Development of novel routes to deliver the required product functionality.

4. Novel catalysis

New types of catalyst to increase selectivity, access new areas of chemistry, and to reduce energy consumption and waste production.

5. Solvents

Solvents represent the biggest pollution risk in many current processes. New processes are required that ensure solvents are properly contained, eliminated or replaced with environmentally benign alternatives.

6. Process improvement

Novel process routes that dramatically improve atom efficiency and energy consumption.

7. Separation technology

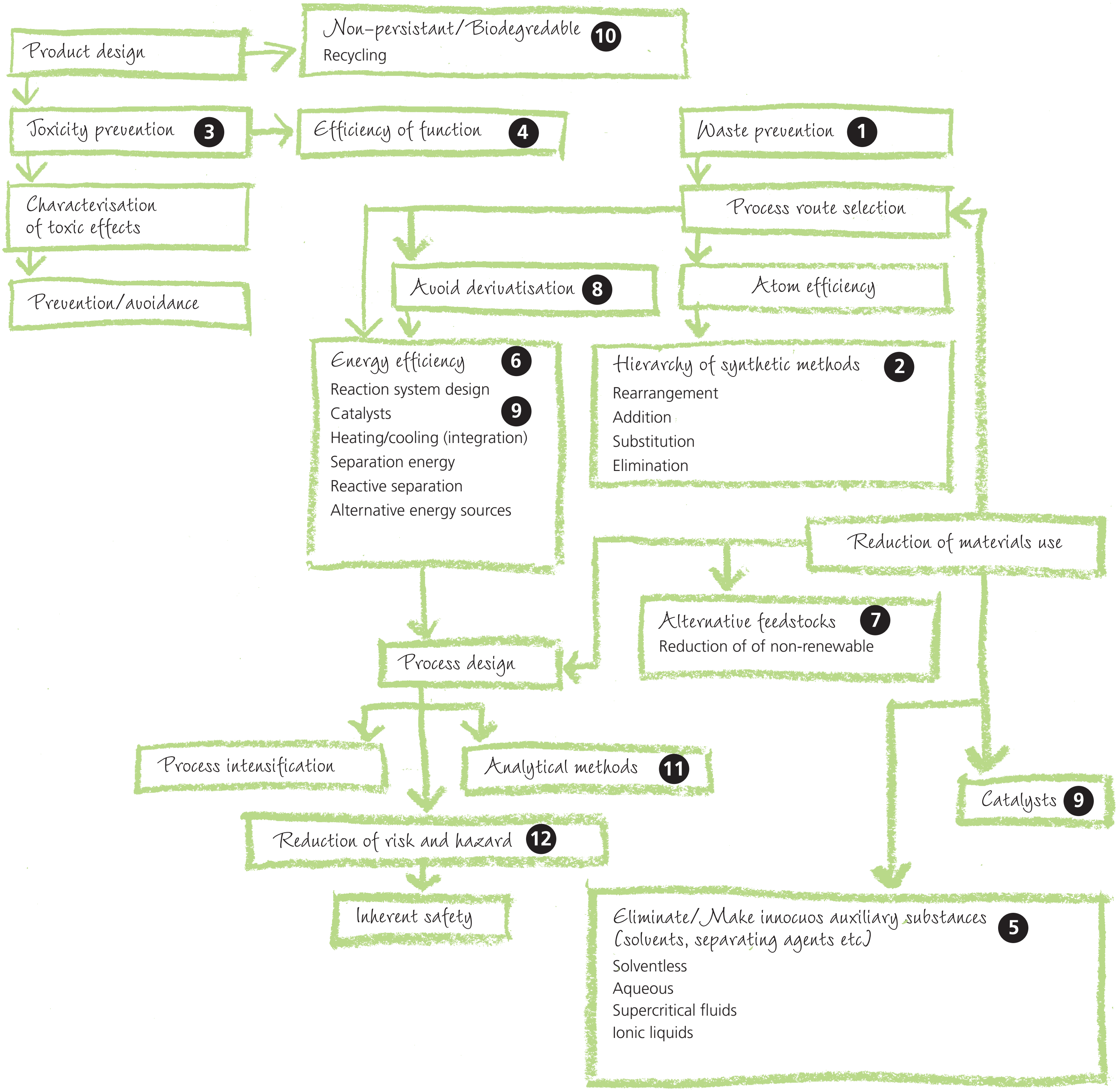
New, highly efficient and selective methods for extracting components from reaction systems.

8. Enabling technologies

A cluster of technologies that will underpin the development of Green Chemistry, including new measurement techniques, informatics and predictive modelling.

For further details of these technology clusters with examples see Appendix 2, page 51.

Figure 1.1 // Green chemical technology model



2. Development of the Roadmap

Technology roadmapping is a technique widely used in industry and public policy to support strategic decision-making. A technology roadmap is a time-line that links the development of technology to future industry or market needs.

Roadmapping can be applied at every level from industry, or industry cluster, to inform government decisions, right down to specific market sectors within a single business.

The basic process is always the same. A relevant group of experts and stakeholders is consulted to identify the key external trends and the market or business needs. These are laid out on a time-line indicating when they are expected to become important. Similarly, forecast developments in relevant technologies are also put on a time-line. The roadmap is formed by joining the two timelines through the product or service attributes that can be delivered by the technologies and the attributes required to meet the needs. The roadmap shows what steps need to be taken in technology development to meet the identified needs and can be used to make decisions about where and how to invest in technology to meet future needs (see Figure 2.1).

2.1 Process Steps

Every technology roadmapping exercise is tailored to the specific application, and this section describes the process used to create the Crystal Green Chemical Technology Roadmap.

The roadmap was developed through a series of workshops and discussions involving representatives of industry, academia and government funding agencies. A full list of participants in the study, together with their affiliation, can be found in Appendix 3 (page 51).

The steps involved in the creation of this roadmap are listed on page 13 and illustrated in Figure 2.2.

Figure 2.1 // Roadmap Overview

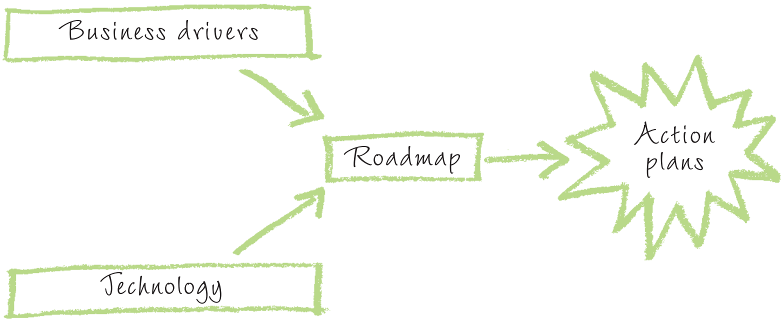
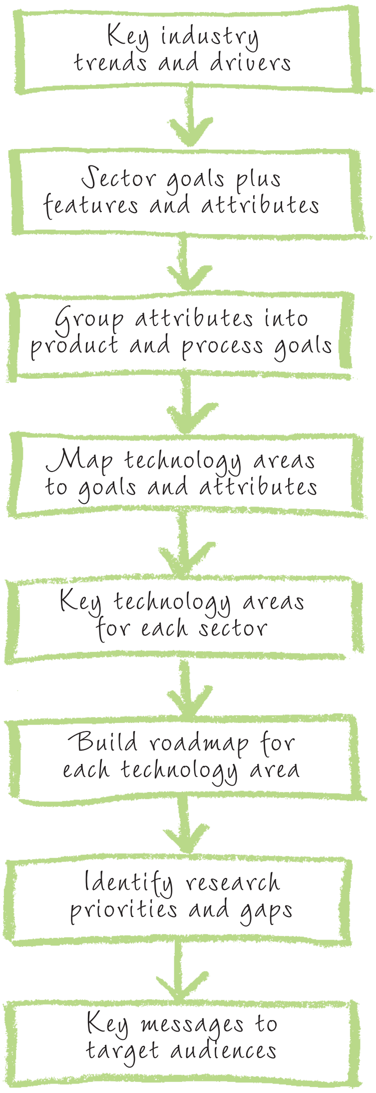


Figure 2.2 // Process Details for Green Chemical Technology Roadmap



Step 1	*Identify key industry trends and drivers* Key industry trends and drivers were identified using the STEEP model (social, technical, economic, environmental and political forces). This was done for general trends and drivers and those specific to a particular sector. Four time periods were considered: • History: 1998-2002 • Short term: 2003-2007 • Medium term: 2008-2012 • Long term: 2013-2023+
Step 2	*Identify goals plus features and attributes by sector* For each of the four sectors in the chemical industry, list the specific sustainability goals of the sector in response to the trends and drivers. Identify the features and attributes required in products, services and manufacturing processes to meet the sector goals. Group these into the three future time horizons.
Step 3	*Group the features and attributes across the sectors* Group the features and attributes identified in Step 2 into a smaller number of product and manufacturing key goals that apply across all sectors.
Step 4	*Map technology areas to key goals and attributes* For each of the eight technology areas rate the impact on the key goals and attributes.
Step 5	*Identify the key technology clusters for each sector* Using the analysis in Step 4 we can identify which technology clusters are most important for each sector of the industry.
Step 6	*Build technology roadmaps for each technology area* For each technology area now identify the technologies that can be implemented in the short term with immediate benefits, and those key technologies that need further development. Dependencies and constraints are recorded for each roadmap.
Step 7	*Identify gaps and priorities* The key technology requirements to meet future industry needs are in the roadmaps. Compare these to existing programmes to identify gaps in the existing portfolio, leading to recommendations for focus and investment.
Step 8	*Key messages for audiences* What are the key messages for the target audiences? • industry; • academia; • government.

3. Trends and Drivers

The roadmap is designed to link technological development to the external trends and drivers that will define the future of the chemical industry.

There are several different ways of classifying trends and drivers. In this study the popular 'STEEP' model has been used. STEEP stands for:

- **S**ocial
- **T**echnological
- **E**conomic
- **E**nvironmental
- **P**olitical

Social factors relate to the society and the social systems we live in. They include demographics, lifestyle aspirations and choices, patterns of work and leisure, mobility and migration, and requirements for security, shelter and food: the elements of Maslow's Hierarchy of Needs [7].

Technological factors relate to the way that broad technological development changes the industrial environment. They include changes in the way we can manipulate materials, delivery systems, packaging, transportation, communication, information systems and new business models.

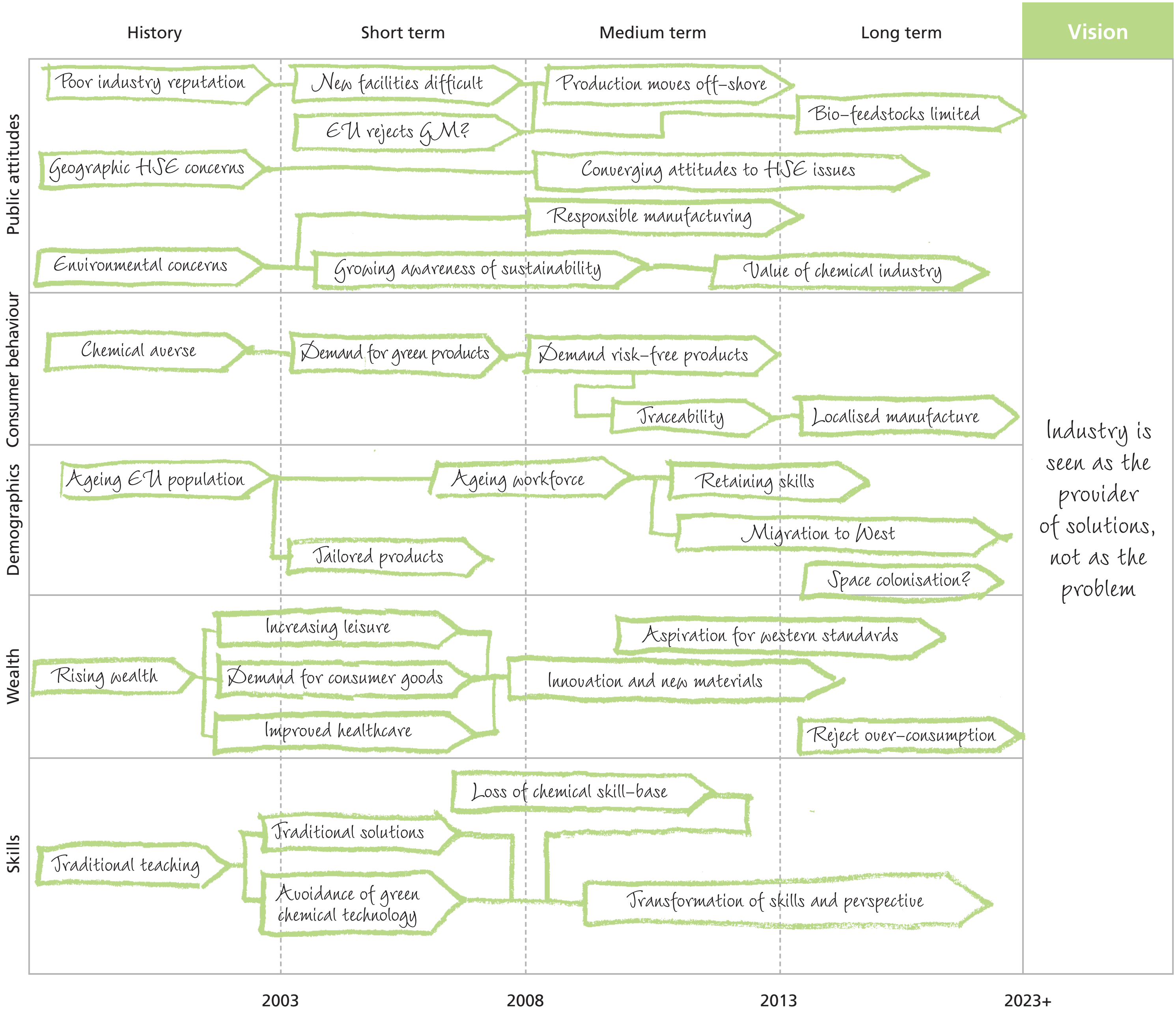
Economic factors relate to the impact of the financial systems on a global, national, corporate and personal level. Access to finance, management of risk, and exploitation of differing cost structures across the globe.

Environmental factors relate to the physical environment in which we live. They include resource consumption, waste generation and disposal, end of life disposal, environmental and health impacts and risks.

Political factors relate to the systems that govern us at the global, national and local levels. They include policy, regulation and legislation, and the political processes that drive them.

For each of the five elements there is a vision and a set of trends and drivers important to the chemical industry.

Figure 3.1 // Social Trends and Drivers



3.1 Social Trends and Drivers

Vision: Industry is seen as a provider of solutions not as the problem		
Public attitudes	The reputation of the chemical industry is already very low with less than 20% of the population in the UK having a favourable attitude. Concerns about the human and environmental impact of chemical products make the development of new facilities difficult. In the medium term this will contribute to a loss of manufacturing capacity as production moves off-shore. Rejection of genetic modification (GM) technology in the EU will also drive manufacturing to other regions. In the long term public resistance to intensive agriculture and changes in the countryside may limit the availability of bio-derived feedstocks for the chemical industry.	Public health and safety concerns are currently very different in different countries. In the medium to long term we can expect more common views to emerge at a regional and finally global level. With increasing discussion of sustainable development, there is a dawning public realisation that the chemical industry can contribute positively through greener products and processes. This awareness will increase over time and in the long term there will be a full appreciation of the value to society of a sustainable chemical industry. In the medium term the pressure of public opinion will demand 'responsible manufacturing' that is not solely profit-driven.
Consumer behaviours	Consumers are already averse to 'chemicals', and are exercising the choice arising from higher incomes to select products they are comfortable with. In the short term consumers will demand products that are more environmentally friendly whilst still delivering high performance. In the medium term they will demand 'risk-free' products.	In the medium to long term, consumers will demand complete traceability of all raw materials and ingredients in products. This may lead to a localisation of production countering the trend to move chemical production off-shore.
Demographics	A wealthy and ageing population in the EU will drive demand for new products tailored to their needs. In the medium term an ageing workforce will create significant problems in retaining expertise In the longer term there will be significant economic migration to the West as birth-rates here continue to fall.	In the very long term colonisation of space may be significant.
Wealth	Rising wealth in the developed world has increased leisure and fuelled demand for non-essential consumer goods. This has driven demand for new materials and functional ingredients to underpin innovation in many sectors. It has also driven demand for improved healthcare products. In the short and medium term this will continue, sustaining the demand for novel functionality right across the industry.	In the long term, the whole world will aspire to Western standards of living, continuing to drive innovation. In the very long term it is possible that public awareness of sustainability issues will lead the West to reject its historically profligate consumption patterns and make compromises on living standards to ensure a sustainable future.
Skills	In recent history traditional teaching of chemistry and chemical engineering has led to traditional solutions being preferred to green chemical technology. Gaining the benefits of green chemical technology will require a transformation of both perspective and skill sets among professional technologists.	In the medium term there is a threat to the chemical skill base in the UK driven by the perceived difficulty of the subject, the poor rewards, and the lack of social acceptability of the industry and profession.

3. Trends and Drivers continued

3.2 Technological Trends and Drivers

Vision: Industry is seen as a provider of solutions not as the problem	
Fast, flexible and low impact manufacture	Much current manufacture uses ‘outdated’ chemistries and process technologies. The short term sees a strong drive to exploit just-in-time manufacturing together with efficiency gains through low- or zero-capex plant optimisation. Mass customisation and the creation of small distributed production units for local production will be important in the medium term. These units will become ‘smarter’ and more flexible over time. Ultimately products will be manufactured on demand at the point of use. Following the existing trends to reduce energy and material consumption, and waste production, plants will in the long term be zero effluent and zero impact.
Green product design	Green product design is at an early stage of development. In the short to medium term products will increasingly be designed for low impact in use, for re-use and recycling. Where loss or disposal to the environment is unavoidable products will be designed for low toxicity and biodegradability.
Renewable raw materials	Today renewable raw materials cannot substitute cost-effectively for most fossil feedstocks. In the short term we will see a shift from naphtha to natural gas. In the longer term fossil hydrocarbons may be reserved for use in chemical manufacturing. There will also be a trend to use more recycled materials in manufacturing, and in the long term we may also ‘mine’ waste dumps for raw materials. Renewable raw materials will gradually emerge from their current niches to become mainstream feedstocks. In the short term this will be in high-value low-volume applications. In the longer term substitution will extend to feedstocks for the commodity sector.
Bio/nano-based materials	Rapid development in bioscience and biotechnology is opening up many new ways to provide novel functionality using low impact manufacturing and renewable raw materials. This is already having a very significant impact on the pharmaceutical sector, and will in the medium to long term have as great an impact on other sectors. Nano-structures and nanotechnology are still at the research phase. In the medium to long term they will have as much impact as biotechnology on the design and manufacture of chemical products.
Rapid product development	Speed to market is already a strong driver. Rapid product development will deliver fast development of niche products and very fast turnover of product ranges.
Computing and communication	Collapsing costs of computing and communications are powerful current drivers for the industry. Ubiquitous computing, deeply embedded computing and new networks will continue to drive new business models, molecular and materials design, exploitation of the knowledge base, and value networks with many participants.

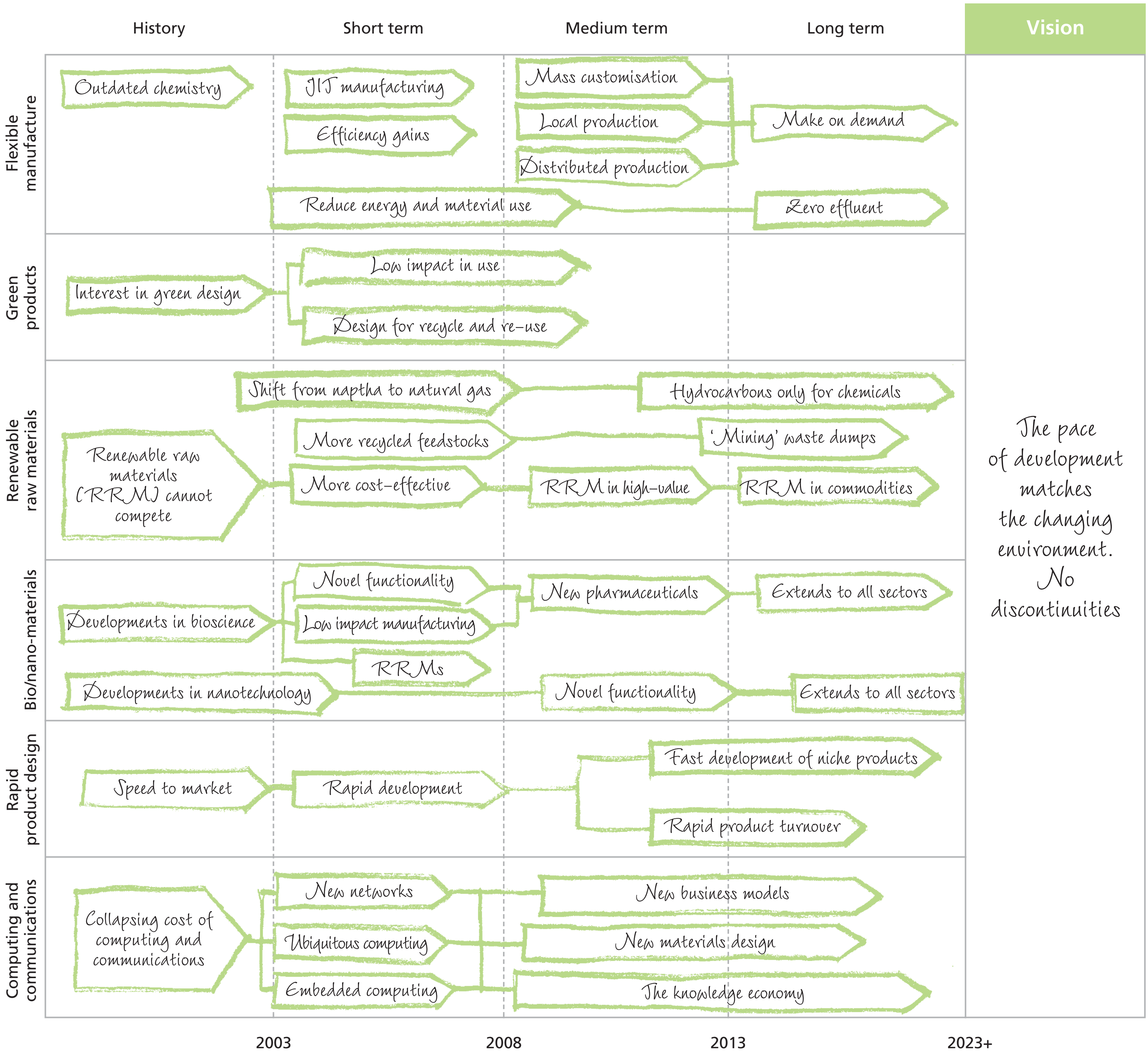


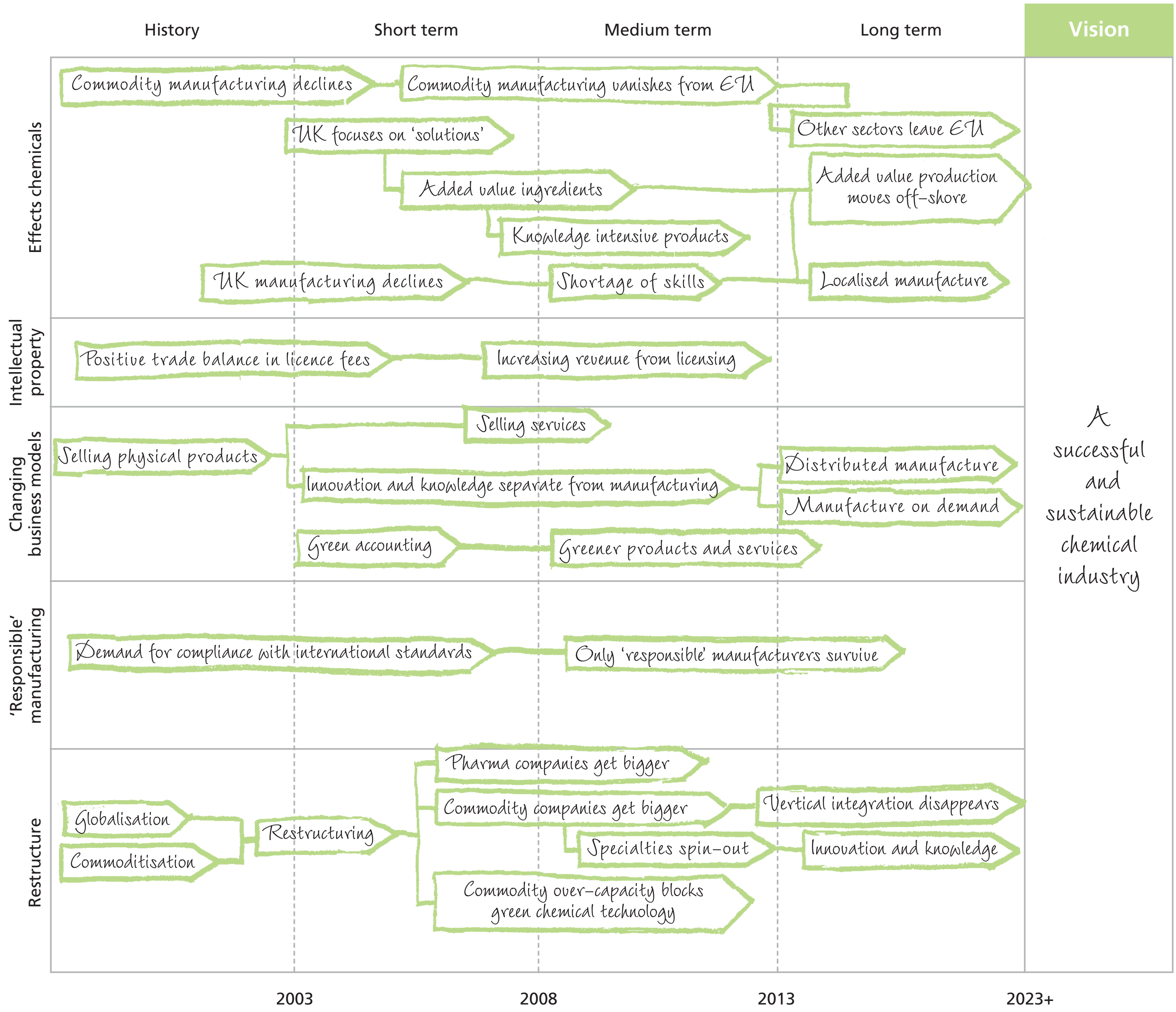
Figure 3.2 // Technological Trends and Drivers

3. Trends and Drivers continued

3.3 Economic Trends and Drivers

	Vision: A successful and sustainable chemical industry
Move to added value "effect" chemicals	The recent past has seen a lot of commodity chemical production moving off-shore. In the medium term commodity chemical production could vanish entirely from the EU. This trend will continue with most sectors feeling increasing pressure from countries with lower production costs. Later in the roadmap higher value chemical manufacturing will follow commodity production offshore. This will lead to a decline in the available pool of skilled and experienced workers. In the short to medium term the UK industry will respond by becoming increasingly focused on selling 'solutions' rather than ingredients, and developing innovative added value products. In the long term the UK chemical industry could add value through innovation, application expertise and the creation and exploitation of intellectual property. The shift is from material-intensive products to knowledge-intensive products. In the long term, development of efficient manufacture on a small scale, and pressures to reduce the environmental impact of global transportation, could lead to a regeneration of chemical manufacturing in the UK based on localised production.
Intellectual property	The UK has a positive trade balance in licensing fees for the exploitation of knowledge and technology. More can be done to develop this source of revenue.
Changing business models	The chemical industry will see a shift from selling physical products to selling services. New business models will evolve in which innovation and knowledge services are separated from manufacturing. In the longer term, further new business concepts will develop that incorporate small-scale distributed manufacturing and manufacture on demand at the point of use. Forced by legislation, accounting processes will change to internalise more of the total whole life costs of a product or service. In the medium to long term this will drive the adoption of greener products and processes.
Demands for 'responsible' manufacturing	Both industrial customers and consumers are demanding ever-higher standards from manufacturers. Already many high profile consumer goods manufacturers require that their suppliers comply with various national and international standards of environmental and sustainable performance (ISO 14000, Forest Stewardship, Marine Stewardship, Global Reporting Initiative, ILO standards on child-labour etc). In the medium term buyers will only work with suppliers with excellent green and sustainability records, and suppliers will only work with buyers with similarly high standards.
Restructuring	Recent history has seen dramatic rationalisation, re-organisation and restructuring of the global chemical industry in response to increasing commoditisation of products and globalisation of trade. Driven by the need to reduce costs and to capture larger market shares to be profitable, commodity companies will get larger. Pharmaceutical companies will continue to grow to provide the cash needed to develop new products. Specialty companies will continue to spin out of larger chemical companies in order to focus on innovation and knowledge services. In the medium term the struggle to maintain the large vertically-integrated chemical companies that dominated the 20th century will be lost. In the commodity sector over-capacity and concerns about return on investment will be a barrier to investment in green chemical technology.

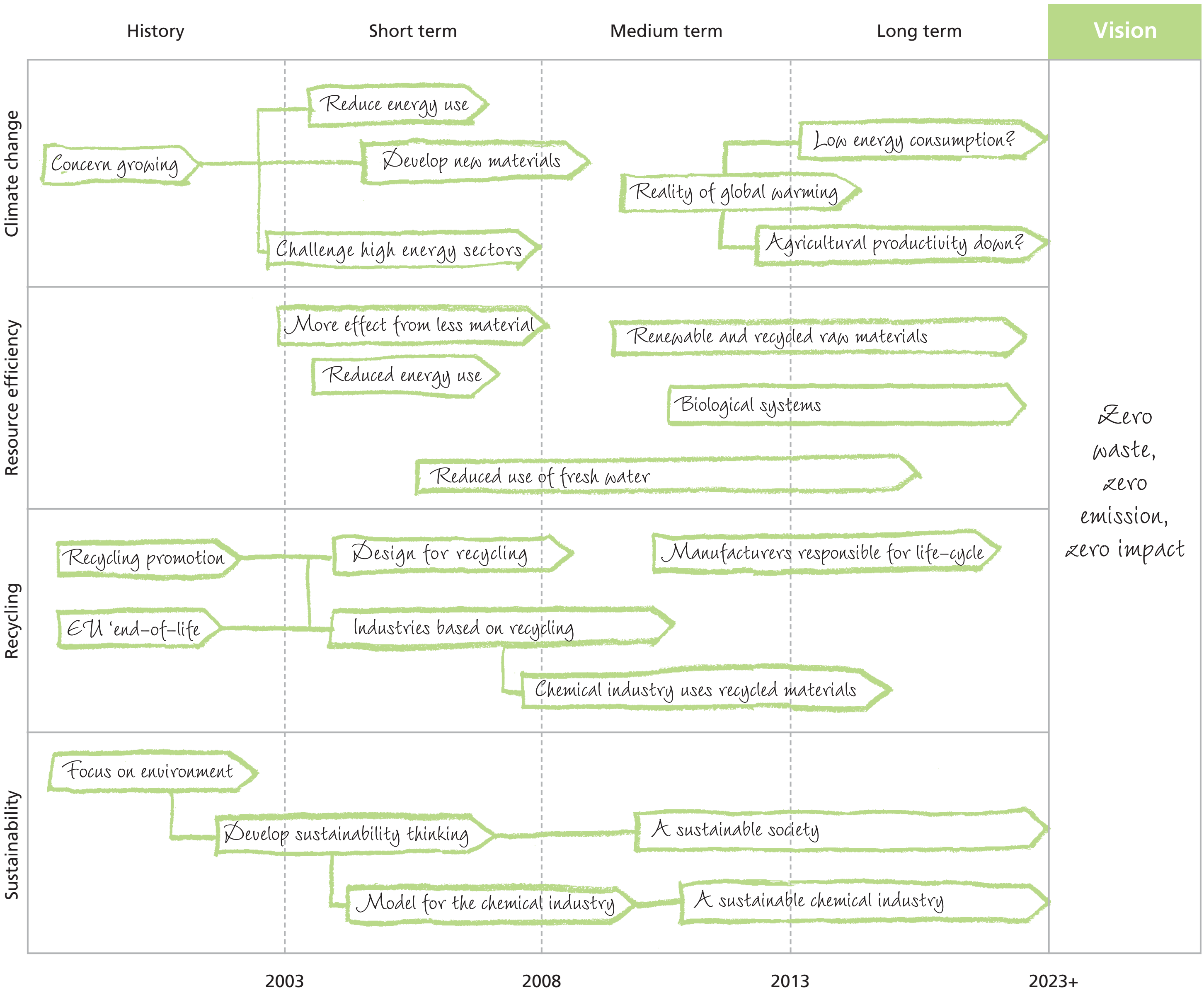
Figure 3.3 // **Economic Trends and Drivers**



3.4 Environmental Trends and Drivers

Vision: Zero waste, zero emissions, zero impact		
Climate change	Concern about climate change is growing. This will drive a growing interest in low energy and low carbon economies. This is already affecting the UK chemical industry (eg, the chlorine industry). The industry will be pressed to reduce energy consumption in manufacturing, and to develop new materials to support low energy systems and energy efficiency throughout the economy (eg, novel materials to allow lightweight vehicles to be built).	In the long term the threat of global warming will be a powerful driver for the adoption of green chemical technology as the need for low energy consumption becomes critical. However, some scenarios for climate change lead to dramatically reduced agricultural productivity in northern countries and this will affect the availability of alternative feedstocks for green chemical technology.
Resource efficiency	Social and public policy drivers are already leading to a focus on the efficiency of resource use. In the short term this will lead to demands for greater effects from less material. It will also lead to a continued focus on energy consumption in manufacture, use and disposal of products. Over the medium to long term, non-renewable resources will gradually be replaced with renewable or recycled raw materials.	In the longer term biological systems will become more important, as sources of raw materials, manufacturing systems and products. Water is a resource under particular stress around the world. Manufacturing processes and products will make progressively lower demands on fresh, clean water.
Recycling	The need to convert society from a ‘use and dispose’ model to more closed systems will lead to more focus on recycling. The various EU end-of-life disposal directives are examples.	This will lead to design for recycling; the development of industries to manage recycling and a chemical industry capable of exploiting recycled materials. Ultimately manufacturers will take responsibility for the entire life-cycle of their products.
Sustainability	Despite being a fashionable word, the concept of sustainability is at a relatively early stage of development in society and the industry. Most of the focus to date has been on environmental performance.	In the medium to long term there will be a drive for a sustainable chemical industry in a sustainable society.

Figure 3.4 // **Environmental Trends and Drivers**



3.5 Political Trends and Drivers

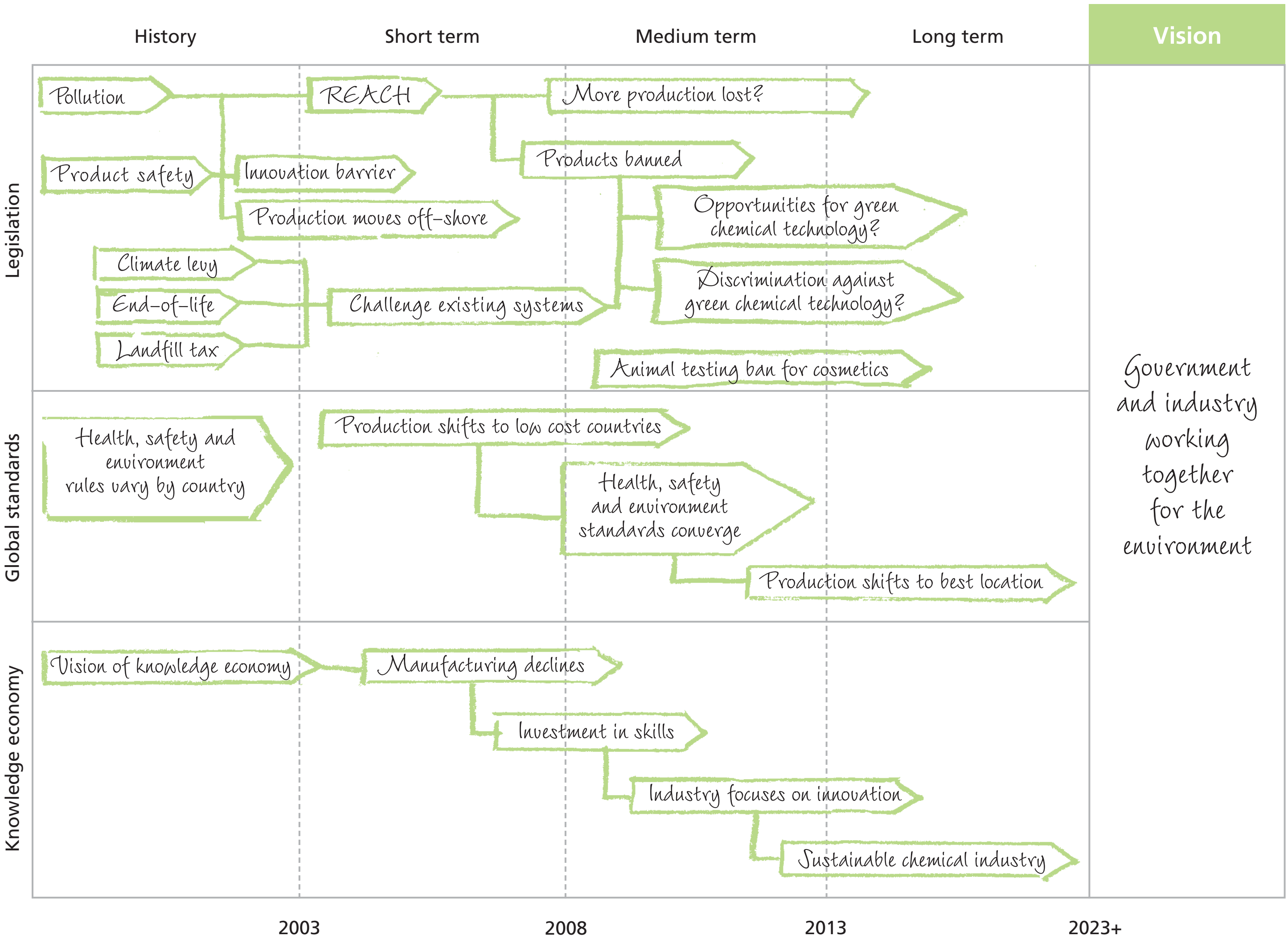
Vision: Government and industry working together for the environment	
Legislation	The industry has experienced strong pressures from product registration and pollution regulations. Many in the industry consider that this has acted as a barrier to innovation and has driven some manufacturing off-shore. This trend will continue with the EU's REACH process. In the short to medium term this could have a profound effect on the viability of the industry in the EU. One outcome will be to drive more manufacturing outside the EU borders. In the medium term many current products will be banned providing an opportunity for green substitutes. However, the cost of registration may prevent these options being brought to market. Similarly, the climate change levy, landfill taxes, end-of-life disposal regulations etc will all challenge existing industry practices providing an opening for green chemical technology. However, regulations developed to protect human health and the environment can also accidentally discriminate against many forms of green chemical technology unless these are explicitly considered during drafting. The EU ban on animal testing for cosmetics and cosmetic ingredients will come into force between 2009 and 2013. This will bring substantial change to the consumer and specialty sectors.
Globalisation of environmental standards	Existing environmental and health and safety legislation varies significantly from country to country. As a result production of many chemicals is able to move location with a significant reduction of cost of production. In the short term this will lead to production moving to areas with a more favourable regulatory environment. World Trade Organisation rules will then allow the products to be sold in the most attractive markets. In the medium to long term, public demand around the world will lead to convergence of environmental and health and safety standards. The driver to move production to more favourable regulatory regimes will vanish.
The 'knowledge economy'	Current focus in the UK and the West generally on the 'knowledge economy' leads to acceptance of a declining manufacturing sector. In the medium to long term, successful investment by the UK government in skills will allow the chemical industry to achieve the levels of innovation required to create a successful, sustainable industry with a radically smaller manufacturing component.

3.5.1 Future legislation

Regulation and legislation is a powerful driver for green chemical technology, particularly in Europe. By questioning existing materials, technologies and practices, regulation opens up the market to alternative solutions and creates gaps where green chemical technology can be profitably exploited. The EU has had a sustained interest, through its political institutions, in regulating to protect the environment and human and animal health.

Although the chemical industry is global, the key legislation affecting the operation of the chemical industry within the EU is EU regulation. This is widely seen as being the most demanding environmental protection and product safety legislation in the world. International organisations such as the United Nations Environment Programme *(www.unep.org)* and the Organisation for Economic Cooperation and Development *(www.oecd.org)* are playing an important role in bringing together developments around the world through initiatives such as the Stockholm Convention on persistent organic pollutants (POPs), and the Co-operation on the Investigation of Existing Chemicals respectively. However, the dominant forces for the European chemical industry come from EU legislation. Appendix 1 (page 49) summarises the future EU legislation of relevance as a driver for green chemical technology.

Figure 3.5 // Political Trends and Drivers



4. Features, Attributes and Technolo

In this section the specific sustainability goals in response to the trends and drivers are described for each of the four sectors in the chemical industry. These are coupled with the features and attributes in products, services and manufacturing processes required to meet the sector goals.

The different sector goals can be combined to give a global set of green chemistry goals. We review the impact of each of the technology areas on the global green chemistry goals and identify the critical technology areas for each industry sector.

4.1. Features and Attributes by Sector

4.1.1 Pharmaceutical Sector Goals

In the short term there is an urgent need to reduce trace toxic metals from pharmaceutical preparations.

There is also a need to reduce toxicity in pharmaceutical actives. Current litigation arising from side effects runs at approximately $1 billion pa. The goal is effectively to eliminate this over the timescale of the roadmap.

At present the pharmaceutical sector is less atom efficient than other sectors. Currently the ratio of waste to useful product is 100-200:1. The goal is to reduce waste by at least an order of magnitude, and at the same time to develop therapies that reduce effective doses from about 100mg to the µg range.

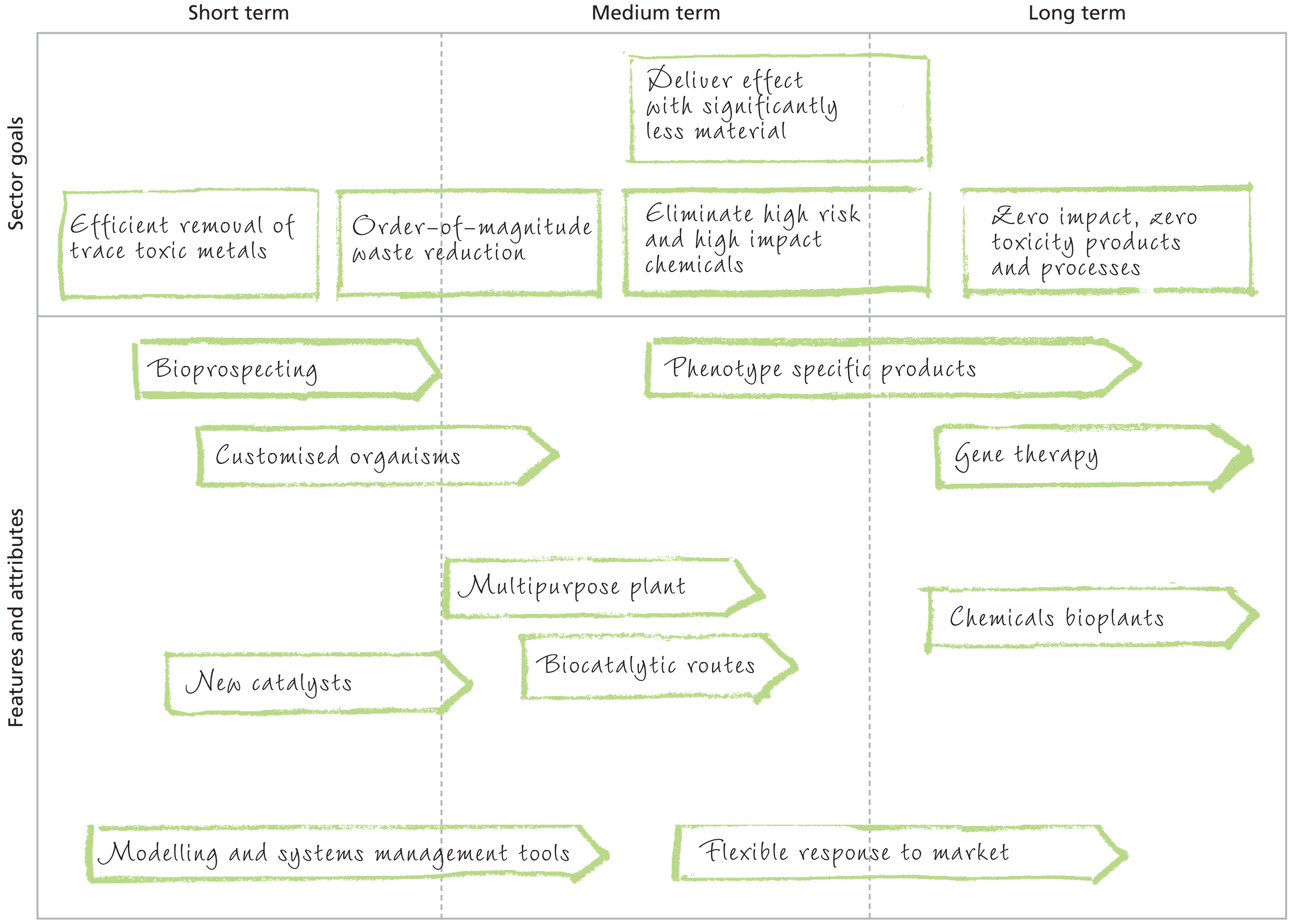
In the medium term legislation and public opinion will drive progressive replacement of high-risk chemicals and those with high environmental impact. This will focus on process intermediates and waste, as many pharmaceutical actives are toxic. In the long term this will lead to interest in zero impact and zero toxicity products and processes.

4.1.2 Pharmaceutical Features and Attributes

The features and attributes required to achieve the pharmaceuticals sector goals can be grouped into three clusters: new therapies, manufacturing and information technology.

New therapies	In the short term, there will be a continued focus on discovering pharmaceutically active molecules in nature. An increasing number of these will be manufactured by fermentation or cell culture using genetically modified organisms. Over time there will be an increased focus on tailoring therapies to the specific needs of an individual. Initially focusing on the individual phenotype, and ultimately leading to gene therapy. As micro- and nano-materials become commercially available they offer a route to enhanced carrying, targeting and delivery for pharmaceuticals. They are likely to be mass efficient, have lower environmental impact, and will be one route to lower effective doses.
Manufacturing	New catalysts for organic synthesis will help to reduce waste and eliminate hazardous materials. Biocatalysts will become progressively more important, leading to the development of chemical bioplants. Because of the low volume and high value of pharmaceutical actives, this sector will drive the development of new types of small, highly efficient, multipurpose plants.
Information technology	Informatics (particularly bio informatics) and modelling are essential for the identification and development of new pharmaceutical actives. The sector has led the introduction and development of advanced informatics and modelling for the identification and development of active molecules. This will continue due to the high value of a successful new therapeutic molecule.

Figure 4.1 // Sector Goals, Features and Attributes – Pharmaceuticals



4.1.3 Consumer Sector Goals

The key goals for this sector are to:

- continuously offer new solutions to customers that improve the perceived quality of life;
- reduce product risk and environmental impact.

The short term will be dominated by a search for novel product functionality. New functionality will come both from new ingredients and from new blends of existing ingredients as manufacturers try to avoid the problems of registering novel molecules. There will be increasing interest in delivering functionality from physical structure rather than from molecular chemistry as another route to avoiding registration and safety testing. This will encompass new carrier and delivery systems, with improved targeting and triggered release.

In the medium term there will be a focus on delivering products that support health and a healthy lifestyle in response to key consumer trends. These products will become more sophisticated and tailored over time until intelligent products are created that are either tailored to the specific individual, or are capable of adjusting performance to the needs of an individual.

In the medium term, legislation and public opinion will drive progressive replacement of high-risk chemicals and those with high environmental impact. This will promote an interest in renewable feedstocks and will ultimately evolve into zero impact and zero toxicity products and processes.

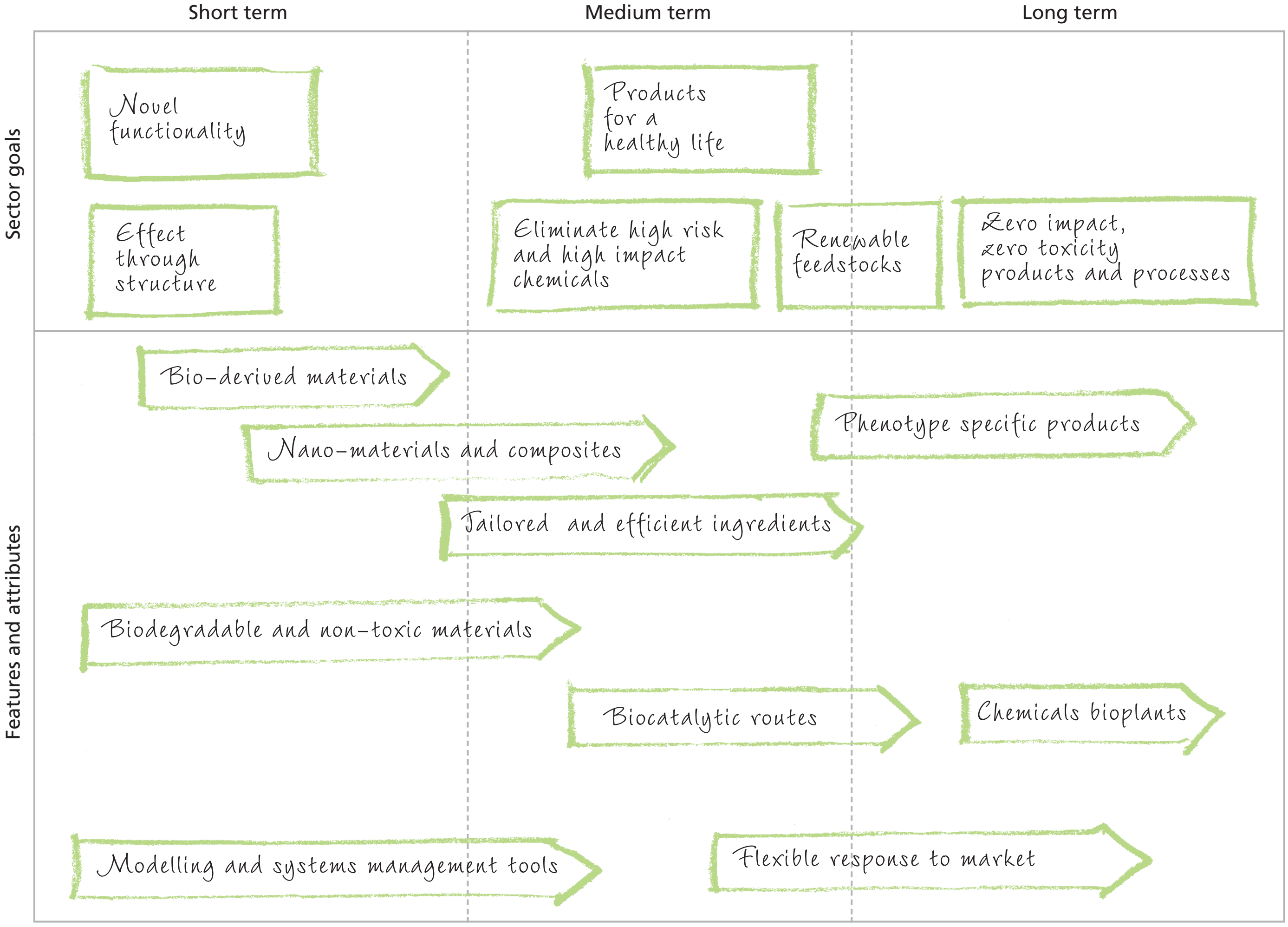
Over the period of the roadmap, the sector is targeting a reduction of several orders of magnitude in the toxicity and sensitisation potential of ingredients, and a four-fold reduction in energy consumption and waste production during manufacture.

4.1.4 Consumer Features and Attributes

The features and attributes required to achieve the consumer sector goals can be grouped into three clusters: new materials, manufacturing and information technology.

New materials	The ability to deliver new functionality to the consumer depends on the availability of new materials, or new ways of using existing materials. Increased regulatory pressure for materials that are released into the environment will increase the consumer sector interest in materials that are more biodegradable and less toxic. This has been an ongoing trend in the industry for many years, and will continue. The sector is a big user of packaging, and there is particular interest in both recycling and alternative materials that can reduce environmental impact. At the same time there is increasing interest in bio-derived materials, either used as extracted or after chemical or biological conversion. These materials offer the combination of new functionality and reduced environmental impact. In some cases, they already offer a sustainable route to delivering functionality to the consumer.	As micro- and nano-materials and composites become commercially available they will find uses in consumer products. They offer a route to enhanced carrying, targeting and delivery, and will probably be a key feature of intelligent products. They are also likely to be mass efficient, and to have lower environmental impact. Consumer chemical manufacturers are also interested in ingredients that are very specific in their effects and mass efficient. This will enable manufacturers to produce products that are highly effective, but produce fewer unintended effects, and a lower environmental impact. In the longer term we are likely to see all of these features come together in intelligent products that are specific to an individual's phenotype. Perhaps the ultimate in mass customisation.
Manufacturing	Most of the developments in manufacturing processes for consumer goods will be found in the commodity and specialty sectors that supply ingredients. However, new biocatalytic processes will be an important feature	of delivering bio-derived ingredients for intelligent products.These processes will evolve into complete chemical bio-plants that will allow flexible manufacturing on a local scale.
Information technology	Informatics and advanced modelling tools will play a key role in the design of consumer products. These tools will not only be used to design or select new materials, but also to design complete formulated products. Modelling of product performance in use will help to design efficient and low impact products.	Modelling and informatics will help to predict environmental impact and will be part of life cycle analysis. It will also help to eliminate animal testing.

Figure 4.2 // Sector Goals, Features and Attributes – Consumer



4.1.5 Specialties Sector Goals

The specialties sector shares many goals with the consumer sector.

The short-term focus will be on delivering functionality from physical structure rather than from molecular chemistry. Effect from structure provides a route to novel functionality as well as being a response to tighter regulations on the registration of new chemicals. In the medium to long term the goal is to deliver an effect with significantly less material.

In the medium term legislation and public opinion will drive progressive replacement of high-risk chemicals and those with high environmental impact. This will promote an interest in renewable feedstocks and will ultimately evolve into zero impact and zero toxicity products and processes.

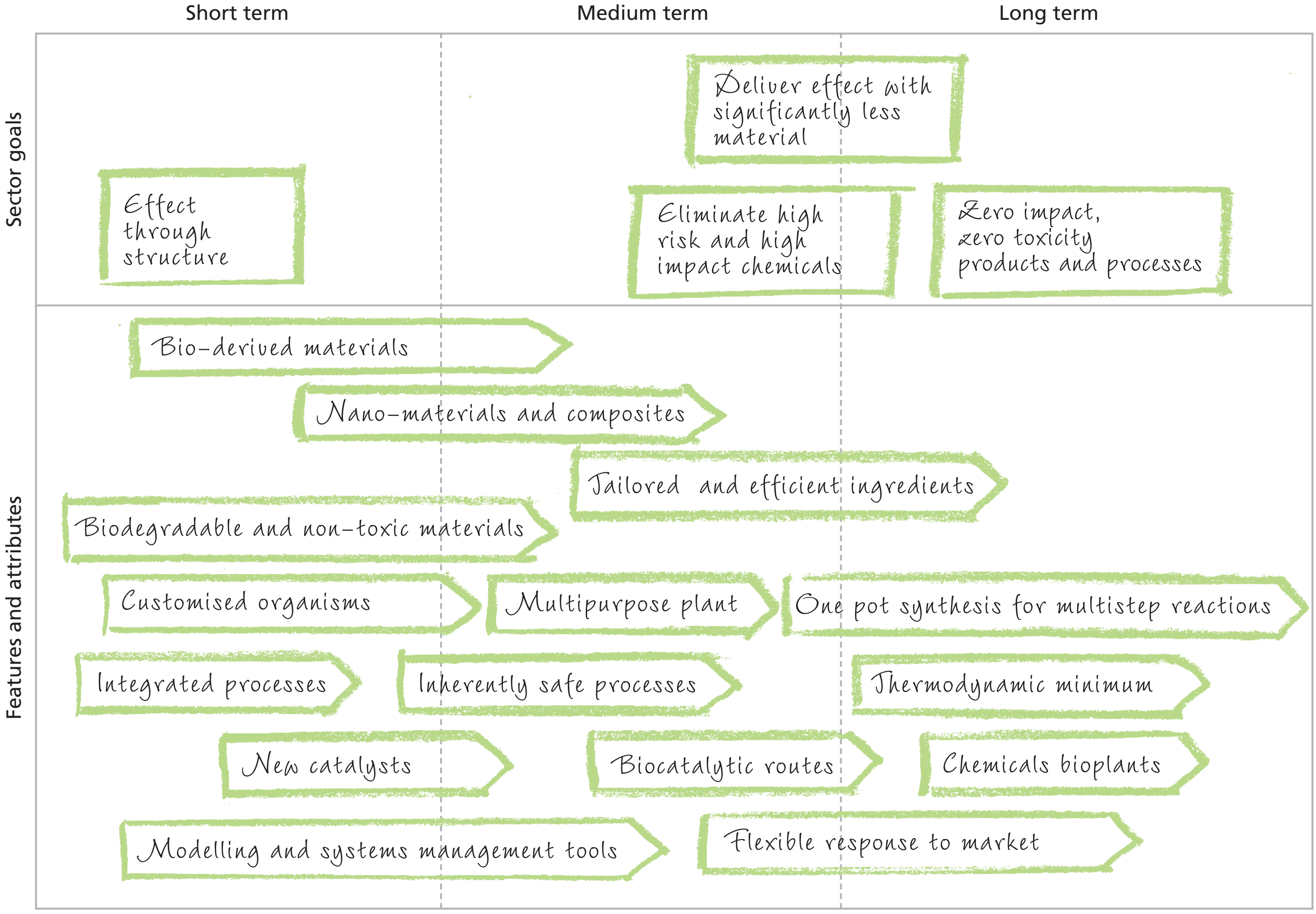
Over the period of the roadmap the specialties sector intends to halve the material needed in a product to deliver a particular effect, and to halve material usage, waste and emissions in manufacturing.

4.1.6 Specialties Features and Attributes

The features and attributes required to achieve the specialties sector goals can be grouped into three clusters: new materials, manufacturing and information technology.

New materials	Many applications of specialties lead to release into the environment. Increased regulatory pressure will lead to interest in materials that are more biodegradable and less toxic. This has been an ongoing trend in the industry for many years, and will continue. At the same time there is increasing interest in bio-derived materials, either used as extracted or after chemical or biological conversion. These materials offer the combination of new functionality and reduced environmental impact.	Micro and nano-materials and composites are attractive in specialties. They offer novel functionality that will benefit the users of specialty chemicals. They are likely to be mass efficient, and to have lower environmental impact. Specialty chemical manufacturers are interested in ingredients that are very specific in their effects and mass efficient. This will enable manufacturers to produce products that are highly effective, but produce fewer unintended effects and a lower environmental impact.
Manufacturing	In the short term we will see greater integration of processes enabling them to run closer to the optimum. Novel catalysts for conventional synthesis will help to improve process performance. We will also see the increasing use of tailored organisms in fermentation to deliver specific molecules. In the medium term there will be a focus on developing new processes that are inherently safe. We will also develop new biocatalytic processes across all sectors.	In the long term we will see the development of processes that approach the thermodynamic minimum, and chemical bioplants that can replace conventional petrochemical and refinery complexes. A particular focus for specialties will be the development of highly flexible multipurpose plants that can efficiently produce a diversity of low volume chemicals. There will also be the development of multistep synthesis in a single reactor to increase the flexibility of plant.
Information technology	Informatics and modelling will play an increasingly important role in the specialties sector. Avoidance of	animal testing, prediction of properties and environmental impact will all draw on these tools.

Figure 4.3 // Sector Goals, Features and Attributes – Specialties



4.1.7 Commodities Sector Goals

The key goals for this sector are to increase process efficiency and to drive towards the goal of zero environmental impact and zero toxicity products and processes.

In the short term the focus will be on improving the overall efficiency of processes and beginning to redesign products for efficient low-impact manufacture and easy recycling.

In the medium term attention will switch to replacing existing feedstocks with suitable alternatives. The goal is to reduce feedstock costs and to replace petrochemical feedstocks with renewable or recycled raw materials.

Legislation and public opinion will drive progressive replacement of high-risk chemicals and those with a high environmental impact.

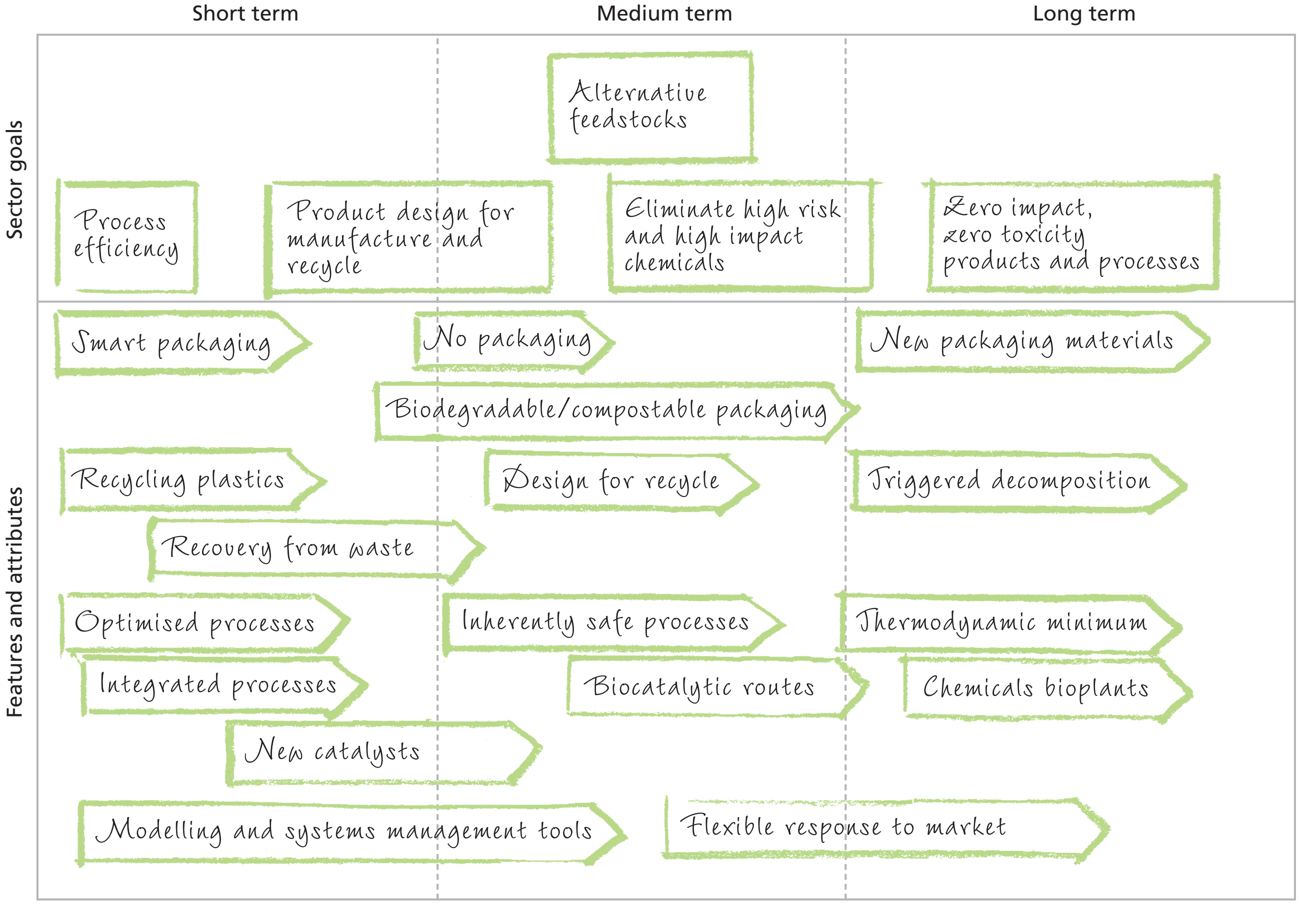
In the long term the goal is to achieve factories and process chemistries with no environmental impact and to produce products with zero toxicity and zero impact.

4.1.8 Commodities Features and Attributes

The features and attributes to achieve these goals can be grouped into four clusters:
recycling, packaging, process improvement and information technology.

Recycling	Recycling will become increasingly important. In the short term we need to improve techniques for chemically recycling plastics, and increase the amount of raw materials that can be recovered from waste. In the medium term we will need to design products for recycling as well as for manufacture.	In the longer term, the sector will require materials that allow triggered decomposition, providing full biodegradability or compostability once the product has been disposed of, but not before.
Packaging	Packaging is an important issue for the commodity sector. Both for use in the supply chain and as a product. In the medium to long term there is a need for 'smart' or intelligent packaging that is part of the product value and not a waste problem. Products will be developed that require no packaging at all, or where the packaging is an integral part of the product, as with some hot-melt adhesives where the protective wrapping dissolves in the adhesive as it melts.	There will also be a move to biodegradable or compostable packaging where disposal of the packaging is unavoidable. New packaging materials will be developed in the longer term that can be disposed of without significant environmental impact, or can be used to support smart and integral packaging solutions.
Process improvement	In the commodity sector a lot of the required features and attributes focus around process development and improvement. In the short term we will see a continued optimisation of existing processes using existing technologies. At the same time there will be increased integration of processes allowing them to run closer to the optimum. Novel catalysts for conventional synthesis will help to improve process performance.	In the medium term there will be a focus on developing new processes that are inherently safe. We will also develop new biocatalytic processes across all sectors. In the long term we will see the development of processes that approach the thermodynamic minimum, and chemical bioplants that can replace conventional petrochemical and refinery complexes.
Information technology	Improved modelling and information management tools will be needed to deliver more efficient processes. In the longer term the sector will need to be able to respond	much more quickly and flexibly to changes in the market. This will be facilitated by information technology developments.

Figure 4.4 // Sector Goals, Features and Attributes – Commodities



4.2 Grouping of Sector Goals

4.2.1 Identifying Key Goals

We can group the various goals for all the sectors to give a list of nine key goals relevant to green chemistry. There are three product and six manufacturing goals.

Product goals:

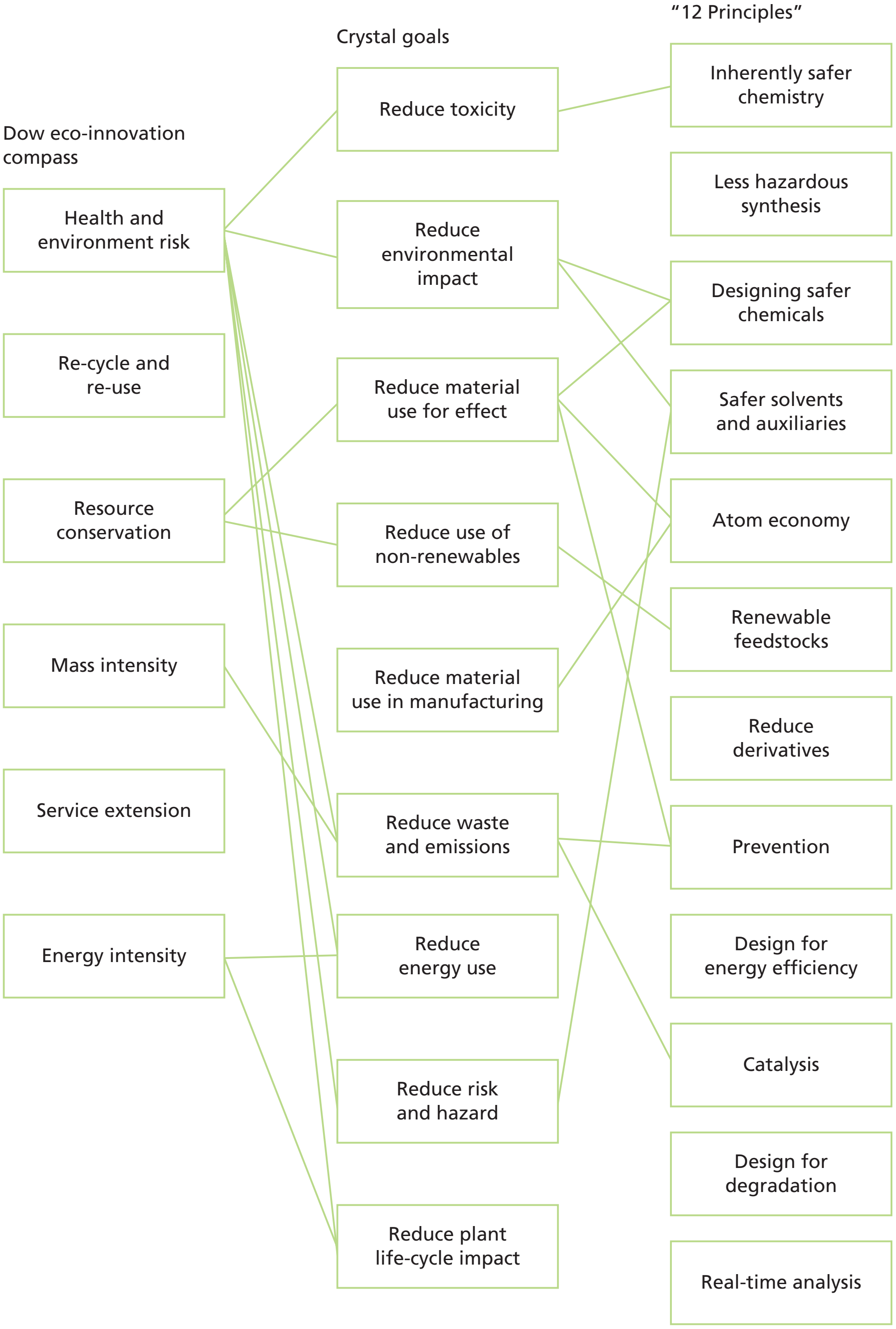
- Reduce toxicity
- Reduce environmental impact
- Reduce materials needed for an effect

Manufacturing goals:

- Reduce materials use
- Reduce use of non-renewable resources
- Reduce waste and emissions
- Reduce energy use
- Reduce risk and hazard
- Reduce life-cycle cost of plant

Several groups have developed key goals and measures for green chemical technology. Figure 4.5 maps the goals that Crystal has used with two popular models for green chemistry, the Dow Eco-Innovation Compass [14] and the 12 Principles.

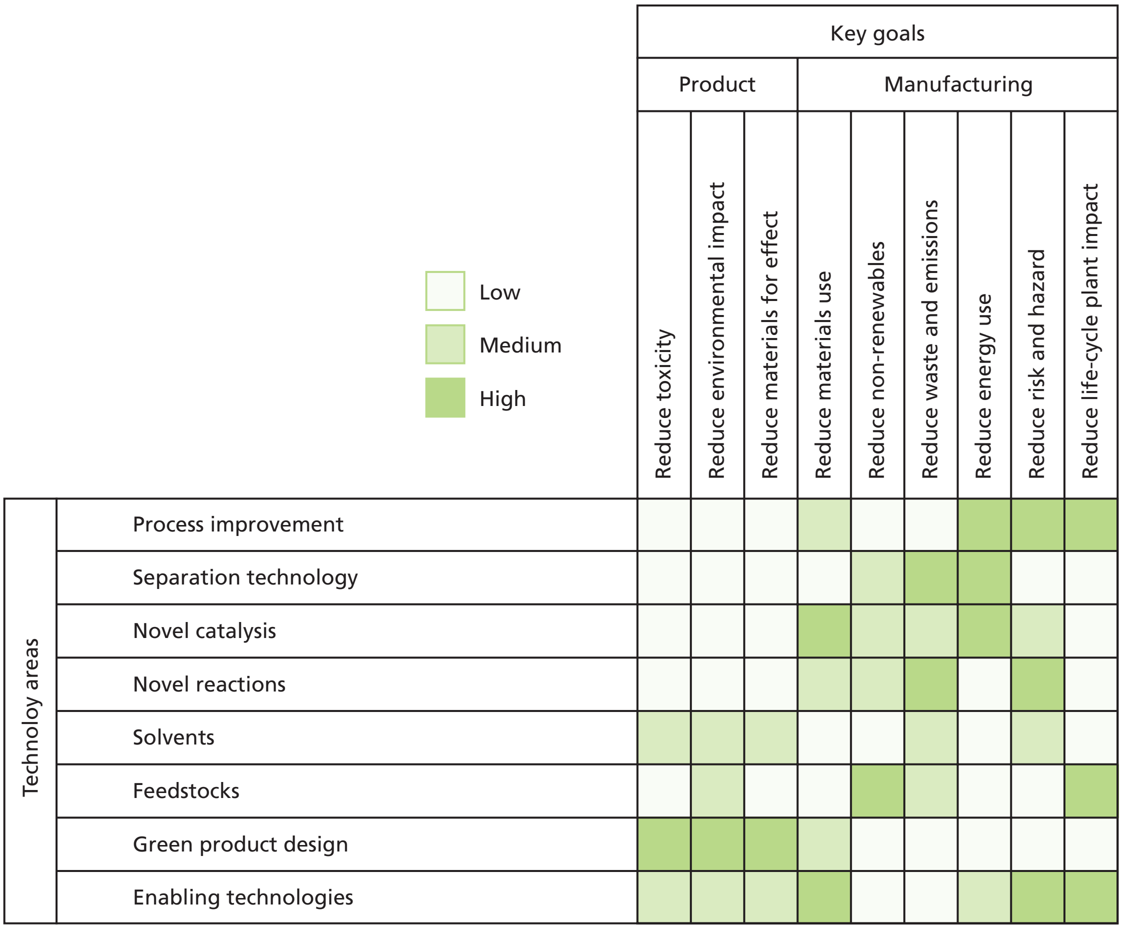
Figure 4.5 // Mapping the Crystal Nine Goals to Other Schemes



4.2.2 Mapping of Technology Areas to Key Goals

Figure 4.6 shows the impact that each of the technology areas can have on the nine key goals.

Figure 4.6 // Impact of Technology Areas on Key Goals



□ Low
▨ Medium
■ High

	Key goals								
	Product			Manufacturing					
Technoloy areas	Reduce toxicity	Reduce environmental impact	Reduce materials for effect	Reduce materials use	Reduce non-renewables	Reduce waste and emissions	Reduce energy use	Reduce risk and hazard	Reduce life-cycle plant impact
Process improvement	□	□	□	▨	□	□	■	■	■
Separation technology	□	□	□	□	▨	■	■	□	□
Novel catalysis	□	□	□	■	▨	▨	■	▨	□
Novel reactions	□	□	□	▨	▨	■	□	■	□
Solvents	▨	▨	▨	□	□	▨	□	▨	□
Feedstocks	□	▨	□	□	■	▨	□	□	■
Green product design	■	■	■	▨	□	□	□	□	□
Enabling technologies	▨	▨	▨	■	□	□	▨	■	■

4.2.3 Mapping of Technology Areas to Features and Attributes

Figure 4.7 is a consolidated list of all the features and attributes from Section 4.1, showing where the eight technology areas will have an impact.

Figure 4.7 // Impact of Technology Areas on Features and Attributes

		Technology areas							
		Process improvement	Separation technology	Novel catalysis	Novel reactions	Solvents	Feedstocks	Green product design	Enabling technologies
Features and attributes	Bio-derived materials		🟩				🟩		
	Nano-materials and composites	🟩	🟩		🟩			🟩	
	Tailored and efficient ingredients	🟩	🟩					🟩	🟩
	Biodegradable and non-toxic materials							🟩	🟩
	Bioprospecting		🟩						🟩
	Phenotype specific products							🟩	
	Gene therapy								
	Recycling plastics			🟩	🟩	🟩	🟩		
	Smart packaging							🟩	
	No packaging							🟩	
	Biodegradable/Compostable packaging				🟩		🟩	🟩	
	New packaging materials							🟩	
	Triggered decomposition				🟩			🟩	
	Design for recycle						🟩	🟩	🟩
	Biocatalytic routes		🟩	🟩					
	Chemical bioplants	🟩	🟩		🟩		🟩		
	Customised organisms			🟩				🟩	
	Multipurpose plant	🟩	🟩			🟩			
	New catalysts			🟩		🟩			
	One pot synthesis for multistep reactions	🟩		🟩					🟩
	Integrated processes	🟩							🟩
	Optimised processes	🟩		🟩					🟩
	Inherently safe processes	🟩			🟩	🟩			
	Processes at thermodynamic equilibrium			🟩				🟩	
	Modelling and system management								🟩
	Flexible market response	🟩							🟩

4.2.4 Interactions between Technology Areas

Many of the technology areas will have an impact not only on the product and service features and attributes, but also on other technology areas. There are synergies and dependencies between technology areas.

For example, to gain the full benefits of the process improvement technology area developments in novel catalysis and reactions are essential. There are also smaller impacts on process improvement from developments in separation technology, solvents, green product design and enabling technologies.

Figure 4.8 shows the interactions between the technology areas.

4.2.5 Key Technologies for Each Sector

From the key sector goals and features and attributes and the impact of the technology areas on goals and attributes, it is possible to identify the key technology areas for each sector of the chemical industry. They are illustrated in Figure 4.9.

For example, the consumer products sector has a target to reduce waste and emissions by a factor of four over the next 20 years. Process improvement, separation technologies, greener product design and novel catalysts and reactions all have a part to play in achieving this objective.

Similarly, in pharmaceuticals it is an objective to reduce the waste material to active ratio from, 100-200:1 today to 10:1 in 20 years' time. In this case, process improvement, separations technology, solvent reduction, novel reactions, greener product design and various enabling technologies are key.

Figure 4.8 // Interactions between Technology Areas

⬜ Low
▒ Medium
🟩 High

		Source of technology							
		Process improvement	Separation technology	Novel catalysis	Novel reactions	Solvents	Feedstocks	Green product design	Enabling technologies
Receiver of technology	Process improvement	🟩	▒	🟩	🟩	▒	⬜	▒	▒
	Separation technology	⬜	🟩	▒	⬜	⬜	⬜	⬜	⬜
	Novel catalysis	⬜	⬜	🟩	▒	▒	⬜	⬜	⬜
	Novel reactions	⬜	⬜	⬜	🟩	⬜	⬜	⬜	⬜
	Solvents	⬜	⬜	⬜	⬜	🟩	⬜	⬜	⬜
	Feedstocks	⬜	▒	🟩	▒	⬜	🟩	▒	⬜
	Green product design	⬜	⬜	⬜	⬜	⬜	⬜	🟩	⬜
	Enabling technologies	⬜	⬜	⬜	⬜	⬜	⬜	⬜	🟩

Figure 4.9 // Priority Areas by Sector

		Technology area							
		Process improvement	Separation technology	Novel catalysis	Novel reactions	Solvents	Feedstocks	Green product design	Enabling technologies
Sector	Consumer products	🟩	🟩	🟩	🟩			🟩	
	Pharmaceuticals	🟩	🟩		🟩	🟩		🟩	🟩
	Specialty chemicals	🟩	🟩	🟩		🟩		🟩	🟩
	Commodity chemicals	🟩	🟩	🟩	🟩		🟩	🟩	

5. Technology Roadmaps

This section covers key developments in each of the eight technology areas. Two groups of specific technologies are identified: technologies that are ready for deployment in industry, but which have for some reason not yet been taken up, and technologies where there have been laboratory demonstrations, but where further development is needed before they can be successfully used in industry. Barriers to exploitation and dependencies on other developments are also noted for each technology area.

The key technology developments for each of the technology areas are summarised in Figure 5.1. Shaded boxes show technologies that are ready for deployment. These are candidates for demonstration projects and raising awareness. Unshaded boxes show technologies that need further development. These are candidates for R&D activities.

The following sections provide more detail.

5.1 Green Product Design

Green product design is at the heart of the development of green chemical technology. It is not sufficient to reduce the cost and impact of the manufacturing process if the products themselves have an unfavourable environmental profile.

The chemical industry needs to think more about the costs and benefits of its products throughout the life cycle. Just as with improvements in manufacturing, reductions in material intensity, waste and energy consumption in use and disposal will bring significant economic benefits.

Thinking about green product design is less well developed in the chemical sector than in other industries. Emerging end-of-life disposal regulations and concerns about total cost of ownership are driving greener product design in the automotive industry and in consumer electronics. The construction industry is another area with a growing focus on sustainable design. The chemical industry can learn from these developments.

Green product design is not so much a set of technologies as a set of capabilities.

Figure 5.1 // Technologies to Deploy or Develop

Green Product Design	Feedstocks	Novel Reactions	Novel Catalysis	Solvents	Process Improvement	Separations	Enabling Technologies
An integrated approach to life-cycle design	Improved routes to olefins from alkanes	Combined bio- and chemical processes	Solid supported catalysts for key reactions	Wider exploitation of closed loop systems	Exploit process synthesis	Better cost and technical data on existing membranes	Integrated approaches to modelling
Extend recycling from lubricants solvents and catalysts	Improved chemistries for recycling plastics	Which greener reagents can be implemented?	Practical enzyme reactions	Supercritical fluids	Alternative energy sources (radio frequency and microwave)	Better membranes for use in organic solvents	Fast, online chemical analysis
Develop design protocols for re-cycle and re-use	Breaking down waste streams to feedstocks	Membrane driven reactions	Chiral synthesis for key reactions	Make ionic liquids a practical tool	Spinning disc reactors	Reduce costs of affinity chromatography	Easier life-cycle analysis for comparing options
Integrate product and process design		Better ways to make small and nano-particles	Ways to develop and scale up catalytic processes	Develop solvent-free reaction schemes	Real-time measurement and control	Develop efficient bio-separations for fermentation systems	Exploiting HTE (high throughput experimentation)
Develop better understanding of downstream chemical use					New reactors – microchannel, catalytic membrane etc		Improved HTE for synthesis and performance testing Exploit small and nano-particles to reduce material intensity
Exploit small and nano-particles to reduce material intensity					Wider exploitation of process modelling		
					Higher fidelity, easier to use modelling		

5.1.1 Green Product Design Capabilities

Design for life-cycle	Designing for the total life-cycle of a product should become standard in the chemical industry. In the consumer sector, where many products are disposed of through the domestic sewage system, biodegradability and low aquatic toxicity are designed into products. Similarly materials supplied to industries with end of life disposal regulations and standards must meet the customer specifications. Tools exist, but there is no generally accepted integrated approach to life-cycle design, and the economic benefits are not being made clear enough.
Design for recycle and re-use	Traditionally, the chemical industry has tried to develop products that are as safe as possible to use. Less attention has been given to ease of recycle and re-use. Within our chemical plants we have developed extensive capabilities in recycling to minimise waste and resource consumption. This needs to be extended to the products in use. Good progress has been made in products such as solvents, lubricants and some catalysts. This experience and thinking needs to be transferred to other product categories.
Efficient process design	Efficient and low impact manufacturing processes are a key part of green product design. Opportunities are discussed in section 5.7. Integrating product and process design, and providing a reliable commercial analysis of the options remain as challenges.
Reducing material intensity	Reducing the amount of material required to produce a specific outcome is an effective way of reducing environmental impact. Overall the chemical industry has been trending to lower material intensity over many years, both in manufacturing and in the product. This has been in response to customer pressure and an effort to reduce costs. There are also many opportunities to develop new products through an active search for ways to produce more mass effective products. Micro- and nano-particles offer new product opportunities for highly effective products. The industry needs to develop a better understanding of downstream user needs.

5.1.2 Barriers and Dependencies

Barriers:

- Thinking about the total product life-cycle is not embedded in the industry. Too many people only think about the parts of the life-cycle they directly control;
- Green product design is seen as a defensive response to an external pressure rather than an opportunity for business improvement;
- A lack of standards;
- A lack of clear models and methodologies;
- Few recognised examples of commercially successful green product design;
- Consumer concern about the safety of nano-technology (the ‘grey goo’ scenario).

Dependencies:

- Green product design is dependent on the opportunities created by all the other technologies in this report.

5.2 Feedstocks

The chemical industry is today based on the use of fossil hydrocarbons as feedstocks. Clearly this is not viable in the long term, and there has been continuous interest in alternative, renewable feedstocks.

The specialty chemical sector has had a long involvement with starch, sugars and plant oils as feedstocks, and will continue to develop new materials where they offer real benefits. Alternative feedstocks in commodity chemicals are less well developed. They have to compete economically with the highly optimised petrochemical product complexes.

For the first generation alternative feedstocks in bulk applications there is a problem of scale. Replacing 5% of the diesel road fuel used in the UK with biodiesel from rape methyl ester would use about a third of the total arable land for intensive rape cultivation.

5.2.1 Feedstock Technologies

Shift to alkanes as feedstock	As liquid petroleum sources become depleted, there is a strong interest in using simple alkanes as feedstocks for the chemical industry instead of olefins obtained from crackers. Catalytic dehydrogenation of propane and isobutane has been practised for a long time, but low conversion efficiencies lead to high capital costs. Alternative oxidative routes have been developed and are beginning to be commercial. BP produces 63 kT/yr of 1, 4-butanediol from butane at its plant in Lima, Ohio. This process has a cost advantage as there are fewer steps and a cheaper feedstock. Saudi Basic Industries Corporation (SABIC) is building a semi-commercial plant to produce 30kT/yr of acetic acid from ethane instead of by methanol carbonylation. If successful a 200 kT/yr plant will be built. Oxidation of methane to provide basic feedstocks remains a challenge.	A similar technology has been commercialised to convert natural gas to diesel via a Fischer-Tropsch synthesis. Shell has a plant in Malaysia capable of producing 12,500 barrels a day of diesel from natural gas by Fischer-Tropsch synthesis. This is an extremely low sulphur fuel with lower emissions than conventional diesel. Shell is currently working to combine Fischer-Tropsch synthesis with biomass gasification to produce biodiesel from renewable resources. Because of the existing investment in established technologies and their low cost, these alternative technologies will need heavy investment to be competitive.
Recycling chemistry	Mechanical recycling of plastics, lubricants solvents and other materials is developing across the world, although more slowly than many would like. However, there is a limit to what can be recovered in this way before the energy consumed exceeds the benefits of re-using the materials.	In addition to mechanical recycling we need access to chemical recycling where the used material is converted back to a feedstock. A good example of the potential is the catalytic cracking of plastics to retrieve the valuable hydrocarbons. Providing plastic can be treated as a single waste stream, 20 MT/year is available in Western Europe alone. Experimental processes are not yet commercially viable and will challenge our catalyst and process development skills.
Converting waste to a feedstock	Another approach with good long-term potential is the conversion of organic waste into a feedstock for the chemical industry. Although the USA is a major importer of fossil hydrocarbons to feed its economy, it is self sufficient in carbon if agricultural production is included. The challenge is to convert domestic and agricultural waste into useful chemicals. One approach being scaled up at the moment is the conversion of lignocellulose from wood, straw, or other plant material, to ethanol via enzymatic degradation followed by fermentation. There are older chemical routes to ethanol and methanol from plant materials, but these are not cost effective. If our existing highly efficient bulk chemical industry can be switched to renewable feedstocks from municipal and agricultural waste, it will be a major step to developing a sustainable industry.	Dow-Cargill is producing a new polymer polylactic acid (PLA) from corn dextrose at a 140 kT/yr plant in Nebraska. The sugars are converted by fermentation to lactic acid and then chemically polymerised. This material can be used for textiles and packaging, and uses 20-50% less energy than conventional plastics. Although currently made from primary agricultural products, there are plans to breakdown cellulose from corn stover (residues from harvesting the maize). This will improve economic and environmental benefits. Corn stover and other waste biomass will also be used to produce bio-ethanol. Iogen Corporation of Canada has recently shipped the first commercial quantities of bio-ethanol made from agricultural waste. The waste is enzyme treated to release sugars and then conventionally fermented and distilled. Estimates of reduced carbon dioxide emissions range from 80-90% for bio-ethanol depending on feedstock source.

5.2.2 Barriers and Dependencies

Barriers:
- Entrenched, low cost technologies
- Currently insufficient pressure to change
- Large sunk investments
- Concerns about strategic availability of alternative feedstocks
- Absence of integrated supply chains

Dependencies:
- New catalytic processes will be required
- Strong link to chemical engineering and process design

5.3 Novel Reactions

Although chemists have a built a vast library of reactions, there is still room for novel routes to particular structures.

Combined bio- and chemical processes	Bio-processes and chemical processes both provide the synthetic chemist with unique capabilities. Developing ways of integrating chemical and biological	transformation will maximise flexibility. Possible examples include enzymes in supercritical carbon dioxide or ionic liquids.
Greener alternatives for standard reactions	Many conventional organic synthesis reactions use hazardous reagents and solvents. A large amount of research has been carried out on greener alternatives to standard reactions. Few of these reactions have transferred to mainstream applications. We need to identify which of these alternatives could be realistically implemented.	Databases of alternatives are beginning to appear, including the Green Chemistry Expert System obtainable from the US Environmental Protection Agency *(www.epa.gov/greenchemistry/tools.html)*. The system helps to analyse the environmental impact of chemical processes, and to identify and design alternatives.
Membrane driven reactions	Membranes can be used to enhance conversion in equilibrium limited reactions by allowing selective removal of one or more products. Where a catalyst is used it can be closely coupled to the separation	membrane to form a catalytic membrane which can deliver even higher yields. This will support compact and intensive manufacturing units.
Better ways to make small and nano-particles	Small particles and nano-particles are providing novel ways to deliver enhanced functionality and nano-particles with reduced mass intensity. This is providing new opportunities in applications from medicine to	industrial coatings. To fully exploit the potential of these technologies we urgently need better and more robust ways to manufacture and handle small and nano-scale particles.

5.3.2 Barriers and Dependencies

Barriers:
- Except for special cases there is insufficient incentive to change existing working processes
- Interesting new reactions are reported and shelved before sufficient data for a realistic evaluation is available

Dependencies:
- Strong link to membrane separations
- Link to novel catalysis

5.4 Novel Catalysis

Catalytic processes have been at the heart of developments in green chemical technology. They have played a key role in reducing energy consumption and waste, and in improving control.

5.4.1 Novel Catalysis Technologies

Solid supports	Supported catalysts are very widely available and offer many advantages in simplifying separation and offering alternative reaction design options. Unfortunately we are still short of robust and reliable supported catalysts for many key reactions.	Zeolites have proved their usefulness with titanium-substituted ZSM-5 (TS-1) allowing the use of atmospheric oxygen as an oxidant in applications like the production of caprolactam. ZSM-5 itself is used in direct oxidation of benzene to phenol, and the zeolite Beta for the production of alpha-terpinyl alkyl ethers. All of these reduce process complexity and eliminate waste streams. Solid state Lewis and Bronsted acids have been successfully used for acylations and alkylations, simplifying the process and reducing waste.
Enzymes	Enzymes offer very mild processing conditions and for the right reactions great specificity. Wild-type and genetically modified enzymes have been available commercially for many years. Yet enzymes are still niche catalysts. Can we define the types of reaction for which enzymes are most suitable, and identify clear performance gaps that it would be worth tackling?	The current palette of industrial enzymes is limited. Only lipases, proteases, cellulases and amylases are used in volume. However, the two biggest players, Genencor and Novozymes, have combined sales of over €1 bn, mostly in enzymes for industrial applications such as washing powders, leather treatment, food processing and producing 'stonewashed' jeans. Tencel fibre is made from the cellulose in wood-pulp. During manufacture the outer sheath of the fibre is opened up into small fibrils. These are removed using cellulose to leave a stronger and smoother fibre core which produces a fabric with good colour, feel and drape.
Chiral synthesis	Chiral synthesis is of obvious importance in bioscience and medicine, and catalysts are already used for this purpose. Chiral synthesis increases mass effectiveness of	active molecules and avoids waste and separation costs. New chiral catalysts are needed to tackle a wider range of reactions.
Catalyst process design	Although a vast range of catalysts have been developed in the laboratory, it can still be difficult for industry to develop a new catalytic process. This is blocking implementation of catalytic processes and superior catalysts to reduce environmental footprint.	We need improved ways to develop catalytic processes from the bench to full scale that deal with issues such as catalyst lifetime and robustness, catalyst removal and control of catalytic processes

5.4.2 Barriers and Dependencies

Barriers:

- Difficulty in transferring new catalysts from laboratory to production
- Problems in knowing how to design effective catalytic processes
- Lack of reliable supplies of development catalysts, particularly for small-scale production

Dependencies:

- Strong link to process design
- Link to modelling

5.5 Solvents

Solvents play a critical role in today's chemical industry both as products and process aids. There has been a long-term focus on preventing solvent loss to the environment, substituting less hazardous and more efficient solvents, and reducing or eliminating solvent use.

5.5.1 Solvent Technologies

Closed loop systems	Concerns about human safety and the environmental impact posed by many common organic solvents has led to the development of recycling and closed loop processes. For many high-volume continuous chemical processes, recycling efficiencies of over 95% are common. Process design and material handling ensure that little solvent is lost to the environment. These best practices need to be transferred to small volume and batch processes where losses are still relatively high. Moving towards closed loop systems will provide cost savings in materials and in effluent treatment and disposal.	Closed loop solvent cleaning systems have been developed for the electronics industry where extremely low levels of contamination are critical. High purity solvents are regenerated using ion exchange and losses are almost zero. Solvent vapours from spray painting of cars are captured and used as a fuel in integrated heat and power systems in the factories of some major car manufacturers.
Supercritical fluids	Supercritical fluids, and in particular supercritical carbon dioxide, are solvents that provide new capabilities, energy savings, and lower health risk and environmental impact. Supercritical carbon dioxide has been very successfully developed for extraction processes, including decaffeination and the preparation of essential oils. Technology introduction has been driven by superior product quality, and plants with feed capacities of several thousands of T/yr are common. However, supercritical fluids are not yet widely used as process solvents in the chemical industry. Demonstrator projects and case studies of successful uses are required to overcome industry perceptions of limited usefulness and high cost.	DuPont has developed a commercial process for fluoropolymers that uses supercritical carbon dioxide as the solvent system instead of ammonium perfluorooctanoate (C-8). There have been growing concerns over the toxicity and environmental impact of C-8 if released. The new process is much lower risk, but has so far only been used for a small percentage of fluoropolymer manufacture. Liquid carbon dioxide is also being used with a new generation of surfactants for dry-cleaning, avoiding the use of organic solvents *(www.washpoint.com)*. Benefits include lower environmental impact and reduced costs.
Ionic liquids	Ionic liquids have been extensively researched for some time, and offer many advantages as process solvents. They are non-volatile and can be 'designed' to have specific properties suited to a reaction or process. Early trials in commercial processes are underway, but a lot of development is still required, particularly around process engineering with ionic liquids. Work needs to be done on:	• Solvent recycle and regeneration • Losses in practical processes • Solvent lifetime • Process design and economics • Toxicity and environmental impact There are also issues with registration of ionic liquids. In principle, separate registration could be required for every ionic liquid used. This is a major barrier to exploitation.
No solvent systems	Designing out the solvent in chemical processes is another approach to developing greener systems. A great deal of research work has been done on solvent-free systems, particularly for standard organic synthesis reactions and in polymer processing. But this is only	slowly transferring to industrial application. The benefits are not clear enough for people to take the risk. New reactor designs such as the spinning disc can offer new routes to solvent-free systems.

5.5.2 Barriers and Dependencies

Barriers:
- Current low cost of conventional organic solvents
- Capital cost of alternative systems perceived as too high for the benefits
- Lack of familiarity with alternative approaches

Dependencies:
- New reactor types for solvent-free systems

5.6 Process Improvement

The process improvement technology area has a potentially very large impact on the development of green chemical technology and a sustainable chemical industry. Many of the technologies are developed enough to be widely exploited now. Yet take-up is disappointing.

These technologies will continue to develop over the coming years and will offer additional opportunities, but the challenge is to take what they offer today. More than any other technology area, process improvement offers the chance to improve economic and environmental performance in the short term.

5.6.1 Process Improvement Technologies

Process synthesis	Process synthesis combines chemistry and chemical engineering into a holistic approach to the problem of producing the desired product from available starting materials with maximum yield with lowest cost and minimum waste generation, energy and resource use.	It is a thoroughly established discipline, with immense potential for delivering a more sustainable chemical industry. Unfortunately it is not as widely used as it could be. Separation of chemistry and chemical engineering into separate disciplines has not helped.
Alternative energy sources	A lot of work has been done on alternative energy sources for chemical processes particularly radio frequency and microwave. Both offer extremely efficient energy transfer with rapid and targeted heating, and direct monitoring of energy uptake. This provides better control of reaction conditions, saving energy and increasing atom efficiency through reduced side reactions. Reactions can be completed more rapidly, increasing reactor throughput. Radio frequency heating is used on an industrial scale for drying in many industries. It is used in food, paper, glass-fibre and ceramics: for example, to dry ceramic	monoliths for exhaust catalysts. Large systems with conveyor belt widths of over 4m are available today. Microwave heating systems exist with capacities of 100kW and have been used to dry continuously poured hydrophilic polyurethane foam, and to pre-heat epoxy resin from 50C to 180C prior to extrusion. Despite these examples, lack of familiarity and confidence in what is seen as a ‘novel’ approach is blocking acceptance. In particular, laboratory-scale experience of microwave assisted synthesis needs to be transferred to industrial use.
Alternative reactor technologies	Many new types of reactors are currently being developed. An important theme for green chemical technology is micro-reactors, small-scale systems that allow rapid, high efficiency chemical processes. These systems can be scaled up by adding identical units, making it possible to go from laboratory scale to full production very quickly. These technologies offer better product consistency and lower waste than batch processes. Typically with short residence time and fast heat and mass transfer, they are particularly suited to fast laboratory-scale reactions. • The spinning disk (also cone or cup) reactor is ready for implementation today Other types need more development work, including: • Microchannel reactors • Catalytic membrane reactors • Reactors with small close-coupled chambers separated by membranes	Spinning disc reactors are beginning to be used commercially. Examples include: Polymerisation of viscous liquids where the yield can be driven from typically 75% to more than 99%. The process is much faster than in conventional reactors with polymerisation occurring in seconds, and downstream processing to remove monomer can be eliminated. Flexible manufacturing of different grades of adhesive. Because it is possible to ‘dial in’ the required viscosity, just-in-time manufacturing with no inventory is possible.
Process modelling	Related to both process synthesis and real-time control, process modelling is a broad technology that has been under-exploited in developing green chemical technology. There are endless case studies showing dramatic improvements in process efficiency and reliability through process modelling, and yet many still see it as difficult, uncertain, expensive and unreliable. Although there are many exciting research developments that promise better and easier modelling in the future, the evidence is clear that process modelling should be a key part of developing green chemical technology today.	Uniqema used process modelling to create a factory out of thin air. Additional capacity was needed for a specific process, but they wanted to avoid significant investment. A comprehensive process modelling exercise was carried out to explore options for improving capacity in this batch process, and it was possible to reduce cycle times by an average of 48% for all products without capital investment Texas Instruments used the same approach to improve throughput in their chip fabrication and squeezed an ‘imaginary factory’ out of the existing capacity.
Real-time control	Real-time measurement and control of plant provides many opportunities for significantly reducing energy and resource consumption, particularly when used with	process modelling. These technologies could be applied today with significant reduction in energy and other resource consumption.

5.6.2 Barriers and Dependencies

Barriers:

- Lack of familiarity amongst industrial scientists
- Difficulties in integrating chemistry and chemical engineering
- Lack of confidence in the real capabilities of these technologies
- Need for demonstrator facilities, particularly mobile units
- Need to make the financial and technical case as a complete package

Dependencies:

- Strong link to modelling in the enabling technology area
- Strong link to advanced analytical technologies
- Link between membrane-based advanced reactors and separations and novel catalyst systems

5.7 Separation Technology

In most chemical manufacturing processes it is necessary to separate a reaction mixture at some point. Better separation technology can improve the efficiency of these processes, reducing energy consumption and waste generation.

5.7.1 Separation Technologies

Membranes	Membranes are already widely used in separations and have proved they can increase efficiency and reduce waste. Better cost data are required to demonstrate the gains possible from wider application of membranes. New membrane separation systems are needed that work in a wider range of organic solvents.	A commercial membrane separation system has been developed to strip aromatic molecules from aqueous media. This has been used for high efficiency recovery of p-cresol from a process stream. The system can handle up to 10kT/yr and brings significant energy savings. Membranes can also be used in the nano-filtration of organic solvents. The process allows for high-efficiency separation of homogenous catalysts, removal of impurities or solvent exchange.
Affinity chromatography	There is always a need for more selective separation techniques. The exquisite selectivity of affinity	chromatography, particularly for separation of bio-molecules, has wider potential if costs can be reduced.
Bioseparations	Bioprocessing is a tool of growing importance in green chemical technology. Unfortunately, many bioprocessing steps take place in conditions that require the recovery of low concentrations of product from large amounts of complex non-Newtonian fluids such as fermenter broths. Industry needs improved separation technologies that can efficiently separate bio-molecules.	There is an enormous opportunity for improved bioseparations. In fermentations for bulk extracellular enzymes, such as proteases, concentrations in the fermenter broth range from 0.001-1g/l and recovery and purification costs 10% of total production cost. Materials such as interferon and human insulin are only found at 10^{-5}-10^{-7}g/l and downstream processing is 90% of total production cost.

5.7.2 Barriers and Dependencies

Barriers:

- Insufficient economic evidence to drive adoption of new techniques.

Dependencies:

- Strong link to process improvement
- Link to novel reactions and novel reactor design

5.8 Enabling Technologies

A cluster of technologies that will underpin the development of green chemical technology.

5.8.1 Enabling Technologies that underpin

Modelling	Modelling is an important tool for developing green chemical technology. It allows 'what-if' experiments to be carried out in the computer faster, and at lower cost, than in the laboratory or plant. With widely available computer power, complex problems of materials and reaction design, process development and financial and business modelling can be studied. Yet modelling is still seen as costly, unreliable and difficult.	We need to develop integrated approaches that allow companies to model materials, manufacturing processes and business processes together. This will support holistic thinking and allow green chemical technology to make its case.
Analysis	A key component of most green chemical technology is fast and accurate chemical analysis. This is particularly important to support process intensification and lean manufacturing. Compact flexible manufacturing units for complex reactions depend on fast, accurate and on-line measurement techniques. Lab-on-a-chip designs will be an important development for this kind of	application, allowing measurement to be cost-effectively brought right into the process. Process optimisation and real-time control also require fast on-line measurement. Although a great deal of work has gone into process analysis over the years, the consensus is that we still lack the tools we need.
Life-cycle analysis	Life-cycle analysis is a key tool in the implementation of green chemical technology. But the international standards and software tools that we have available for life-cycle analysis are difficult to implement, and are not suited to practical decision-making in the chemical industry. The prescribed methodologies usually require the services of an expert to implement, are costly and time-consuming to use, and very sensitive to boundary conditions. Life-cycle analysis has found its best	application in discussions about public policy, where the use of industry average data and standardised assumptions are valid. To support green product and process design, we need simpler tools that can be used by an individual scientist or development team. An appropriately simplified life-cycle analysis process that can be used to compare design options would be a powerful addition to the green technologist's toolbox.
High throughput experimentation	High throughput experimentation allows large numbers of experimental trials to be carried out in parallel using robotics and automation. High throughput experimentation is one of the tools that make experimental design a viable choice for chemists in industry instead of a distant ideal.	Industry needs to know more about what can already be done in high throughput experimentation, and the technique needs to be developed to cover more areas of synthesis and performance testing.

6. Priority Activity Areas

During the development of the roadmap, it became clear that there were some areas where specific focus would have the greatest impact on the development of green chemical technology.

6.1 Exploiting Existing Technologies

In a number of technology areas there are well established technologies that have been successfully used to 'green' chemical processes. However, these are not used as widely as they could be. This can be due to lack of awareness, difficulty in demonstrating the risk/value equation for a given application, or the need to tailor technology to a specific use. Getting what we already have into industrial use deserves greater focus.

The experts involved in developing this roadmap identified many technologies that could be implemented today to help the development of a more sustainable chemical industry. This is particularly true in the areas of modelling and process design. Continuing to invest in developing further new technologies will be of little value if these technologies experience the same problems in breaking through to wide industrial application.

A high priority activity should be helping industry to evaluate and implement known technologies that will reduce environmental impact and improve economic performance.

6.2 Developing Complete Packages for the Industry

Much of the chemical industry lacks the resources and expertise to evaluate green chemical technology options properly.

It is not sufficient for inventors to describe the general features and benefits of a technology. Industry needs demonstration facilities, data, design guidelines, process and financial models. All of this needs to be packaged together so that the case for using a technology can be thoroughly and realistically examined.

Mobile demonstrator facilities are needed that will allow industry to try out real processes on site. Scale up is a key issue and the information and models to develop and cost a design are a critical part of the package.

Industry also needs to be able to integrate the new process into their business models and financial planning. Providing good data and models plays an important part in encouraging the take up of new technology. A good example is the use of liquid carbon dioxide for dry-cleaning. Commercial spread of this technology has been supported by a website *www.washpoint.com* that provides on-line calculators that help interested cleaning companies to evaluate the likely cost/benefit for their specific situation.

There is a key role for intermediary companies and integrators to develop these complete packages and support implementation of these technologies.

There is a lack of such companies in the UK willing to take up new technologies and further support is needed to bridge this gap.

6.3 Demonstrating the Business Case

For most of the chemical industry, green chemical technology is not successfully making the case that this will be a more profitable way to work. It is too often seen as either a response to external public and regulatory pressures or a commitment to corporate social responsibility that is 'nice to have'.

Green chemical technology needs to win its place on the business agenda as a tool for improved competitiveness.

There is plenty of evidence available, but not well organised and communicated. Crystal can play a key role in collecting, organising and distributing the evidence to make the business case for green chemical technology.

6.4 Green Product Design for the Chemical Industry

Green product design is the only technology area identified that has direct relevance to products, both in use and at end of life. The chemical industry has been relatively slow to develop a coherent picture of what green product design means and how it might be implemented.

The chemical industry needs to develop its own model of green product design that is appropriate to the types of products, their typical risks, hazards and impacts.

This will draw on:

- all of the work that has been done on eco-innovation;
- successful practice from more advanced industry sectors such as automobiles, white goods and consumer electronics;
- industry experience with topics such as eco-toxicity and biodegradability.

The goal would be to build a coherent collection of theory, models and skills that can be taught to existing product developers as well as through universities to the next generation of developers.

A key part of this will be developing more usable methods for life-cycle analysis.

Crystal is in an excellent position to lead the development of green product design for the chemical industry in the UK.

7. Key Messages

Here are the key messages for stakeholders in green chemical technology:

7.1 Government

- Demonstrators are valuable, but we need to create complete packages for industry

To introduce green chemical technology successfully we need to build complete demonstration and information packages. Government has a role to support and encourage this (see Section 6.2).

- There is a gap between universities and user industries that needs to be bridged by technology implementers/integrators

At the moment there is support to academia to develop green chemical technology and support to industry to exploit them. However, there is a lack of intermediate providers who can commercialise technology and provide a full service to the chemical industry. For green chemical technology to be taken up more widely, a specialist technology provider sector needs to develop (see Section 6.2).

- Be consistent and patient in funding research

Making a significant change to the sustainability of the chemical industry will take time and require continued focus. Regular changes in research priorities and funding schemes may be mistaken for a lack of commitment on the part of the Government to sustainable development.

- Joined-up thinking in regulation

Rightly or wrongly, industry feels itself to be facing a tidal wave of regulation that often appears to have contradictory policy goals. Horizontal initiatives, such as REACH, may collide with vertical initiatives, such as the Cosmetic Directives. Clarity about the policy goals around a sustainable chemical industry, and a consistent and coherent picture of current and projected regulation would help industry to focus on this key topic (see Section 3.5 and Appendix 1).

- Government procurement can create market pull

Central and local government represent a very large sector of the UK economy. Through procurement policies such as the Sustainable Procurement Initiative, the Government can create a market for the goods and services delivered through green chemical technology.

7.2 Industry

- Green chemical technology is a route to improved profitability

Green chemical technology is not just about meeting regulatory requirements or responding to public pressure. By increasing efficiency and reducing resource consumption it represents a more profitable way to do business.

A sustainable industry must be an economic success as well as being environmentally acceptable and socially responsible.

- Let the world know what you need

Industry must engage with those trying to develop green chemical technology. Industry is not providing clear enough guidance on its needs. It is not sufficient to sit back and look at what academia and technology providers offer; industry must be fully engaged in defining, promoting and supporting programmes targeted at the tools that will enable the development of a sustainable chemical industry.

- Being too conservative brings real risks

It is tempting to delay changing manufacturing processes until forced to do so by regulation. Unfortunately, competitors may see the opportunity to increase their overall efficiency dramatically through the exploitation of green chemical technology. While we are defending the *status quo* they could be dramatically shifting their supply chain costs.

Green chemical technology represents a real shift in practice. Smart companies will exploit it for competitive advantage.

7.3 Academia

- We need better multidisciplinary working between chemistry and chemical engineering

Successful deployment of green chemical technology requires close integration of chemistry and chemical engineering. The academic sector should be actively supporting this kind of interdisciplinary approach. As an example, the next call for green chemistry proposals by the EPSRC will be jointly managed by the chemistry and engineering panels.

- Publicise academia's capabilities

Finding out about the technological capabilities academia is developing is a problem for the other stakeholders in green chemical technology. We need to find ways to showcase our capabilities. This needs to go beyond papers and posters and into demonstrators and case studies using realistic reactions. Organisations such as Crystal with a technology transfer capability are one route.

- Industry needs to know the scope and boundaries of technology

Industry needs to be able to assess whether a new technology is applicable to their circumstances. It needs to know where the boundaries of a new technology are. Where can it be used and where not? What are the limitations? How does performance degrade as we approach the limits of the technology?

Showing a proof of concept on a few standardised reactions is not sufficient. Academia can play a vital role in developing the complete technology packages required by industry.

- We are teaching the workforce of the future

Give them the understanding of what green chemical technology is, what it can do and how new technology is implemented in the chemical industry. It will enable them to change the industry.

8. Next Steps

The strategy contained in this roadmap provides key decision makers in industry, academia and government with a clear picture of the role that green chemical technology can play in developing a vibrant and sustainable chemical industry in the UK. As such it provides a valuable communication tool between these major stakeholders in the industry but it will only maintain its value if it is kept under review to reflect the social, economic and political changes in the industry's operating environment and developments in technology arising from research activity.

The roadmap and technology strategy will be continually refreshed based on new inputs.

The roadmap identifies a number of clear priority issues which could have an impact in the short term on the sustainability of the chemical industry (see Section 6).

The key issues identified will be addressed in priority order through workshops, the facilitation of collaborative research and development projects etc.

The industry's need for a toolkit on "how to do sustainability" which will provide the protocols and procedures to focus and prioritise activities has been highlighted here. Crystal has already developed the Sustainable Manufacturing Protocol as a starting point.

Additional areas such as sharing best practice, performance improvement measures and accounting for sustainability have also been addressed by Crystal and others.

Crystal, in partnership with others, will develop a toolkit to assist industry define the business case for sustainable development and provide a framework for action.

The lack of demonstration facilities to provide detailed design information for the evaluation and implementation of new technologies in specific applications is also highlighted in the roadmap and in Crystal's report on the barriers to implementation of green chemical technology.

Crystal will work with industry, government, including RDAs, learned societies etc to address this issue of demonstration facilities.

The adoption of sustainable management practices by the industry and the resulting improvement in its social, environmental and economic performance will impact positively on its currently poor reputation.

Crystal will be the focal point in the UK for the development, implementation and dissemination of best practice in green chemical technology.

9. References

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10. Appendices

Appendix 1: Future Legislation

Regulation and legislation is a powerful driver for green chemical technology, particularly in Europe. By questioning existing materials, technologies and practices, regulation opens up the market to alternative solutions and creates gaps where green chemical technology can be profitably exploited. The EU has had a sustained interest, through its political institutions, in regulating to protect the environment and human and animal health. Towards the end of the last century there was a growing interest in the use of the precautionary principle and the recognition that the population needs to be convinced that the EU is taking positive steps to protect them.

The tension between the precautionary principle on one side and a strong belief in an evidence-based approach by the industry dominates the debate about strategies for the future use of chemicals in the EU. Although the chemical industry is global, the key legislation affecting the operation of the chemical industry within the EU is EU regulation. This is widely seen as being the most demanding environmental protection and product safety legislation in the world. International organisations such as the United Nations Environment Programme *(www.unep.org)* and the Organisation for Economic Cooperation and Development *(www.oecd.org)* are playing an important role in bringing together developments around the world through initiatives such as the Stockholm Convention on persistent organic pollutants (POPs), and the Co-operation on the Investigation of Existing Chemicals respectively. However, the dominant forces for the European chemical industry come from EU legislation.

This Appendix therefore deals almost entirely with EU legislation and its implications.

Even focusing on EU legislation it is not easy to create a clear picture of what regulatory framework will come into being and on what timescale. The political process of developing and agreeing new laws means constant changes to both the scope and the key dates for almost all the relevant EU legislation. Although all of the documentation relating to legislation is available through a number of websites [8] it is not easy to understand the implications and timetables for each specific piece of legislation. At the moment there is no publicly accessible website that provides an up-to-date overview of the forthcoming regulations that will impact the chemical industry.

Legislation can be divided into two types. Horizontal legislation has implications across the whole of industry, for example the Climate Change Levy, Integrated Product Policy and the Hazardous Waste Directive. Vertical legislation applies to a specific industry, product or application, for example the Biocidal Products Directive or the End of Life Vehicle Directive. A number of these vertical regulatory frameworks apply directly to the chemical industry, and more to the customers of the industry.

The mix of horizontal and vertical regulation presents difficulties for many companies. It is not easy to be sure what rules apply where, and case law takes time to develop. Although the direction and intention of many initiatives is clear, the practical details are often obscure.

The following is an incomplete list of future legislation of relevance as a driver for green chemical technology.

The list is divided into two groups:

- Regulation that has been enacted and has defined milestones for implementation, or is in advanced draft and milestones can be inferred.
- Regulation that is under discussion, but where the preliminary assessments have not yet been completed. In this case it is not possible to list milestones.

Legislation enacted or in draft:

• Stockholm Convention on Persistent Organic Pollutants (POPs)

The Stockholm Convention entered into force in May 2004. It targets the production and use of persistent organic pollutants [9]. It starts with 12 of the most toxic POPs. These cover 9 pesticides, 2 industrial chemicals and 1 group of by-product pollutants. Some of the pesticides are banned with immediate effect; others must be phased out where alternatives become available. For the 10 intentionally produced POPs transport across borders is banned except for environmentally sound disposal.

One class of POP is PCBs, and these are permitted to be used in existing equipment until 2025.

Although initially targeted at the 12 chemicals of most concern, the convention provides for new POPs to be added to the action plan and adopts the precautionary principle that, “where there are threats of serious or irreversible damage, the lack of full scientific certainty shall not be used as a reason for postponing cost-effective measures to prevent environmental degradation”.

• Biocidal Products Directive (BPD)

The Biocidal Products Directive defines biocides as chemical preparations containing one or more active substances that are intended to control harmful organisms by either chemical or biological means. All active ingredients used for this purpose must be tested, evaluated and placed on a positive list if found acceptable. The existence of a less harmful alternative will mean that the ingredient will not be placed on the list. All testing of existing materials must be completed by 2010, and manufacturers will not be able to use active ingredients not on the list. Because of the costs of completing the testing programme, it has been estimated that up to 75% of existing biocides will disappear.

• Cosmetics Directive

The Cosmetics Directive has been in force for many years and is constantly updated. The 7th Amendment is currently working through the EU institutions and will probably ban the testing of cosmetic ingredients on animals and the marketing of cosmetics containing ingredients tested on animals between 2009 and 2013.

As the scientific understanding of risk changes, there is a continuous stream of small changes to the Directive changing the materials and processes that can be used in cosmetics.

• Restriction of Hazardous Substances in Electrical and Electronic Equipment Directive (RoHS)

From July 2006 new electrical equipment will not be able to contain lead, mercury, cadmium, hexavalent chromium, polybrominated biphenyls or polybrominated diphenyl ethers.

• Waste Electrical and Electronic Equipment Directive (WEEE)

From August 2005 private householders will be able to dispose of WEEE at collection facilities free of charge and producers will be responsible for collection, treatment, recovery and disposal. arrangements will exist for commercial users.

From December 2006, producers will be required to meet recycling and recovery targets for different classes of appliance.

The Directive will push producers to avoid materials that cause problems in recycling and recovery and to substitute materials that are easier to handle.

• End of Life Vehicle Directive (ELV)

The ELV Directive requires that at least 85% of the weight of all vehicles must be recoverable (recycling plus incineration with energy recovery) by 2006. By 2015 at least 95% must be recoverable.

The automotive industry will avoid materials that will block achievement of the targets, or which are difficult or expensive to recover.

• Proposed Directive on Batteries and Accumulators and Spent Batteries and Accumulators

Batteries and accumulators are not currently covered adequately by the RoHS Directive, the ELV Directive or other legislation. This draft aims at a significant reduction on the quantities of spent batteries going to disposal and at the highest possible re-introduction of wastes into the economic cycle.

Each year more than 1 MT of batteries and accumulators are sold in the EU. This is not a hazard in use, but on disposal becomes a major problem. Disposal through landfill or incineration both create significant environmental damage.

It is proposed that all batteries and accumulators be recovered and recycled. Within 1 year of the directive being adopted all collected batteries and accumulators must enter a recycling process. Within 3 years, all of the lead and cadmium and the bulk of other materials should be recycled. Within 4 years portable NiCd batteries should be being collected from domestic users at the rate of 160g per person per year.

• Registration Evaluation and Authorisation of Chemicals (REACH)

The EU Commission published a White Paper “Strategy for a Future Chemicals Policy” in 2001 [10]. This proposed a new process for the registration and authorisation of chemicals in the EU (REACH). This is a major change to regulation affecting the chemical industry and is creating a lot of activity both in the chemical industry and in downstream user sectors.

“Companies will be required to register all substances produced or imported in volumes of 1 tonne and more per year per manufacturer or importer”. Substances of specific concern must also be authorised for particular applications.

Substances of concern include:

- CMRs (carcinogenic, mutagenic or toxic to reproduction), category 1 and 2,
- PBTs (persistent, bio-accumulative and toxic),
- vPvBs (very persistent, very bio-accumulative).
- Substances identified as having serious and irreversible effects to humans and the environment equivalent to the other three categories, for example certain endocrine disrupting substances.

For the first time materials that were accepted into use before 1981 will have to submit safety dossiers. Given expected dates for agreement on a directive, the likely milestones for registration of existing substances are:

- 2009 substances used in volumes > 1000 T/yr
- 2012 substances used in volumes > 100 T/yr
- 2017 substances used in volumes > 1 T/yr.

As substances are registered for an application, the system will have impact all the way down the supply chain to the end user.

Polymers and intermediates that are not separated from the reaction mix do not need to be registered.

REACH does not apply to finished products allowing for manufacture in another area of the world and importation.

The Commission estimates that 1-2% of existing materials may be lost through this process as it would not be cost effective to compile the dossier. Industry estimates are much higher.

The chemical industry has a number of concerns about the workability of the proposals [11, 12]. There are fears that implementation could drive part of the chemical industry off-shore, and may stifle innovation.

A study carried out by Arthur D Little for the German chemical industry estimated that the September 2003 draft legislation would reduce the German economy's gross added value by 3% and cost approximately 1 million jobs.

The diagram shows the timeline for legislation enacted or in draft.

Legislation under discussion:

• Sustainable use of pesticides

The EU is developing a strategy for the sustainable use of pesticides. This involves:

- Minimising the hazards and risks to health and environment from the use of pesticides through national plans for reduction of hazards, risks and dependence on chemical control
- Improved controls on the use and distribution of pesticides
- Application of the substitution principle to move to lower impact actives
- Encouraging low-input or pesticide-free crop production
- Supporting accession countries to eliminate obsolete pesticides
- Working through international initiatives such as the Stockholm Convention and the Protocol on Informed Consent.

• Endocrine disruptors

Reflecting public and scientific concern about endocrine disruptors, the Commission, is developing an action programme. This is divided into short, medium and long-term activities.

- Short-term actions – focused on the need to gather up-to-date information about the science of endocrine disruption, the extent to which it was affecting people and wildlife, and identification of substances for further evaluation of their role in endocrine disruption.
- Medium-term actions – develop and validate test methods through cooperation with member states and the OECD
- Long-term actions – review and adaptation of existing laws and legislation, governing the testing, assessment and use of chemicals and substances within the EU.

Changes in legislation are seen as a long-term activity.

• Pharmaceutical preparations

Although pharmaceutical actives and products are subject to stringent regulation, the focus is around human health not environmental impact. However, many commentators have noted that many pharmaceutical products are highly ecotoxic and have questioned the fact that this is not taken into account in the registration process [13]. Various bodies in the EU and the UK are beginning the process of evaluating what regulatory changes might be needed.

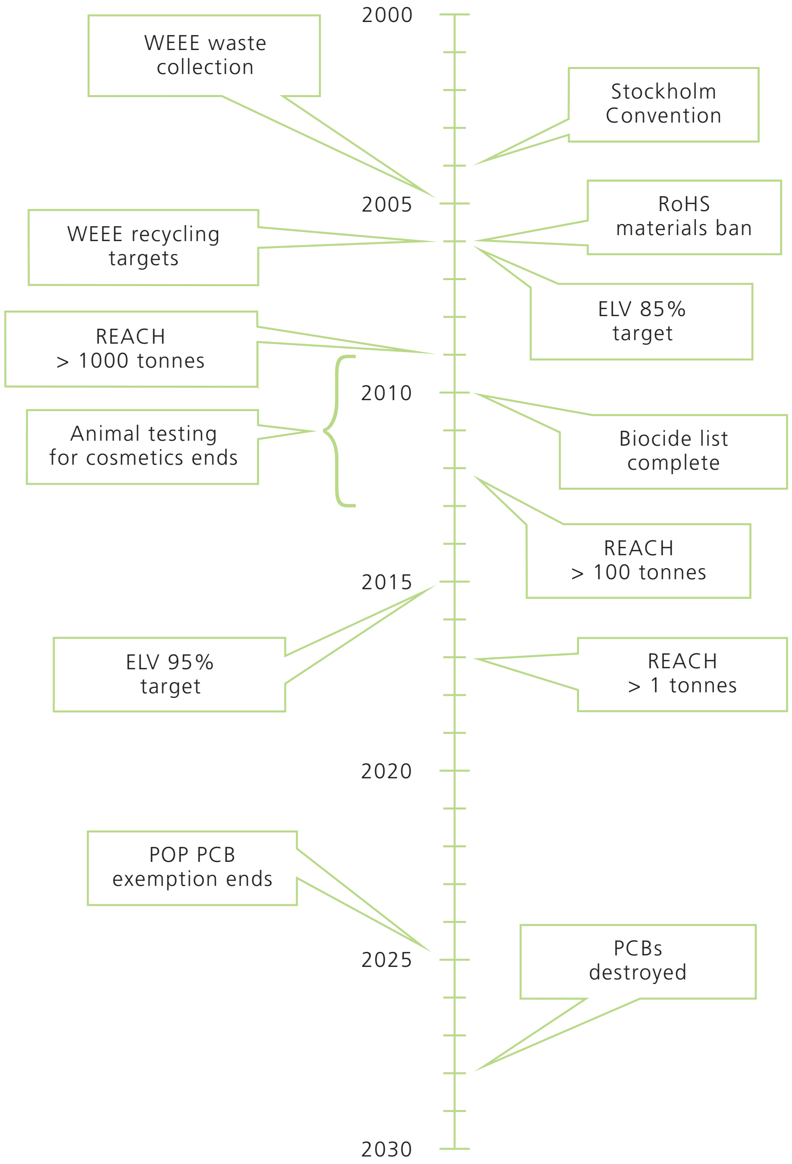
• Priority substances under the Water Framework Directive

32 substances or group of substances have been identified that are of major concern for European waters. Once the list of priority substances is adopted, the Commission will propose community-wide water quality standards and emission controls for the priority substances.

Within the list of priority substances the Commission has identified the priority hazardous substances which are of particular concern for the freshwater, coastal and marine environment. Discharges, emissions and losses of these substances will be phased out within 20 years.

In addition to the proposed legislation listed above, there are constant updates to European Directives as new information becomes available about the environmental impact and safety profile of substances, processes and patterns of use.

Timeline for Key Legislation



Appendix 2: Green Chemical Technology Areas

Crystal has defined the following key technology areas in green chemical technology:

1. Green product design

Designing products to minimise environmental impact. Including use of life-cycle analysis in the design process and design for recycling and re-use:
- Design for efficient manufacture and recycling
- Reducing mass and energy intensity
- Biodegradable and compostable products
- Products with intrinsically lower toxicity
- Smart materials that save energy in manufacture and use, eg greenhouse coatings that control heat absorption and loss
- Nanomaterials that use less mass to deliver a specific effect

2. Feedstocks

Use of unconventional feedstocks to substitute for non-renewable or hazardous materials.
- Agricultural crops
- Biomass for manufacture of building blocks: eg ethylene and propylene.
- Carbon dioxide as a feedstock
- Biomimetic routes

3. Novel reactions

Development of novel routes to deliver the required product functionality.
- Rapid processes pushing kinetic limits
- Enzymatic processes
- Genetic modification for production of functional molecules
- Single molecule manipulation
- Nanoscale manufacture – molecules on demand

4. Novel catalysis

New types of catalyst to increase selectivity, access new areas of chemistry, and to reduce energy consumption and waste production.
- Biocatalysis
- Self-assembling catalyst systems
- Solar energy and visible light catalysis

5. Solvents

Solvents represent the biggest pollution risk in many current processes. New processes are required that ensure solvents are properly contained, eliminated or replaced with environmentally benign alternatives
- Closed solvent processes
- No solvent processes
- Dry reactions – microwaves, mechanical action
- Alternative solvents
- Supercritical carbon dioxide, ionic liquids and beyond

6. Process improvement

Novel process routes that dramatically improve atom efficiency and energy consumption.
- High throughput techniques
- Microchannel reactors
- New reactor technologies
- Spinning disk
- Micro-reactors using enzymes, ribozymes and cellular systems
- Process integration
- Novel energy sources
- Pipeless plants

7. Separation technology

New methods for extracting components from reaction systems that are highly efficient and selective.
- Membranes
- Reactive separation

8. Enabling technologies

A cluster of technologies that will underpin the development of Green Chemistry, including new measurement techniques, informatics and predictive modelling:
- Analytical science
- Cheminformatics and bioinformatics
- Improved modelling, prediction and knowledge management
- Robust non-animal testing methods
- Nanotechnologies
- Sensors for feedback systems

Appendix 3: Core Participants

Core Participant	Affiliation
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Dr Nick Hazel	BP
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