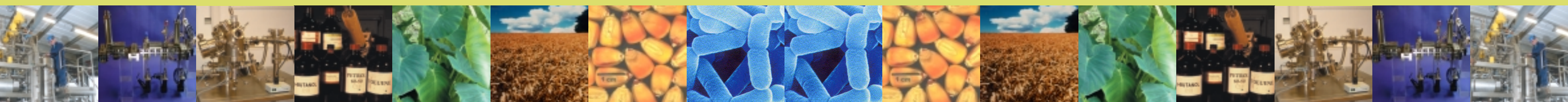


BENIGN AND SUSTAINABLE CHEMICAL TECHNOLOGIES



*A Workshop sponsored by the
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This report summarises the proceedings, conclusions and recommendations of a research workshop on Benign and Sustainable Chemical Technologies organised by the RSC and held at King's Manor, York, 20–21 October 2003. It is not intended as the final word on the status and prospects for Green Chemistry and Sustainable Technology Research in the UK. Rather, it represents what the workshop participants — collectively — identified as gaps, opportunities and areas that should be promoted in order to stimulate further development and innovation in green chemistry. We are indebted to the participants for giving their time, effort and energy, for their enthusiasm, and for their lively contributions to the discussions, formal and informal. This document does not necessarily represent the views of the RSC.

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The Royal Society of Chemistry is pleased to present this composite picture of discussions that took place at the RSC-sponsored Workshop on Benign and Sustainable Chemical Technologies, held at King's Manor, York, on 20-21 October 2003. In the near future, RSC will collaborate with the Institution of Chemical Engineers in producing a short policy document arising out of the recommendations reported here.

*Rodney Townsend
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FOREWORD

The “*Whitesides Report*”, as it is informally known, summarised the findings of the International Assessment of UK Chemistry Research. In this document the review panel drew particular attention to the current state of UK green and sustainable chemistry research and stressed the importance of developing these activities further, propelling them beyond industrially driven initiatives towards truly innovative research. Multidisciplinary and collaborative research were seen as essential elements in any such development. This implies, among other things, bringing new people into the field. Green chemistry research is indeed intrinsically multidisciplinary—therefore the framework of this RSC-organised workshop extended beyond chemistry itself.

The aims of the workshop were to raise further the research profile of benign and sustainable chemical technologies, to respond to the recommendations of the International Assessment and to set the context for future RSC action. Leading researchers already active in this area joined other key players in order to examine current research activity and identify major challenges and opportunities for the future.

An invited panel of 31 UK chemists, engineers, agricultural chemists, biologists and biochemists from both academia and industry participated in the workshop. Keynote lecturers opened the proceedings by reviewing important areas, emphasising how these fitted into the wider context of science and technology. The workshop was structured around two sets of breakout sessions to maximise individual participation and encourage discussion across discipline boundaries.

The topics discussed were:

- *Raw Materials, Agriculture and Chemistry*
- *New Chemical Routes—Solvents and Chemicals.*
- *Catalysis, Biocatalysis and Materials*
- *New Process and Process Strategies*
- *Environmental Biotechnology*

The chairs of the first set of breakout sessions reported their findings at a plenary session where they were debated in order to define the issues to be addressed during the second set of breakout sessions. Accordingly, on the second day the panel divided into three groups to discuss raw materials, products, and processes.

Funding modes were also discussed, including topics such as the relative merits of single investigator grants *versus* collaborative projects, and there was a good level of interaction between panel members and the Research Councils’ representatives. We welcome this participation by the EPSRC and the BBSRC, which constitute the principal governmental sources of support for academic research in the chemical sciences. Their contribution to the meeting was very valuable in enabling the formulation of shared strategies and identifying new opportunities for the research community. EPSRC’s financial support of the workshop is also gratefully acknowledged.

This report summarises the conclusions and recommendations emerging from the workshop.

What was achieved? Through dialogue between industry and academia a wide range of topics deserving further attention from the research community has been identified. Multidisciplinary debate on a common theme involving chemists, biologists and engineers—and the recognition that more needs to be done here. Another step towards bringing the Research Councils and the research community closer together. Moreover, the RSC’s strong commitment to the subject area was clearly demonstrated.

Exciting science based on multidisciplinary research programmes is anticipated—such projects should also attract newcomers into the field and will complement and extend activities currently carried out under the Faraday Partnerships.

A final word. One of the most encouraging aspects of organising this event has been the enthusiastic support received from the community *before, during* and *after* the workshop.

Alejandra Palermo and Colin Webb



From left to right. John Pierce, Neil Bruce, Rodney Townsend, Adisa Azapagic, Roshan Jachuck, Alejandra Palermo, Gary Sheldrake, James Clark, Colin Webb and Brian Hayden.



Martyn Poliakoff

Lynne Macaskie, Neil Bruce, Chris Knowles, Jonathan Spencer, Cliff Burton and Ben Sykes.



1. EXECUTIVE SUMMARY

A wide-ranging workshop on “*Benign and Sustainable Chemical Technologies*” held at King’s Manor, York, 20-21 October 2003 was organised by the RSC as part of its strategic response to the recommendations of the 2002 EPSRC-sponsored International Review of University Chemistry Research in the UK. This workshop’s principal findings and recommendations are summarised below.

- 1) The UK needs to attract more investigators from a range of disciplines into Benign and Sustainable Chemical Technology research. Multidisciplinary teams will be very important drivers for developing new technologies within both academia and industry. Chemistry will play a vital role in formulating the new concepts necessary to understand and exploit highly complex systems—leading to revolutionary advances.
- 2) Chemical engineers and chemists should work together closely from the earliest stages of a project. For instance, in the development of greener technologies, improved separation methods can have as much impact as synthetic strategies. Therefore one promising strategy is integrated design from the macroscopic scale down to the molecular scale—for example by combining reaction and separation. Clearly, such advances will depend critically on close collaboration.
- 3) Agricultural crops can provide a new range of *platform chemicals* that may be used as intermediates; hence there is a need to focus chemical research in this area, in both upstream and downstream directions. The goal of whole crop utilisation requires crop optimisation: it is critically important for government to initiate relevant research.
- 4) The potential of catalysis and biocatalysis as tools for sustainable chemical technologies is very great. Integration or combination of bioconversion with chemical conversion offers exciting prospects and is an area that should be strongly encouraged: it is essential that chemists learn to regard enzymes as part of the standard tool kit for synthesis.
- 5) The creation of new material structures aimed at sustainability requires focused and precise synthesis of building blocks using, for example, biological processes. Such activity is lacking in the UK.
- 6) A major barrier to implementation of new, greener solvents is the relative lack of data on fundamental physical properties and information about toxicity. These gaps need to be addressed urgently.
- 7) Ways should be found to publicise within the industrial arena the economic benefits of new greener technology.

Specific Recommendations

- 1) ***Stimulate the further development of Benign and Sustainable Chemical Technologies through focussed Research Workshops.***
 - ❖ Act to bring more organic chemists into green chemistry research: *most industrial processes consist of organic chemical reactions but most organic chemists do not automatically think “green”.*
 - ❖ Organise meetings designed to bring together the distinct and currently separate

catalytic communities (homogeneous, heterogeneous, biocatalysis, photocatalysis, electrocatalysis, bio-electrocatalysis) from both industry and academe. *This will be an important step towards fostering creativity.*

- ❖ Bring chemical engineers and chemists together at an early stage in the development of greener processes. *Both groups should play a key role in scaling-down and decentralising the production of chemicals—miniaturisation, intensification and the use of sophisticated technologies calls for an early dialogue and a common language.*
 - ❖ Encourage further the involvement of chemists in environmental biotechnology research. *Bioremediation and marine biotechnology are important areas that require chemistry. Development of transducers for communication between cells and devices and the use of information technology are examples of exciting opportunities in this area. Understanding the concept of bioavailability.*
- 2) Provide the right forum for chemists and engineers to begin a dialogue; recognise common aspirations and identify opportunities that can be exploited by collaboration. IChemE and the RSC working together may have a role here. This could be achieved by means of**
- ❖ summer schools
 - ❖ focussed research workshops
 - ❖ devising appropriate training modules for chemists in, for example, process technology
 - ❖ continuing and expanding the joint accreditation of courses
- 3) Continue allocation of Research Councils' resources to "Benign and Sustainable Chemical Technologies". Optimise the use of these resources by**
- ❖ facilitating collaborations across research council boundaries
 - ❖ attracting newcomers to the field by promoting increased awareness of the subject within the research community as a whole.

2. INTRODUCTION

In October 2002 the EPSRC sponsored a major review of the state of academic chemistry in the UK. This review—managed by the RSC—was carried out by an international group of thirteen leading scientists and industrialists chaired by George Whitesides of Harvard University. The Panel's report *Chemistry at the Centre—An International Assessment of University Research in Chemistry in the UK* was published in December 2002, followed by a public presentation in January 2003 (<http://www.rsc.org/lap/polacts/uniresearch.htm>). The report could not have appeared at a more opportune time. Its public release almost coincided with the DfEs White Paper on *The Future of Higher Education* and with the appearance, a month earlier, of the report produced for the Science Minister, Lord Sainsbury, by the Chemicals Innovation and Growth Team on the Chemicals Industry in the UK. The White Paper acknowledges that current strength in UK research cannot be maintained unless substantial changes are implemented; it also recognises the continued growth in competition from other countries. The CIGT report establishes that the UK chemical industry needs to (i) earn a better public reputation, (ii) respond to the challenges of sustainable development, (iii) increase innovation by improved use of science and technology, (iv) recruit a more diverse workforce to ensure availability of the right sets of skills and competences. These three reports convey a very similar message, though in different ways and with different emphasis. Together, they represent a clear wake-up call for the scientific community in general and for the chemistry community in particular.

Some of the major scientific concerns expressed in the “*Whitesides Report*” were:

- Creativity is perceived to be slipping: the quality of scholarship in chemistry in the UK is comparable with the world's best; levels of innovation, step changes in thinking and ground breaking discovery are declining.
- Financial/organisational structures favour conservative research. The system does not encourage revolutionary, multidisciplinary and exploratory research. It does not facilitate the links with chemical engineering, physics, biology, medicine and materials science.

The report made key recommendations that were intended to address the perceived decline in creativity within academe,

*“Work with the chemical community to develop and articulate opportunities, and formulate a strategy for academic chemistry:
—develop a rolling strategic plan for academic chemistry
—encourage the academic chemical community to generate initiatives, rather than responding to those developed by government
—use the power of the top departments to strengthen departments at the next level and increase the number of internationally first-tier departments;
preserve the strength of current top-tier departments”*

Undoubtedly, it is the community itself that should foster creativity by generating initiatives, and helping the research councils to focus more effectively their resources. Hence the role that RSC sees for itself is as *facilitator*, providing the forum that makes possible effective dialogues between the academic community and the Research Councils, between academia and industry, and between universities and government, enabling constructive interactions between all of these groups. In this respect, the RSC is unique in that it is *the* professional organisation that represents the chemical sciences in the UK.

The *Whitesides Report* affirmed that the chemical sciences are central for the achievement of scientific innovation advances in the 21st century. Particular note was made of the current state of green chemistry research, emphasising its importance and encouraging further development of these activities, thus: “*If the UK wishes, as a matter of public policy,*

seriously to address environmental issues, it must engage some of the most able research groups in academic chemistry". And more specifically: "Multidisciplinary and collaborative research involving multiple departments and universities, and specifically including chemical engineering, are essential for significant progress".

A number of projects have been identified by the RSC with the aim of ensuring that the major recommendations of the International Review are carried forward. The first of these was the two-day Research Workshop in **Benign and Sustainable Chemical Technologies** that took place on 20/21 October 2003 at King's Manor, York. This event emphasises the RSC's commitment to this area and its intention to raise its profile within the academic and industrial communities.

Over the last five years the RSC has committed significant resources to this area, supporting the establishment of the Green Chemistry Network at York University as well as providing substantial effort towards the development of the Crystal Faraday Partnership where the RSC is one of three hub partners, along with the Chemical Industries Association and the Institution of Chemical Engineers. In addition, the RSC has led the way by introducing two new journals related to the areas of benign and sustainable chemistry, *Green Chemistry* and *Journal of Environmental Monitoring*. The attitude of the RSC towards green chemical technology is therefore one of public commitment and active support through:

- the further development and incorporation of benign, chemical technological thinking into education at all levels;
- the inculcation of best practice wherever the profession of chemistry is practised;
- the encouragement of creative and innovative research on benign chemical technology;
- a campaign that chemistry is *the central solution* to the needs of society: sustainability, human health, the environment and economic goals

Thus, in response to the Whitesides Review, the overall aims of the York workshop were to raise the national profile of the field and to sharpen the RSC's own related objectives.

WHAT IS GREEN CHEMISTRY?

During the 1990s, the US Environmental Protection Agency (EPA) developed a pioneering concept that became known as green chemistry. Green chemistry involves promoting the design of environmentally benign processes that minimise or eliminate the use of toxic substances (feedstocks, reagents, solvents) and maximise overall efficiency (reduction of unwanted by-products, especially toxic materials). The guiding principle is prevention rather than cure—it is far better to prevent toxic waste from being produced in the first place, rather than cleaning up after the fact. Green chemistry encompasses all aspects and all types of chemical processing—including synthesis, catalysis, reaction conditions, separations, monitoring and analysis—that reduce negative impacts on human health and the environment. The current challenge is to expand the concept of green chemistry to encompass a broader view of sustainable development. And this was one of the guiding principles of the workshop.

STRUCTURE AND CONTENT OF THE WORKSHOP

An invited panel of 31 UK chemists, engineers, agricultural chemists, biologists and biochemists and included representatives from both academe and industry attended the workshop (see Appendix 1). These participants were selected after wide consultation within RSC and with other organisations (Research Councils, IChemE, Green Chemistry Network and the Crystal Faraday Partnership).

Biotechnology is becoming more important to the future of the chemical industry as biotechnological strategies become increasingly viable, both environmentally and economically. This is highlighted by the 2003 Presidential Green Chemistry Challenge Awards (Washington, USA), where three of the five winners were honoured for their bio-based developments in innovative syntheses, process improvements and new products that promote pollution prevention. One of the winners was DuPont who developed a commercially viable bioprocess for production of 1,3-propanediol from corn-derived glucose. In this context, Dr John Pierce, Director of Biochemical Sciences and Engineering Central Research, DuPont USA, agreed to open the workshop and gave a superb address entitled “Green and Sustainable—a Work in Progress”.

Day One began with a series of keynote lectures. These did not address the speakers’ own research achievements but instead gave a broader view of the state of the art in the relevant area, facilitating the ensuing discussions. The speakers were: Professor Rodney Townsend, RSC Director of Science and Technology, Malcolm Wilkinson, Crystal Faraday Director, Dr Jeremy Tomkinson, National Non-Food Crops Centre, Dr Cliff Burton, Viridian EnviroSolutions Ltd., Professor Keith Smith, Chemistry Department, Swansea University, Professor Andrew Livingston, Chemical Engineering Department, Imperial College of Science, Technology and Medicine, Dr Roshan Jachuck, Chemical Engineering Department, University of Newcastle upon Tyne, and Professor Martyn Poliakoff, School of Chemistry, Nottingham University.

The workshop emphasised discussion and brainstorming, partly through small multidisciplinary working groups. First, the panel divided into 5 groups structured so as to fully engage the participation of all concerned. These were:

- *Raw Materials, Agriculture and Chemistry*, chaired by Professor Colin Webb, Chemical Engineering Department, UMIST
- *New Chemical Routes—Solvents and Chemicals*, chaired by Dr Gary Sheldrake, Chemistry Department, Queen Belfast University.
- *Catalysis, Biocatalysis and Materials*, chaired by Professor Brian Hayden, Chemistry Department, Southampton University
- *New Process and Process Strategies*, chaired by Dr Roshan Jachuck, Chemical Engineering Department, University of Newcastle upon Tyne
- *Environmental Biotechnology*, chaired by Professor Neil Bruce, Biology Department, York University

In each area, the discussion focussed on (i) recognising gaps, (ii) identifying potential advances and (iii) spotting key areas that should be promoted. The relative merits of single investigator grants *versus* collaborative projects were also considered.

Findings from these group sessions were discussed in a plenary session which served to define the issues to be addressed in a second set of three breakout sessions on Day Two: *Raw Materials*, chaired by Dr John Pierce, Dupont USA, *Products*, chaired by Dr Ian MacKinnon, Thomas Swan & Co. Ltd. and *Processes* chaired by Dr Adisa Azapagic, School of Engineering, Surrey University. Conclusions from these were also presented to the workshop as a whole and formed the basis for a final discussion.

The following sections highlight the outcomes of the various discussions held during the workshop. Whilst they represent fairly extensive views, based on the wide range of experience of the participants, they are not intended to be exhaustive nor definitive. Rather they offer a basis for further discussion and debate.

3. RATIONALE FOR MULTIDISCIPLINARITY

The report of the 2003 Royal Commission on Environmental Pollution on *Chemicals in Products—Safeguarding the Environment and Human Health* makes a strong case for Green Chemistry. The EU Chemicals Policy Review—REACH—hailed as the most important chemicals related regulation in 20 years, focuses very much on products. Significantly, this is also reflected in the Royal Commission report:

“We recommend that the government together with the chemical industry continue to promote programmes for the development and promotion of green chemistry but with a new emphasis on its application to product design and use.”

Green Chemistry thus requires consideration of all parts of the life cycle of chemical products – from feedstocks through process to product fate. Important factors include product toxicity and environmental impact, biodegradability, and recyclability. The challenge for chemists in collaboration with toxicologists and environmental scientists is to design new chemical products that provide the required effects at a price the market can bear, while not threatening human health or the environment. There will be a need to distinguish between performance products (formulations) and specification products (molecules). Other challenges include:

- increasing the use of sustainable resources, hence improving environmental acceptability
- increasing the current rate of substitution of undesirable (toxic/environmentally hazardous) chemicals
- intensifying and simplifying production processes
- development of “*destructor*” technologies for organic compounds to prevent their accumulation in the environment
- introducing legislation—inevitably leading to winners and losers—that will drive these developments.

Sustainable development clearly requires a complex balance between use of resources, economic growth and competitiveness, and socio-environmental impact. Progress in science and technology can address these challenges locally and globally, in terms of global environmental sustainability—climate change, transport, energy and food production, depletion of non-renewables, bioaccumulation of contaminants, and accumulation of toxins such as endocrine disrupters. However, the technologies required to accomplish these goals are many and varied and involve much more than just the core of chemistry, including for example: agricultural sciences, biotechnology and biological sciences, economics, engineering, social awareness and public policy.

Petrochemical processes have provided low cost production routes for fuels, plastics and chemicals for well over 50 years but the escalating impact on the environment and the inevitable future depletion of fossil feedstocks make it essential that benign, sustainable, alternatives be developed commercially in the very near future. We already have the means to develop advanced technologies to overcome environmental burdens, improve the quality of life and create new business opportunities. But this can only happen with full co-operation between a wide range of currently disparate disciplines. An effective way to replace many hazardous and noxious chemical processes may be through bioprocessing, yet the development of biotechnology has largely been limited to the production of high-value low-volume products because of relatively poor production economics. There is much to be gained by the synergistic combination of chemistry, biotechnology and process engineering in undertaking the difficult restructuring of the organic chemical industry for the production of commodities (fuels, chemicals and plastics) from alternative raw materials.

4 RESEARCH OPPORTUNITIES

4.1 Raw Materials, Agriculture and Chemistry

The raw materials for benign and sustainable chemical technologies need not necessarily be renewable but must be available on a sustainable basis. In other words, there must be a balance between their production and consumption that does not threaten the availability of future supplies. Ultimately this does lead to the need for renewable feedstocks and, in the limit, this implies chemicals produced through photosynthesis along with fresh water and greenhouse gases such as carbon dioxide and methane.

Plant-derived renewable raw materials can be divided into starchy crops, sugar crops, oil seeds crops and lignocellulosic biomass including agricultural residues. The selection of the appropriate raw material to supply industry is dependent on infrastructural, economical and technological factors (*e.g.* availability, skilled workforce, pre-treatment technology and costs, and transportation). In much of the world, the best candidates to meet these prerequisites are cereals, while the economic and efficient utilisation of lignocellulosic biomass (*e.g.* agricultural wastes, wood, straw, municipal solid wastes) is a “holy grail”, the pursuit of which calls for significant further research.

The approach to the utilisation of renewable raw materials can be either to extract valuable end products directly (most crops are, after all, rich and complex in terms of their chemistry) or to break them down to relatively simple molecules from which desired end products can be synthesised (a kind of *cracking* and *reforming*). In practice both approaches will likely be used, often in combination. The technological challenges then become: to optimise crops to produce specific end products; to develop suitable extraction processes (which must themselves be benign and sustainable); to develop the chemistry necessary to synthesise the molecules that we are familiar with (*e.g.* aromatic hydrocarbons, ammonia) from a new raw material and/or to develop new set of chemistry based on the chemicals that are readily available (*e.g.* starch, sugars, oils, proteins and their derivatives).

Interesting new commercial challenges will also arise from the switch to renewable raw materials. Many of the high-value end products that can be extracted from crops are available or required in only kilogram per annum amounts. Alongside them, however, will be tonnes of by-product materials of significantly lower value, which must also be processed to end products. This will need commercial structures that can handle the production and distribution of very wide ranges (in terms of quantity and value) of materials. On top of this, it is likely that supplies of the raw material will be seasonal and so continuity of supply will have to be addressed; however examples such as sucrose extraction from sugar beet show this to be viable on an annual basis. Transportation over long distances can in some cases be an issue if low bulk densities are encountered; therefore primary processing close to the site of collection should if applicable be developed and endorsed.

Recognising Gaps. Given that the feedstocks for the organic chemical industry of the future are likely to be produced through agriculture it is reasonable to consider whether conventional technologies are appropriate. Intensified, local small-scale processes might therefore be appropriate, even for the production of large volume (commodity) products. Agricultural crops are an excellent source of oxygenated molecules and there is a need therefore to focus chemistry research on these. Rather than simply trying to produce petrochemical substitutes, the opportunity exists to create a whole new range of platform chemicals, which can be used as intermediates. To identify potential candidates, research is required in both downstream and upstream directions (*i.e.* what intermediates can be easily produced from the raw materials? and what intermediates would be required to produce

particular end products?). The former could involve, for example, bioconversion research, while the latter would benefit from retro-synthetic analysis. Whatever products and processes are developed it is clear that as much of the raw material as possible should be used and that the crop should therefore be optimised (*e.g.* in terms of the relative mass of vegetative to seed material) for whole crop utilisation.

Whole crop utilisation may be achieved by alternative strategies. Crops may either be tailor-made for a specific sector, or consortia of industrial end users created that can use the chemical fractions present in a particular crop. There is currently little activity in this area, partly because the kind of crops envisaged for industrial chemical use (*e.g.* cereals, potatoes and oilseeds) are primarily food crops and the incentive to improve them for their food-use is clearly much greater. However, where crops are used only for industrial purposes, (*e.g.* cotton) optimisation for improved processing is already well underway. This would suggest that such investment would occur if a return were likely. To pump-prime this process it will be essential for governments to initiate relevant research and provide incentives for industry to change the reliance on petrochemical feedstocks. This has already happened to some extent, though not particularly in the UK, in creating the biofuel economy. Such developments will lead wholesale advances in fermentation technology, from which other bioconversions will benefit. There is a strong analogy here with the development of the petrochemicals industry, which was driven by advances in petroleum refining for fuels production. Once agricultural crops become competitive with non-renewable resources commercial activity will proliferate. This is beginning to occur in the case of maize (corn) where the corn:oil price ratio is near to unity again after 150 years of being considerably greater than one.

Despite the potential to improve crops for non-food uses there will always be the dilemma of having to balance food and non-food needs for those crops that can serve both purposes. Even for those crops that only have non-food uses the dilemma still exists based on land usage. Whilst this is an emotive issue it must be accepted that, ultimately, market forces will control the balance, as farmers will plant the crops that they perceive as being the most profitable. Hence, in the US considerable acreage is given over to the production of established industrial crops such as cotton, while in the EU agricultural policies currently encourage the planting of some non-food crops, *e.g.* oilseeds. This is likely to increase with the expansion of the EU through the inclusion of countries in Eastern Europe, where there is much under-utilised land.

Identifying Potential Advances. Whilst there is enormous potential for the development of new chemical technologies based on the processing of agricultural raw materials it is also clear that this must in many cases be undertaken in close collaboration with biotechnological disciplines. Primary biotechnological processing, *e.g.* fermentation or biocatalysis, will lead to a more *natural* and cost-effective means of converting complicated natural feedstocks such as starch into single *platform* chemicals like levulenic acid that can be further derivatised through chemical synthesis into a wide range of high added value chemicals/materials, *i.e.* the biorefinery concept. These too, in some cases, could be produced biologically and it is therefore essential that chemists learn to regard enzymes (biocatalysts) as part of the standard tool kit for synthesis. Considerable benefit will come from the collaboration of chemists, biotechnologists and biochemical/bioprocess engineers but specific programmes or projects are required to provide the generic forum for this cross fertilisation to occur.

Platform chemicals that can be produced in large quantities by microorganisms include acetic acid, ethanol, glycerol, succinic acid, pyruvic acid, 2,3-butanediol and 1,3-propanediol. They are different from the building blocks currently used by petrochemical processes (*e.g.* ethylene, propylene and butadiene) and therefore require significant research in order to accomplish the technological breakthroughs necessary to the development of commercially viable processes. Other platform chemicals attracting the interest of scientific communities

(and significant government funding, outside the UK) and large-scale industries include lactic acid, levulinic acid and pyruvic acid. In the United States *The National Sustainable Fuels and Chemicals Act* of 1999 authorized \$49 million per year for six years in new Federal funds to “support research focused on improving the fundamental understanding of biomass conversion technologies and environmental impacts and lowering the processing costs by technology advances”.

Key Areas that Should be Promoted. These include the identification of the full range of platform chemicals obtainable from agricultural raw materials. This will involve a combination of bio-related research directed downstream from the raw material and retro-synthetic chemical analysis, starting from the other end. Having identified the platform chemicals there will be a need for the development of new synthetic protocols and methodologies, to produce both traditional and new products. Plant breeding focussing on obtaining the optimum raw materials will be essential to improve the commercial viability of subsequent processing activities. Further development of fermentation and associated biotechnology, including modelling and control of bioprocesses and improved understanding of enzyme mediated biosynthesis, will also be required. Given that it may be necessary to carry out processing at source, research into process technology for appropriate scales of production would be beneficial.

The commercialisation of products based on renewable raw materials will clearly be dependent on the co-operation of numerous disciplines, such as chemistry (agricultural, synthetic, bio-organic, physical organic), agronomy, biology, biochemistry, biochemical/biomolecular engineering, materials science, process engineering, computer science and mathematics. Novel and highly useful tools could be provided from each of the above disciplines, the effective utilisation of which could lead to the development of viable processes for the production of fuels, plastics and chemicals. Bio-related disciplines could provide the knowledge of how case-specific microorganisms function. Engineers could develop novel reaction and separation equipment that can meet the needs of specific processes. Computer science and mathematics could assist in the modelling, control, simulation and optimisation of processes, especially in the absence of pilot scale trials and intensive laboratory experiments. For bioconversion reactions, metabolic engineering is a most appropriate tool, derived from the co-operation of many of the above disciplines, which can assist in the understanding of industrial microorganisms, the optimisation of bioconversion feedstocks and the increase of bioconversion productivity and yield.

A very important factor that will determine the sustainability of any process is detailed life cycle analysis. Only by carrying out such analyses can the *real* cost-effectiveness of renewable resources be properly assessed. The true ratio of energy output to energy input for each process is crucial for the creation of sustainable technologies. It is evident that any large-scale operation requires large amounts of energy, which is currently provided by fossil fuels. Energy could be generated by utilising components of the renewable raw materials (*e.g.* ligno-cellulosic residues). It is also important to conduct a CO₂ mass balance for each process, incorporating the cost of both energy and carbon, so that the true technical and commercial benefits are clearly apparent. Some reactions can achieve CO₂ fixation in the production of specific platform chemicals (*e.g.* microbial production of succinic acid and fumaric acid). This means that the constructive application of specific bioprocessing could not only reduce CO₂ emissions but also utilise CO₂ produced from other bioprocesses. Therefore developing a financial model that allows for the internalisation of the true cost of production, use and disposal for any material is crucial if wholesale adoption of renewables technology is to be realised. Currently, little or none of the costs associated with disposal, renewable carbon content and energy inputs are applied to commodity materials. If these factors were included in the overall price then chemicals derived from renewable resources would be cost advantageous already as their carbon neutral nature allows the carbon fixed in the structure to be released through biodegradation for reuse in the following cycle.

4.2 New Chemical Routes: Solvents and Chemicals

Recognising Gaps. Successful research in reducing the environmental impact of solvents in chemical manufacture has included the development of new benign reaction media, new processes and reactor design, and the elimination of organic solvents by the use of aqueous catalytic and biocatalytic transformations. Future progress in the area of sustainable development will require a more integrated collaboration across the disciplines of organic synthesis, physical-organic chemistry and chemical engineering.

Solvents are a natural starting point for a chemist or engineer wishing to improve the environmental performance of a multistage chemical process. Solvents have an important role in many processes and may be chosen to influence the mechanism or selectivity of a reaction or to facilitate product isolation thereby assisting overall process efficiency. However, solvents are often present to act mainly as a heat sink or as an inert medium to facilitate mixing of reagents. They are not usually incorporated into the molecular structure of the product but often form the major component of the mixture and so make the most significant adverse contribution to atom efficiency, especially if recovery is poor.

Much improvement in solvent usage can be achieved by traditional process chemistry and engineering approaches such as telescoping of stages, avoiding solvent changes between reactions, more efficient recovery and recycling and process intensification. Indeed, these simple “housekeeping” approaches have been responsible for some of the most impressive improvements in environmental performance by fine chemical companies during the last two decades. These improvements are often a testament to the co-operation between chemists and engineers in industry and can provide valuable lessons for interdisciplinary research approaches in academia.

Identifying Potential Advances. Improving environmental performance through better process development, *e.g.* process intensification and reactor design to reduce solvent inventory and innovative reactor design continues to provide new opportunities. These are explored in more detail in the section *New Processes and Process Strategies*.

Solventless reactions, in which reactants are mixed in close to equimolar proportions as eutectic mixtures or as liquids rather than using one reactant in excess as a surrogate solvent, have always played a small but important role in the design of new reactions. In these cases, the product can usually be readily isolated from the excess reagent (*e.g.* by precipitation or distillation) and the excess reactant re-used in the next batch. The scope of such reactions is, however, often limited for conventional large-scale batch reactions due to poor control of exotherms and problems associated with mixing. A combination of novel reactor designs and continuous processing can provide new opportunities for solventless reactions. A number of international research groups are active in this area and significant niche applications are emerging.

The proliferation of biocatalysts has greatly extended the range of chemical transformations that are available in aqueous medium and this has been matched by the development of water-tolerant, non-biological catalysts and reagents. The drive towards the use of water as a reaction solvent has probably been the largest common theme of “green” research programmes over the last two or three decades. However, while water can be regarded as a benign solvent, water contaminated with even small amounts of organic or inorganic components can pose a greater environmental control problem than a properly contained and managed organic solvent. For any aqueous process there is also the issue of product isolation, often particularly problematic with whole-cell biotransformations where large volumes of solvent are used for extraction. Furthermore, the efficient recovery of organic solvents from such extractions is frequently made more difficult by the entrainment of water.

Aqueous reactions are environmentally benign only if the water can be recovered easily in a non-contaminated state at the end of the process.

Solid-phase synthesis has provided many potential benefits for creating more benign chemical processes. The main benefits are in the simplification of work-up and product isolation because of the separation of the phases, either solid-supported product from reaction solution or solid-supported reagents from product solutions. A recent advance is that of polymers with switchable properties. Supported reagents can be dissolved in the reaction mixture and then precipitated prior to work-up by changing physical properties such as temperature or pH. This overcomes one of the main disadvantages of solid-supported synthesis, the poor efficiency of diffusion of reactants through the solid matrix.

There have been other successful approaches to the total phase separation of reagents/catalysts from reactants and products. Fluorous biphasic systems and ionic liquids are two of the main areas of research in this field. There are many elegant examples which exploit the total immiscibility of fluorinated solvents with water to reduce cross-contamination of reagents/catalysts with products essentially to zero. However, there are concerns about the environmental impact of the manufacture of these materials and their potential "greenhouse" effect if released to the atmosphere. Research on ionic liquids has resulted in a nearly infinite array of potential *designer* solvents. In principle, these materials can be produced to satisfy the demands of most chemical reactions by varying the combinations of anions and cations to suit the requirements of the processes. There is considerable industrial interest in the use of ionic liquids in organic synthesis, given the zero vapour pressure and high potential for recycling of these compounds. The biggest barrier to implementation is the relative lack of fundamental physical property data and toxicity information compared with that available for conventional solvents.

Another approach is the use of supercritical fluids, especially supercritical carbon dioxide. Reactions are carried out under relatively mild temperatures and pressures and the solvent can often be recovered by low temperature evaporation/condensation. In the case of supercritical (or near-critical) water based processes technological problems exist because of the high temperatures and pressures involved. This area will require the continued partnership of chemists and engineers for future development.

There is a need to derive organic solvents from sustainable feedstocks but such solvents must still be regarded with caution. They may be benign in terms of renewable raw materials but all the other environmental concerns about solvent use still apply. Bioethanol has been available as a commercially competitive commodity for some time and it has already been demonstrated that esters, *e.g.* ethyl lactate, can be produced relatively economically from renewable raw materials. There have also been some studies on the use of CO₂ as a sustainable raw material. Esters such as diethyl carbonate have been produced in multi-tonne quantities for various solvent applications.

Key Areas that Should be Promoted. When introducing a "greener" solvent into a process, the chemical community must be sure that the problem is not simply shifted up- or down-stream. A benign solvent may provide an immediate and measurable environmental benefit if emissions are reduced, the reaction can be carried out more selectively and under less extreme conditions or if the solvent is completely recovered at the end of the process. However, these benefits may be negated if a multi-stage synthesis is required to produce the solvent or if it generates environmental or toxicological problems. Many industries have begun to look at the total life cycle of materials associated with their processes. It is no longer acceptable to become green simply by shifting the responsibility to a third party.

There is no single, ideal approach to solving the problems of a sustainable chemical industry. Research in several unconnected areas has provided practical, applicable technologies for

industry and so support for diversity in research is strongly endorsed. Technology that industry has been able to apply to solve environmental problems has often arisen from research that had completely different aims.

The chemical industry, which will be the ultimate major consumer of new solvents, clearly desires a wide choice of possible solutions to a given problem. Currently there is a diverse array of new reaction media but insufficient predictive criteria for selecting a solvent for a given reaction largely because of the lack of physical property data for these media.

Transfer of technology and ideas from academia to industry is often an unstructured process. Commercial organisations rely on protecting their intellectual property to remain competitive and it is thus difficult for industry to share their most important strategic aims with academia. Collaboration between industry and academia is, however, important for both parties and this is best achieved by wide dissemination and effective communication of academic research to the industrial community.

Lastly, most research and development chemists think of solvents in the context of media for supporting chemical reactions. However, in the broader context, the major uses of solvents in terms of volume would be in non-chemical applications such as cleaning, lubrication and the basis of fluid media for a huge array of industrial processes. These applications are, arguably, beyond the remit of this workshop but many of the general conclusions would apply equally, especially the production of solvents from renewable raw materials.

4.3 Catalysis, Biocatalysis and Materials

Recognising Gaps. The applications of catalysis in current chemical technology—from fuels processing, commodity chemicals and polymers to fine chemicals and pharmaceuticals—are all pervasive. Nearly 90% of all industrial processes are catalytic. The potential for new applications of catalysis in the field of benign and sustainable chemical technologies is very great. This is not unexpected, given that nature itself relies on the extraordinary efficiency of a wide range of catalysts to sustain all aspects of the life cycle. Existing industrial applications of catalysis are however often associated with one or more of the following drawbacks: the use of large quantities of solvents in complex separations; high temperatures and pressures; catalyst materials that are difficult to separate from the products, cannot be recycled after usage or are environmentally hazardous. The pressing need for and the technical challenges imposed by the development of clean catalytic systems are therefore clear.

Identifying Potential Advances. The effective application of catalytic solutions to sustainable chemical technologies encompasses two broad areas. Firstly, non-incremental improvements in existing processes. This should be by means of waste elimination and reduction of emissions at source rather than end of pipe treatments. Also the use of alternative forms of energy and the development of gentler processes (lower temperatures and pressures). A good example of non-incremental improvement is the new catalyst developed for selective production of phosgene which meets tighter regulations by reducing CCl_4 waste.

Secondly, the development of new catalysts to drive new processes based on alternative raw materials derived from sustainable resources. A recent important example in the production of high value intermediates is provided by the large scale, low cost production of levulinic acid (used in fragrances, food, and speciality chemicals) by a new direct hydrolytic route from cellulose. The production of pyrrolidinones (high value solvents, surfactants and agrichemical intermediates) by heterogeneously catalysed reaction with amines provides a further example. The invention of new syntheses that exploit alternative reaction media—especially aqueous media—will require new catalysts.

Key Areas that Should be Promoted. In the development of new catalytic pathways certain general principles should be followed as indicated below.

- Broad initial assessments of possible routes to products should be undertaken. Correspondingly, premature choice of final solutions should be avoided.
- Strategies to decrease dependence on protecting groups leading to improved atom efficiencies are highly desirable. Possible solutions include increased reliance on enzyme catalysis and temporary immobilisation of reactants by adsorption during conversion.
- Reduction of the temperatures and pressures required for sustained catalytic conversion would be highly advantageous. Here, enzymatic routes could be especially valuable.
- Catalyst immobilisation without loss of activity or selectivity so as to reduce subsequent separation requirements would be very beneficial. This calls for development of new supports, especially organic and inorganic micro and mesoporous structures.
- Enzyme immobilization is an effective means of providing more stable biocatalysts. Another approach to overcoming enzyme instability would be to use whole cell (organism) reactors and directed evolution techniques. This is attractive when the desired products are secreted into the growth medium.
- Catalysis must play a key role in the process of scaling-down and decentralising the production of chemicals in order to reduce and ultimately eliminate the environmental impact of conventional large-scale plants. This will require new approaches involving miniaturisation (micro-fluidics, thin-film processing) and the use of more sophisticated technologies (e.g. polymer-based membrane reactors).
- Development of new methods for heterogenising homogeneous catalysts.

Important reactions requiring further development include; C-H bond activation, especially in the case of methane; use of methane monooxygenase; the feasibility of creating simple analogues that would catalyse the conversion of methane to methanol; enantioselective catalysis (e.g. in epoxidation reactions or Diels-Alder reaction); selective oxidation (e.g. $\text{H}_2 + \text{O}_2 \rightarrow \text{H}_2\text{O}_2$, selective oxidation of CO in reformat); and the bio-conversion of glycerol to glyceric acid.

The genomic approach to access novel biocatalysts is becoming important because enabling technologies are now available that permit synthesis of “designer” enzymes. Bioinformatics will facilitate the identification of gene sequences encoding potentially useful enzymes or binding domains. By exploiting this approach in combination with directed evolution methods it should be possible to invent stable biocatalysts with specific desired properties, optimised to perform under the required conditions (temperature, pH, solvent...). The performance of these systems at different scales of operation should also be carefully considered.

A potentially important opportunity is the development of non-aqueous enzyme chemistry, where the enzyme is stabilised by only a thin layer of water. This would open up alternatives to, for example, aqueous-organic systems. The integration or combination of bioconversion with chemical conversion offers exciting prospects and is an area that should be encouraged.

The stable immobilisation of homogenous and enzymatic catalysts without loss of performance represents a major challenge. Fundamental issues and strategically important research themes include the following:

- Studying, understanding, controlling and optimising the catalyst/surface interaction.
- Creation of new high surface area support materials.

- Controlled sequential attachment of enzymes so as to achieve the desired overall conversion.
- The use of membranes for both support and separation.
- Identifying important target reactions for immobilised catalysts: *e.g.* enantioselective oxidations.

Progress towards the development of radically different catalysts, materials and processes requires a strategic approach. Pre-requisites include the supply of relevant information by industry to academia to answer questions such as: what is already possible but well worth improving? What is desirable but not yet possible? Ways should be devised for stimulating this exchange without compromising commercial needs. There can be little doubt that multidisciplinary should be an essential component of ambitious research programmes. Therefore, academic researchers should cultivate critical awareness of key subjects that may be used to leverage the technological impact of their own specialisations. This will require a willingness and an ability to communicate across subject boundaries.

As a first step, to stimulate innovation, meetings involving the various distinct catalysis communities, both from academia and industry (homogeneous, heterogeneous, biocatalysis, photocatalysis, electrocatalysis, bio-electrocatalysis) must be organised.

4.4 New Processes and Process Strategies

Improved reactor and process design are needed in order to increase yield and selectivity and to reduce environmentally unfriendly by-products. New systems that provide for product separation during reaction, such as reactor-separator combinations, alternative energy sources for reaction initiation (such as UV radiation) and in-process sensing and control, are important goals.

The application of Life Cycle Assessment to study material and energy flows in products and processes can identify hidden production costs and predict the environmental impact of a product or process over the entire life cycle. Factors such as waste treatment and disposal, site remediation, regulatory compliance, public relations, and legal consultation should all be included in the analysis.

Recognising Gaps. At the initial stage of process design there is a need for more fundamental understanding, including physico-chemical data on both existing and new materials. Efficient design of new processes also requires early identification of the most promising routes, rate-limiting step, and technologies that allow the process to run at its kinetic speed. This calls for the development of tools for preliminary screening, identification and assessment of potential processes in terms of technical performance and sustainability.

In this context, environmental monitoring has become hugely complicated, as a result of the increasingly complex data required (*e.g.* composition of micrometer-size particulates, synergistic effects among trace pollutants). This necessitates greater sophistication of analytical instrumentation including measurements at the single-molecule level. Development of practical tools for rapid process screening and design in new applications is crucially important.

Chemistry that uses new, tailored processes represents one way forward for green chemical technology. Minimization and intensification often result in a simplified plant that is more efficient and less prone to failure. New reactor types may come about through applying the principles of process intensification or indeed through process simplification. New sustainable chemistry routes for synthesis coupled with the high transport rates offered by novel reactor and separator technology have the potential for not only improving commercial

competitiveness but also speed to market, new product development, process flexibility and distributed manufacturing.

Despite research council initiatives, obstacles to improved collaboration between chemists and chemical engineers persist. Here, training plays a major part. Undergraduate courses in chemical engineering do not include enough chemistry, while chemistry students tend to have low levels of attainment in mathematics and do not encounter appropriate engineering principles. There is a need to provide the right forum for chemists and engineers to begin a dialogue, recognise common aspirations and identify opportunities that can be exploited by collaboration.

Identifying Potential Advances. There is an urgent requirement for facilities that can be used as demonstrators for green chemical technology. High-risk expenditure to construct pilot scale facilities can be a problem for prospective technology developers which should be addressed. These demonstrators would have a process plant using the concepts of modern reactor and process design and using green chemistry for synthesising and producing products in a sustainable manner. Such facilities will not only be used to carry out proof of concept studies for industrial collaborators and therefore reduce the risk of introducing new technology but will also play a major role in promoting the perception of chemical processing in general.

Miniaturised and intensified reactor systems (*e.g.* micro and spinning reactors) which reduce the inventory requirements of a reaction or screening process can be developed. These may be based on conventional or novel reactor types and can function as high throughput rapid screening devices. This latter feature can lead to faster routes to market. The concept can be applied to a range of generic processes such as catalytic reactions, supercritical reactions/extraction, membrane separations and renewable/novel feedstocks processing.

Key Areas that Should be Promoted. Separations remain an important field in process design involving new reactor systems. One of the keys to success in this area lies in designing from the macroscopic scale (devices and systems) down to the molecular scale through self-organisation, catalyst selectivity to avoid the need for separation, specific interactions with solid phase reagents, and importantly continuous flow separation processes. Here, effective communication between engineers and chemists will play a vital role. One important principle of green chemistry is the development of catalytic processes. This could favour new homogeneous-heterogeneous hybrid catalysts and an understanding of how they can be incorporated into new reactor systems.

In promoting new processes the following general principles practices should be borne in mind.

- Chemists should think twice before using stirred tanks for their research—as it dictates the subsequent process development.
- Composition of the research team/consortium is critical—*Smaller teams are often more productive*, although the multicentre *Lab on a Chip* LINK programme was highly successful and led to the commercialisation of a high throughput screening micro reactor system using plug and play technology.
- Construction of a list of strategically important green chemical technologies and novel reactor/mixer/micro technologies backed with appropriate facilities to enable rapid development to large scale at low cost.
- Run process workshops in specific technology areas to identify strategically important areas of development.
- Effective management of intellectual property to attain industrial confidence.
- Availability of generic demonstration facilities.

- Easily accessible tool kit for chemists to play with intensified modules
- The role of technology developers should not be underestimated—hence involvement of the Faraday Partnerships, especially Crystal Faraday should be encouraged.
- Bring together the RSC and IChemE to consolidate interactions between chemists and chemical engineers, particularly in the areas of curriculum development and accreditation.

4.5 Environmental Biotechnology

Recognising Gaps. Biotechnology has the potential to improve and sustain the environment, thereby enhancing quality of life and contributing to wealth creation. A wide range of technologies based on the understanding of natural processes has facilitated improved approaches to sustainable development. Over the last ten years much progress has been made in the development, use and regulation of biological systems for the remediation of contaminated air, soil and ground water. In particular, development of biological science and technology and process engineering has now resulted in bioremediation being a low cost and generally environmentally benign means of cleaning-up the environment. Some of the main barriers to the implementation of bioremediation are the lack of compelling legislation, scepticism about biotechnology and the often site specific nature of the remedy.

Recent developments in molecular biology have provided new tools and approaches for monitoring the environment. *In-situ* monitored natural attenuation (MNA) bioremediation processes should be enhanced further and the development of biosensors promises to revolutionize the way pollutants are monitored. Currently, biosensors provide an effective way of monitoring general toxicity. However, methods for the detection and monitoring of specific pollutants are urgently required.

The biological and physical complexity of many contaminated sites requires a multidisciplinary approach including chemistry, microbiology, engineering and geology. Microorganisms, primarily bacteria and fungi, tend to be the organisms of choice to degrade or transform pollutants, although the use of plants (phytoremediation) is an emerging area. Currently, the successful development and application of bioremediation technologies depends on field-based research and the underpinning science is poorly understood. Natural attenuation is often the only available approach. A major problem facing the development of bioremediation technology is lack of scientific understanding with respect to environmental systems such as the bioavailability of pollutants and how toxic wastes interact with the hydrosphere. The effect of micropollutants (such as oestrogens and oestrogen mimics) in the environment is unknown and extremely difficult to deal with. Solid wastes such as conventional plastics are probably too recalcitrant ever to be biologically degraded, however biodegradable plastics are being developed. Environmental biotechnology also has an important role to play in the development of environmentally friendly processes such as green manufacturing technologies and sustainable growth.

Identifying Potential Advances. Biotechnology can be used to convert toxic compounds into benign materials, monitor environmental systems, produce novel biomaterials (including biodegradable plastics), to develop new methods of energy production, as a source of 'naturalness' and raw materials. While some successes have been achieved, advances in environmental remediation have been delayed by the lack of knowledge of organisms or microbial ecosystems/communities that can be used for bioremediation and the ecology of the environment where these systems are to be deployed. Promising new approaches involve the use of microorganisms to create supported metal nanocrystals effective for the heterogeneously catalysed degradation of pollutants. Here, bacterial cell surfaces provide the scaffolding and templating functions that allow the

engineering of highly active metal crystallites. This 'hybrid' approach can succeed where traditional bio- and chemical technologies fail, e.g. in the treatment of polychlorinated biphenyls (PCB).

The atmosphere is also a focus for environmental biotechnology. Greenhouse gas emissions need to be cut substantially. Hydrogen is an alternative 'clean' fuel; the only product of its utilisation is water. There are several ways to make hydrogen using biological systems (often using food wastes, reducing the amount of these to landfill or combustion) and hydrogen biotechnology is developing in parallel with the development of fuel cells and the hydrogen infrastructure (storage and transport capabilities). Low temperature proton exchange membrane (PEM) fuel cells use hydrogen to make electricity but high temperature solid oxide fuel cells (SOFC) can also use methane. There is clear potential for the harnessing of methane produced by anaerobic digestion, but gas filtration may be needed to remove potential catalyst poisons. The high cost of the materials for a PEM fuel cell (e.g. precious metal catalysts) may be problematic but recent studies have shown potential for the use of bacteria to recover precious metals in a re-usable form from scrap.

A particularly important issue that needs to be addressed is the determination of pollutant toxicity. What is the effect of a single pollutant versus complex mixtures and how are emerging chemicals to be tested for toxicity? Research priorities in the bioremediation/clean technology area include:

- Developing mathematical models for the evaluation of polluted sites
- Developing an understanding of the microbial ecology of polluted sites in terms of community structures and their response to pollutants
- Elucidating of biochemical mechanisms in plants and microorganisms, including enzymology
- Gaining a better understanding of bioavailability
- Determining the effects of pollutants on soil chemistry and soil health
- Developing an understanding of microbial genetics to facilitate *in situ* degradation of pollutants
- Developing innovative technologies such as biosensors for monitoring and evaluating toxicity of pollutants and effectiveness of remediation systems
- Developing hybrid technologies that are not site specific, embracing the interfaces between biocatalysis, chemical catalysis and chemical engineering
- Developing applications of bio-nanotechnology in remediation and clean technology
- Developing biotechnologies for atmospheric protection and their integration into the hydrogen technology infrastructure

Biotechnology offers a sustainable way of utilising biodiversity resources with limited or no impact on the environment. The use of recombinant DNA technology allows the possibility of delocalising the site of production of useful chemicals and materials. A certain organism, which harbours useful genes, chemicals or enzymes etc, may only be present in restricted environments in the biosphere; however, biotechnology can enable the production of these materials in any location. Biotechnology therefore has the potential to add-value to untapped biological resources and to reduce pressure on threatened species. The marine environment has been identified as an important area for the discovery of novel bioactive compounds, enzymes and biomaterials (such as mussel glues). A potential important opportunity involves making use of biologically derived nano structures; for example, an understanding of the mechanisms of silica frustule formation in diatoms may lead to the development of self-assembly of electrically conducting nanomaterials. It has been estimated that less than 1% of the microorganisms present in the biosphere have been isolated. Therefore, apart from opportunities in developing new remediation technologies, this natural diversity offers tremendous opportunities in terms of small molecule and enzyme discovery for the

pharmaceutical, agricultural, chemical sectors. Likewise plants produce a plethora of complex chemicals as secondary metabolites; elucidation of these pathways will furnish new biocatalysts and provide new therapeutics. Importantly, plants offer alternative strategies to extract, sequester and detoxify pollutants from soil, water and air. We still have a very poor and incomplete picture of biological diversity, in terms of species richness, biogeography and ecosystem function.

The ability to monitor and control processes at the molecular level so as to achieve real-time information in complex environmental systems would be a revolutionary advance. Such systems would need to be sensitive, highly selective, and capable of being used *in situ*. Microorganisms and plants survive in a wide variety of harsh environments by processing information. Can these processes be accessed by bio-micro or bio-nano devices? The new concepts necessary to understand these highly complex systems can only come from chemistry. Any such advances will require the development of novel transducers for communication between cells and devices and the invention of algorithms for exploiting the information processing systems of the cells.

Key Areas that Should be Promoted. Environmental biotechnology is a highly interdisciplinary area of science and mechanisms need to be put in place to foster and stimulate collaborative and highly creative research. Solutions will not be provided by chemists or biologists working in isolation. The emphasis should be placed on truly interdisciplinary teams consisting of microbiologists, chemists, biochemical engineers, hydrogeologists, soil scientists and environmental modellers. Ultimately, it will be necessary to plan for environmentally benign products rather than rely on new technologies for end of pipe treatment. Indeed, the 'new environmental biotechnology' should give greater emphasis to forestalling the problems of environmental contamination by design of processes giving less waste, or production of wastes that can be used as source materials for other processes. This approach should also be applied to mitigating the effects of terrorist attack by chemical, radiological or bio-agents. In this connection, 'end of pipe' or 'clean up' technologies should still be encouraged where this will add to the UK's portfolio of countermeasures.

5 THE WAY FORWARD

For decades the chemical industry has invested heavily in plant and equipment designed for production by traditional process technologies. Reduced turnover in the West has led to massive overcapacity and consequent pressure to maximise return on current assets. In this context, capital investment in new technologies is difficult to justify in purely economic terms, unless incentives are provided. Tax incentives designed to encourage investment in cleaner technologies could provide a spur—and current consultations in this area being carried out by the government should be seen as an opportunity.

To remain competitive, the UK needs to advance the causes of green chemistry and sustainability within both academia and industry. This will inevitably require a larger investment in relevant R&D so as to achieve internationally competitive levels of expenditure. The average UK R&D investment is currently only about 2% of turnover compares unfavourably with figures of ~4% for top international companies and ~5% in the USA. In the non-pharmaceutical sector, the situation is even worse. R&D activity in the USA, stimulated by significant financial support earmarked for green and sustainable technologies, could further marginalize the UK's position. Therefore appropriately targeted funding and strongly improved cooperation between industry and academia should be seen as strategic imperatives for UK plc.

Strikingly, with respect to new reactions and new catalysis, the recent Crystal Faraday Partnership survey revealed a substantial mismatch between relatively high levels of academic research activity and relatively low perceived industrial needs. Equally striking, when it comes to new feedstocks, the picture is reversed: industry's demand outstrips research activity. The message is clear—there is an urgent need to find ways of bringing the two cultures closer together: industry and academia.

The RSC, Research Councils, the Faraday Partnerships and other funding bodies have an important role to play in promoting closer collaboration between academic chemists, biologists and engineers, and between academia and industry. More generally, the chemical community at large should be educated in the principles and aims of "*benign and sustainable chemical processes*".

Research involving environmental sustainability issues often requires the analysis and evaluation of scientific and engineering information and complex phenomena over large spatial and time domains. Here, the application of modern information technology and high-end computing resources present exciting opportunities for the research community. Analytical methodologies need to be developed for real-time in-process monitoring and control to minimise the formation of hazardous substances. This is a key element in the development of greener routes, and is crucially important in continuous processes. The UK needs to attract more investigators from a wider spectrum of disciplines into green chemistry. Thus, for example, whilst most industrial reactions are organic, most green chemists are not organic chemists.

If benign and sustainable chemical technologies are to become a reality then dialogue between process engineers and chemists is essential. A major factor that impedes such dialogue is the imbalance between UK strength in synthetic organic chemistry and the low level of activity in physical organic chemistry. Therefore it is important to reinvigorate physical organic chemistry in UK universities, whilst maintaining strength in synthetic organic chemistry. An example of this is the pressing need for developing better predictive criteria for choosing solvents for industrial application from the vast array of new possibilities available. This requires a greater emphasis being placed on the gathering of fundamental physical data for new materials, which requires the specialist skills of the physical organic chemist. It should be kept in mind that physical organic chemistry is a very broad area whose potential impact on the chemical sciences is large. It involves the application of physical ways of thinking and measuring (thermodynamics, simulations, kinetics, spectroscopy) to the solution of complex problems. The mechanism of action of enzymes, the structure of signalling networks in cells, the mechanisms of environmental degradation of pesticides—all these are encompassed by physical organic chemistry.

Support could be provided in this area through the provision of interdisciplinary summer schools and courses in green chemistry aimed particularly at graduate students in chemistry and chemical engineering. The RSC and the Research Councils could have a role in facilitating this.

Through initiatives, the Research Councils have supported collaboration between chemical engineers and chemists. Although such ventures have generally been successful and some have produced internationally leading research, they are relatively few in number. Successful joint ventures are most likely to emerge if created and driven by the common interests of well-informed collaborators—how best to stimulate such a state of affairs? Clearly, initial barriers due to reciprocal ignorance of disciplines need to be overcome in order to open the dialogue between potentially interested parties. We need the right forum within which chemists and engineers may begin the conversation, recognise common aspirations and identify opportunities that can be exploited by collaboration. In regard to education, greater interaction between the RSC and IChemE in curriculum development and professional

accreditation would provide an effective strategy for the longer term. Such actions should not dilute the existing curriculum but extend it beyond current levels—RSC and IChemE are already accrediting courses jointly and this welcome trend should be strongly encouraged.

Continued support for a diverse range of research programmes is sought. The resources recently allocated to sustainable technology and green chemistry research should stimulate the participation of a greater cross-section of the academic and industrial community. In order to capitalise on the strong interest in Green Chemical Technologies that emerged at the York workshop, favoured projects should involve collaboration between chemists, biochemists, biologists and engineers in both industry and academia. Given this, it is likely that interdisciplinary programmes will emerge more frequently in the short to medium term.

Joint projects always require clearly defined goals and agreed strategies. In the present context of strongly interdisciplinary research, these requirements are absolutely essential. When they are met, the chances of such projects from becoming too cumbersome, wasteful, difficult to manage or liable to fail are minimised.

In conclusion, unless we begin to think in terms of global solutions to problems of resources and the environment, navigating the future technology landscape may be more difficult than any of us imagined. Chemists as a whole—and biochemists, biologists and engineers—both in academia and industry, need to develop a new “thinking culture” in terms of benign and sustainable issues in relation to their own research, teaching, and technical applications. The use of new solvents, catalysts, materials, processes and biotechnologies will surely benefit both the environment and the national economy in the short term. But difficult choices could be called for—selecting products and processes that maximise long-term environmental benefits may not necessarily enhance short-term profitability, and it is here where the responsibility for the environment must be shared by all of us.

Our goal for the near future should be a scientific and technological culture in which the concept of sustainability is embedded in the thinking and practices of the chemical sciences wherever they are applied.

A MESSAGE FROM EPSRC Chemistry Programme—funding opportunities

We would like to thank the RSC for the invitation to attend the workshop on “*Benign and Sustainable Chemical Technologies*”.

EPSRC is keen to receive proposals for pre-competitive research projects and related activities in this area. Proposals for research projects, sandpits, national or international workshops or summer schools are welcome at any time. Collaboration between disciplines is particularly sought to address research in this field and proposals with industry involvement are also welcome where appropriate. EPSRC funding is highly flexible and we are always happy to discuss ideas for specific proposals or for wider programme development.

Together with the CRYSTAL Faraday Partnership, EPSRC is actively seeking to develop a research portfolio of highly speculative research leading to greener chemistry.

After a specific call for proposals, twelve projects were funded in 2002 with a total value of £2M. The projects included research into atomistic simulations of processes leading to greener chemistry, the development of various greener catalysts, catalytic oxidation in supercritical CO₂ and the development of new micro reactor based electrochemical methodology.

Proposals submitted to a second call are being assessed at the moment. Up to £2M is available for this and a third call for proposals is planned for 2004.

EPSRC has also provided £1M of earmarked funding for research selected by the CRYSTAL Faraday Partnership and continues to provide CRYSTAL with industrial CASE studentships.

Please see our website (www.epsrc.ac.uk) for more information or contact Dr Paula Duxbury, paula.duxbury@epsrc.ac.uk.

A MESSAGE FROM BBSRC

The BBSRC would like to thank the RSC for the invitation to attend its workshop on Benign and Sustainable Chemical Technology.

BBSRC continues to fund applied biological research in the fields of environmental biotechnology and biocatalysis of relevance to this workshop. The former includes harnessing biological systems both for environmental remediation and for clean technology processes which eliminate pollution at source. BBSRC continues to work with EPSRC and NERC at these multidisciplinary research interfaces, through for example its Engineering and Biological Systems (EBS) Committee.

For more information, please contact Dr Ben Sykes, ben.sykes@bbsrc.ac.uk.

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APPENDIX

List of panel members and observers to the RSC Research Workshop on Benign and Sustainable Chemical Technologies.

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