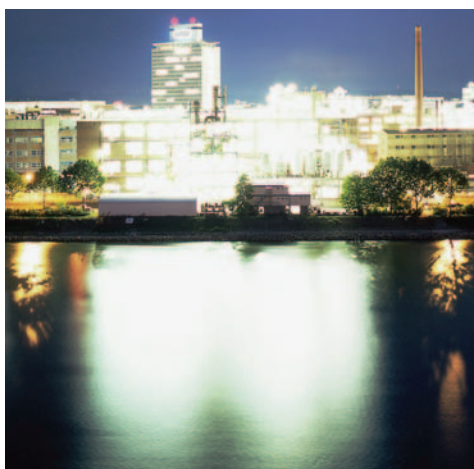
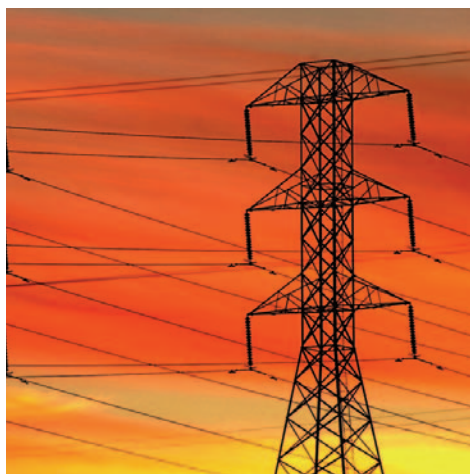


Chemical Science Priorities for Sustainable Energy Solutions



Statement of Intent

In 2004, the RSC's Environment Sustainability and Energy Forum established a committee to develop an outlook for chemical science research in the context of energy. The group met with the goal of defining the challenges and key priority areas for the chemical sciences – across the energy distribution system and all major energy sources – that are needed to support technological breakthroughs. The group focused on presenting sound scientific evidence to support the key recommendations. The report is intended to provide guidance to funding bodies and policy makers on:

- the pivotal role that the chemical sciences will play in the transformations that are needed to achieve a sustainable energy system so that funding bodies and policy makers can support chemical science research;
- the priority areas for the chemical sciences that need to be supported to advance the fundamental knowledge necessary to address key challenges in the energy system.

Contents

1. Executive Summary	4
2. Conclusions and Recommendations	6
3. Summary of Chemical Science Priorities	8
4. Introduction	10
5. Primary Energy Production	12
5.1 Petroleum	12
5.2 Coal	14
5.3 Natural Gas	20
5.4 Renewable Energy	21
5.5 Nuclear	26
6. Energy Distribution and Storage	30
6.1 Transition to a Hydrogen Economy	30
6.2 Energy Storage	36
7. The Efficient Use of Energy	40
7.1 Transport	40
7.2 Industrial Energy Use	42
7.3 Buildings	44
7.4 Domestic Applications	46
8. Products – Waste – Recycling	47
8.1 Emissions from Combustion	47
8.2 CO ₂ Capture and Storage	50
8.3 Nuclear Waste	55
9. Working Party	57
Appendix I	58

1. Executive Summary

An adequate and secure supply of energy is fundamental to our quality of life, but this needs to be achieved with minimum adverse environmental impact. As society moves from an economy based on fossil fuels to a more sustainable energy mix, considerable ingenuity from scientists and engineers will be required not only to develop sustainable energy solutions but also to find more efficient ways of producing, refining and using fossil fuels during the transition. This report defines the challenges and key R&D areas for the chemical sciences that are needed to support the sustainable development of energy supply, distribution and use and to assist in the transition to a sustainable energy future.

The chemical sciences will be at the heart of multidisciplinary initiatives, since much value will be gained from an improved molecular-level understanding of chemical processes. The opportunities for chemical scientists to transform the energy system are substantial, including, for example, the clean and efficient combustion of fossil fuels without formation and release of unwanted pollutants, greater efficiency in renewable energy technologies and greater capacity in energy storage.

Primary Energy Production

The future energy portfolio will comprise a mix of primary energy sources including fossil fuels, renewable energy and nuclear power. Scientists and engineers are needed to work on developing processes to use our remaining fossil fuel resources more efficiently and more cleanly. In particular, a fundamental understanding of the reaction chemistry underlying complex gas-phase combustion systems will offer opportunities for improved efficiency in fossil fuel combustion. For renewable energy sources to achieve a bigger share of energy supply, continued reductions in cost (per unit of energy supplied) are needed. Chemists will play their part in delivering cost effective and highly efficient renewable energy technologies through the provision of, for example, third generation photovoltaic materials, improved feedstock conversion and new lightweight, durable materials and coatings for turbines. Nuclear power, a carbon-free energy pathway, will comprise an important component of the energy mix. A key priority for the nuclear industry is to redress the run down in nuclear fission research and education skills in UK universities.

Energy Distribution and Storage

Hydrogen is increasingly regarded as the energy vector of the future: providing a suitable means of storage and transmission of energy from fossil fuels, renewables or nuclear power. However, before the commercialisation of hydrogen is realised, many technological barriers need to be overcome. Short-term requirements include the need for more rugged and more cost effective materials for fuel cells and for storage of hydrogen on-board vehicles. As demand for hydrogen grows, steam reforming of methane (with subsequent release of CO₂) is likely to form the predominant production route. Consequently, development and deployment of carbon capture and storage technologies will become an important issue. For a true hydrogen economy, large-scale, renewably produced hydrogen using renewable or low-carbon energy sources will need to be developed and commercialised which is competitive on the energy market.

The need for energy storage will increase by orders of magnitude as the energy landscape changes to include a much greater proportion of renewables. The storage technologies that are likely to make an impact on static electrical energy storage include batteries, flywheels and superconductors. In the transport sector, as hybrid vehicles gain increasing penetration, small, lightweight battery technologies with superior energy density are required. New strides in developments in lithium-ion batteries will offer significant improvements in performance. Supercapacitors are particularly attractive technologies in hybrid vehicles or direct electric traction. They can act as important power buffers, absorbing energy at a high rate, which is then transferred to devices such as batteries or flywheels. Developments in materials chemistry (e.g. new electrode and electrolyte materials) will be pivotal in driving the breakthroughs needed to optimise energy density and performance of these various storage mechanisms.

The Efficient Use of Energy

Major opportunities exist for improvements in the conversion of primary energy in transport, industrial energy use, buildings and domestic applications. Changes in vehicle design, for both road vehicles and in the aviation sector, are being driven by the need to improve efficiency and reduce emissions. Chemists, engineers and material scientists must be encouraged to work together to develop the next generation of fuels and lightweight hybrid vehicles capable of two or threefold improvements in fuel economy.

In the chemical manufacturing industry, where energy costs will become of increasing importance, research chemists should be encouraged to consider alternative energy sources (e.g. photochemical, microwave and ultrasonic energy sources) to initiate chemical reactions, as these may offer advantages over other more conventional energy sources.

In building materials there is considerable scope for developing safer and more environmentally benign alternatives to current insulating materials. Organic insulating materials and bio-fibre products offer advantages in terms of end of life disposal and improved performance for controlling humidity.

The provision of advanced highly energy-efficient technologies (e.g. solid-state lighting technologies) for household appliances that are cost competitive, longer lasting and more energy-efficient will significantly reduce energy use in the domestic sector.

Products – Waste – Recycling

An improved understanding of combustion chemistry (i.e. chemical kinetics, reaction dynamics, thermodynamics) is essential before one can predict what by-products are formed and in what quantities they are released to the atmosphere. Continuing atmospheric chemistry research is required to understand how gaseous and particulate emissions from combustion processes interact with the environment and potentially impact on human health. Advances are needed in the control of product quality and research to find a wider range of uses for solid wastes (e.g. ash from coal and biomass) from combustion processes.

The capture and storage of CO₂ could play a significant role in reducing the release of CO₂ to the atmosphere. The major thrust of research in CO₂ capture technologies, which will require input from chemists, is in the optimisation of solvent absorption systems, development of new separation systems and more concentrated gas streams. For CO₂ storage, collaborative research by chemists, geologists and engineers is essential to tackle such issues as long term sealing, maximising storage potential and surveillance and monitoring.

Nuclear waste research spans waste management, waste storage and dispersal, decommissioning and contaminated land management. Environmental chemistry (including hydro-geochemistry, radio-biogeochemistry and biosphere science) and wasteform chemistry (which includes the fundamental science of materials used in the immobilisation of nuclear waste materials) will have a pivotal role to play in providing solutions to nuclear waste management.

2. Conclusions and Recommendations

A transition to a sustainable energy system requires a 'systems approach' rather than focussing on individual technologies and products in isolation. Driving innovation across the energy system will require the expertise of chemical scientists since an understanding at the molecular level is essential. However, there are few chemical scientists working in the energy industry, and this will impinge on the delivery of sustainable energy solutions for the future. Action is needed now to realise and deliver long-term solutions.

Government support, that is a combination of regulation and incentives, will provide the market pull to encourage more energy related R&D. As government support increases, the market incentive and funding for energy research will increase and demand for a continual stream of world-class scientists will rise. More generally, building public awareness of the issues surrounding energy needs to start now. Education will play a major role in providing the necessary scientists and engineers to work on energy related R&D and in raising public awareness to enable the public to make informed choices on the issues surrounding the use of and preference for different energy technologies.

Recommendations

Education

- Key influencers involved in developing and advising on the school curriculum (e.g. RSC, The Association for Science Education, Institute of Physics) must work together to influence government and the regulatory authorities to include areas relating to chemistry and energy in the school curriculum. Currently energy education is covered mainly in areas most closely identified with physics.
- Chemistry in the context of energy must be better represented in the undergraduate chemistry curriculum (e.g. chemistry of energy production and use, natural energy flows, carbon cycle of oil, coal and gas, radiochemistry) to encourage chemists to pursue careers and R&D in this area. The undergraduate curriculum needs to be adapted to highlight this application for chemists.
- Continual professional development for school teachers must be provided so that their knowledge and professional skills are being kept up to date with current developments related to sustainable energy.

Government and Funding Bodies

- Government needs to put in place a framework to provide incentives (most likely fiscal incentives such as R&D tax credits) to promote R&D associated with sustainable energy technologies.
- Significant¹ long-term funding is required for fundamental chemistry and application specific chemistry to stimulate and encourage energy related research. Innovative, ground-breaking energy related R&D will rely on a strong chemical science base (e.g. materials chemistry, catalysis, combustion chemistry, radiochemistry) in the UK.
- Incentives are required to recruit and retain outstanding, internationally competitive scientists to work on energy related research in the UK. Incentives to attract international researchers to work in these areas are required to ensure that R&D happens now.

¹The RSC has calculated that £300 million is needed to secure the future of the physical sciences in the UK. The 2004 Spending Review has provided a total of £70 million to enhance UK capabilities in areas such as physical sciences and engineering - Royal Society of Chemistry response to the Comprehensive Spending Review outcome, including Science and Innovation Investment Framework 2004-2014 <http://www.rsc.org/pdf/policy/csrsept04.pdf>.

Learned Societies

- Greater interactions are required between the various scientific and engineering learned and professional societies to bring academic communities together.
- An international conference to highlight the deficiencies and weaknesses in the context of the energy system is required – this should involve key organisations including learned and professional societies.
- Active steps are required to change attitudes and values amongst the public and key decision makers. Learned societies such as the RSC must work to raise public awareness by disseminating key scientific data in an accessible manner on climate change and energy options for the future.

3. Summary of Chemical Science Priorities

Underpinning Chemistry	Applications
<p style="text-align: center;">Materials Chemistry</p>	<ul style="list-style-type: none"> • Breakthroughs in membrane separations could dramatically reduce capital and operating costs for the separation of gases and monomers. • Improved materials and coatings for supercritical and advanced gasification plants to extend temperature of operation and resistance to corrosion under reducing conditions and in the presence of species remaining after coal gasification. • High-temperature materials for improved efficiency and high performance in gas turbines. • New lightweight coatings and materials for wind turbines. • Development of third-generation photovoltaic materials based on molecular, polymeric and nano-phase materials. • Development of high performance, low cost materials for fuel cells (e.g. nano-scale materials and new cathode and anode materials). • Hydrogen storage materials (e.g. development of processes using materials that can be reversibly hydrogenated, chemical hydrides, reversible hydrogenation/de-hydrogenation systems as well as nanotubes and other organic/inorganic lattices). • Identification of new membranes and materials for superconductors that combine high conductivity with good mechanical stability. • Polymer and synthetic chemists are needed to create new structural materials and designs to radically reduce vehicle weight for both air and road transport without compromising safety. • Development of safer and more environmentally benign alternatives to current insulating building materials. • For CO₂ sequestration, new materials with enhanced capacity and CO₂ selectivity need to be developed. Adsorbents that can withstand extreme conditions (e.g. high temperatures and presence of steam) are needed. • Development of new materials (e.g. nanomaterials) for advanced battery technology.
<p style="text-align: center;">Catalysis</p>	<ul style="list-style-type: none"> • Improved catalysts, separation and conversion processes for the conversion of a wide range of feed-stocks, including crude oil, heavy oil, natural gas, coal and biomass, to a tailored range of gas and liquid fuels and chemicals through synthesis gas (syngas) chemistry. • High performance and multifunctional catalysts to yield cost effective production of ultra low-sulphur transport fuels. • Developments in zeolite catalysts to increase the yield of petrol per barrel of crude. • New catalysts required for both improved combustion of a range of gas types and qualities and for emissions clean-up. • For the Proton Exchange Membrane Fuel Cell better catalysts and membranes and better systems integration of the various Membrane Electrode Assemblies components are required. • Catalysts that can chemically reduce NO_x under the oxidising conditions of a diesel exhaust over a wide operating temperature range and sorbents that adsorb emissions during cold start operations. • Further developments in catalysts with lower thermal mass and light-off temperature that can be coupled to the exhaust manifold. • Improvements in catalysts and sorbents for reducing post-combustion emissions of NO_x and SO₂ from power plant, particularly for smaller plant that requires systems available at low capital and operating cost.

<p>High-temperature gas-phase kinetics</p>	<ul style="list-style-type: none"> • Increased understanding of the high-temperature chemistry in gas flames for efficient conversion of the fuel and limiting pollutant production. • Improved understanding of the effects of gas properties on combustion as import of gas becomes the norm. • Development and improvement of combustion technologies (e.g. pyrolysis and gasification) capable of operating with different fuels and co-firing. • Integration of fuel science, combustion chemistry, thermodynamics and the kinetics of NO_x and particulate formation will be required to address particulate emissions from diesel engines. • Sophisticated models of combustion and engine operation must be developed that can deliver precise individual-cylinder air/fuel control and minimise emissions.
<p>Radiochemistry</p>	<ul style="list-style-type: none"> • Study of the nuclear and chemical properties of the actinide and lanthanide elements. • Developments required in reprocessing chemistry (i.e. recycling of spent fuel into its constituents of U, Pu and fission products) include, for example, improved dissolution methods, control and abatement of volatile fission products (I-129, C-14), understanding solids formation and precipitation behaviour and a reduction in the number and volume of secondary waste streams through the development of non-aqueous processes. • Development of radiochemical separation techniques such as liquid-liquid extraction. • Actinide separation chemistry in nuclear waste streams (e.g. zeolites for sorption, membranes, supercritical fluids, molten salts).
<p>Radiation Chemistry</p>	<ul style="list-style-type: none"> • Improved understanding of radiation effects on polymers, rubbers and ion exchange materials. • Better understanding of the physio-chemical effects of radiation on material fatigue, stresses and corrosion in nuclear power stations will help optimise the performance of materials. • High performance materials to withstand high radiation fields for use in nuclear fusion.
<p>Waste Immobilisation Chemistry</p>	<ul style="list-style-type: none"> • Improved understanding of long term ageing and development of micro-structural properties of cements, waste/cement interaction and the corrosion of metallic components in cement materials used in the storage of intermediate level waste. • High level waste is bonded with glass in a process called vitrification. Chemical research challenges include defining and understanding the calcine/frit reaction and related melt behaviour, vitrified product performance, structure/property relationships in complex waste glasses and identification of suitable mineral/ceramic phases for the immobilisation of actinides based on natural analogues.
<p>Geochemistry</p>	<ul style="list-style-type: none"> • Effective enhanced oil recovery processes require a detailed understanding of the complex physical and chemical interactions between the oil, the injected fluid and the rock matrix. • Hydro-geochemistry and radio-biogeochemistry will improve our understanding of the relevant chemical and physical processes in the storage of nuclear material.
<p>Integration of biosciences with chemistry</p>	<ul style="list-style-type: none"> • The cost effective hydrolysis of lignocelluloses to fermentable sugars would considerably increase the source of biomass for bioethanol production; this source could include woody and grass crops as well as bio-waste. • Considerable innovation will be required by chemists, botanists and chemical engineers for the development of transport fuels from biomass.
<p>Electrochemistry</p>	<ul style="list-style-type: none"> • Cheap non-toxic emulsion breakers and crystal, hydrate and corrosion inhibitors. • Identification, development and scale up of appropriate electrochemical processes for advanced battery technology.

4. Introduction

The RSC supports the wider aims of society to improve quality of life through the provision of energy and electricity with minimum environmental impact. This support is realised by the RSC through the encouragement of, *inter alia*, education, research and development by professional chemists to contribute to this goal. The RSC supports the view that a balanced portfolio of energy supply technologies is required for the on-going prosperity of the UK.

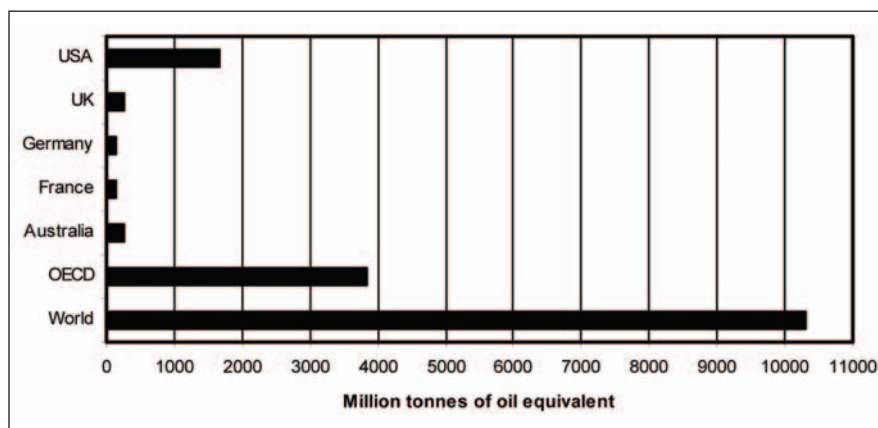
This report adopts a lifecycle approach, giving consideration to primary energy production, energy distribution, energy use and handling of waste products. Lifecycle assessment provides a useful tool to draw-out the unified and whole system approach, which is required when discussing the future energy landscape. Furthermore, when assessing different energy options, which will ultimately comprise the energy portfolio for the UK, each component of the energy system (be it energy production, distribution, energy use or waste) will need to be considered and analysed. The best overall approach for assessment is to apply the resources efficiency Life Cycle Assessment. (In the UK, the resources efficiency Life Cycle Assessment was developed as part of ISO14001 (1996)²).

Energy use is across a range of market sectors (industrial, commercial and domestic) and is necessarily of many types (heat, power, transport, etc). The RSC endorses the aims of:

- energy efficiency – to minimise energy demand whilst maintaining output;
- reduced environmental burden – lower emissions to land, water and air;
- reduced waste production – better management of resources and improved process operation to minimise waste.

Most commentators agree that energy demand will increase over the next few decades, as the world's population grows and the developing world economies expand. Figure 1 shows total global energy production in 2002 and compares it to energy production in selected countries and regions.

Figure 1: Total Primary Energy Supply, 2002



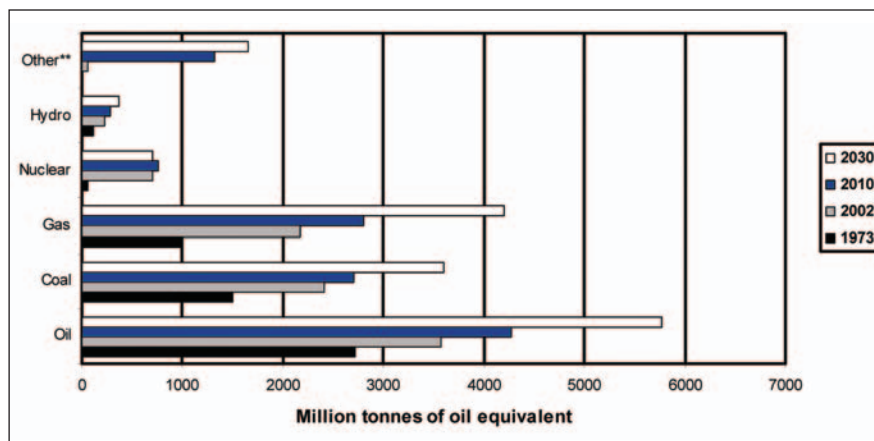
Source : IEA (2004). *Key World Energy Statistics*.

The economic development of the OECD countries during the 20th century has been greatly facilitated by the availability of cheap fossil fuels. However, this has come at a price, and most long term scenarios suggest that the introduction of alternatives to oil will be required in the coming decades. In addition, there is concern that the rate of investment in new wells and field development will not be fast enough to meet growing demand in the next few decades. The oil industry may need to add some 80 million oil-equivalent barrels per day to production by 2010 to meet projected demand. The cost of doing so could reach \$1 trillion or about \$100 billion a year, which is substantially more than the industry is spending

² ISO 14001 (1996), Environmental Management Systems, International Standards Organization, October 1996.

at present.³ Figure 2 shows the 1973 and 2002 fuel shares of total global primary energy supply and projections of fuel shares of total global primary energy supply for 2010 and 2020.

Figure 2: 1973, 2002, projected 2010 and projected 2030 Fuel Shares of Total Global Primary Energy Supply*



Source :IEA (2004). *Key World Energy Statistics*.

* includes bunkers

** other includes combustible renewables and waste, geothermal, solar, wind, tide etc

Reductions in greenhouse gases are imperative to halt the gradual rise in global temperatures and projected extreme weather events. There is now strong evidence that the combustion of fossil fuels and subsequent emission of CO₂ and other greenhouse gases is the major cause of global warming.⁴ Temperature observations show that the Earth has warmed since the pre-industrial era – during the 20th century the increase has been $0.6 \pm 0.2^\circ\text{C}$.⁴ The atmospheric concentration of CO₂ has increased by 31% since 1750 and continues to increase. The Intergovernmental Panel on Climate Change (IPCC) reports in its third assessment that ‘there is new and stronger evidence that most of the warming observed over the last 50 years is attributable to human activities’. Climate models suggest that in order to stabilise CO₂ levels at reasonable concentrations, it will be necessary for cuts to be made such that CO₂ atmospheric concentrations return to pre-1990 levels in a timeframe of a few decades. Therefore the case for seeking zero emission fossil fuel technologies or carbon-neutral alternatives is very strong, whilst at the same time utilising our remaining reserves of fossil fuels more efficiently and in a cleaner way. The chemical sciences will underpin many of the innovations required in the transition to a low-carbon economy.

There are very few predictions we can make with any certainty but it seems reasonable to suggest that the next half-century will be a period of significant change. This will be brought about by the likelihood of high oil and natural gas prices, more cost effective renewable energy technologies, improved predictions of the consequences and costs of climate change, and new lower energy demand technologies to provide the basic energy services of heat, light, mobility and information transfer. The transition from an economy based on fossil fuels to a more sustainable energy mix will require considerable ingenuity from chemists and the other science disciplines to develop sustainable energy systems and also to find more efficient ways of producing, refining and using fossil fuels during the transition.

³ H. J. Longwell (2002). *World Energy*, 5, 3.

⁴ IPCC (2001). *Climate Change. Synthesis Report*.

5. Primary Energy Production

5.1 Petroleum

Pessimistic estimates of the world's conventional oil reserves are 2000 gigabarrels, implying that global oil production will peak between 2010 and 2030. Higher estimates suggest that peak production will be deferred until 2060.⁵ The amount of the world's primary energy supply provided by renewable energy technologies will grow, but without further breakthroughs in technology or dramatic environmental deterioration, most estimates predict that it is unlikely to provide more than 10% by 2050. As a result, fossil fuels will continue to be an important part of the energy mix for many decades.

5.1.1 Oil Exploration and Production

Chemists are needed to work on extracting the remaining oil reserves from existing fields using new enhanced oil recovery technology based on a better understanding of the physical chemistry of oil, water and porous rock systems and novel chemical additives to improve water flooding and miscible gas injection.

Oil is currently being produced from increasingly inhospitable environments and water depths approaching one mile, which both increases cost and also acts as a brake on supply. These factors are stimulating research into enhanced oil recovery and the exploitation of heavy oil reserves.

As oil fields develop it becomes increasingly difficult to maintain the flow of oil and enhanced oil recovery techniques are usually employed. These involve increasing the pressure in the reservoir by injecting water. This is often a mixture of water co-produced with oil from the reservoir and seawater. Alternatively, co-produced gas may be injected into the reservoir to provide pressure and in some cases to reduce the viscosity of the residual oil. Some fields use CO₂ taken from natural CO₂ reservoirs to enhance oil production. This technique can also provide a means of storing CO₂ underground at the end of field life (see section 8.2 on CO₂ capture and storage). Power stations and other large industrial plants are now being considered as potential sources of CO₂ injectant. Effective enhanced oil recovery processes require a detailed understanding of the complex physical and chemical interactions between the oil, the injected fluid and the rock matrix. Other significant problems associated with enhancing the recovery of residual oil includes creating a detailed flow model of the reservoir and being able to control the flow patterns of the oil and injectant. Pioneering work by BP, Chevron Texaco and Nalco has shown that the injection of polymer gel particles, designed to expand under the influence of time and the higher temperatures in the oil bearing parts of the reservoir, can be used to exert some control over the flow pattern and hence increase oil recovery factors.⁶

Water and gas co-produced with oil create significant additional production costs due to inefficient separation and emulsion breaking processes. Corrosion, the precipitation of insoluble barium and calcium salts, and hydrate formation also create operational integrity problems and blockages in wells and flow lines. Whilst these are traditional process industry problems, the development of cheap non-toxic emulsion breakers and crystal, hydrate and corrosion inhibitors would considerably reduce production costs.

These issues, whilst perhaps mundane, will require effective solutions if the vision of fully automated and unmanned production facilities is to be realised, particularly for sub-sea operation. The dream of many oil company executives is to create closer integration between the producing oilfield and the refinery and to develop technology to produce oil while leaving undesirable components such as sulphur and asphaltenes behind in the reservoir. These remain considerable challenges for chemists and engineers.

⁵ Royal Commission on Environmental Pollution (2000). Appendix D 3. *Energy-The Changing Climate*.

⁶ H. Frampton, J. C. Morgan, S. K. Cheung, L. Munson, K. T. Chang and D. Williams (2004). *Development of a novel waterflood conformance control system*. (SPE . 89391, Tulsa).

5.1.2 The Refinery of the Future

The development of improved catalysts and separation and conversion processes will require the expertise of chemists for the production of ultra-low sulphur transport fuels, to increase the yield of petrol per barrel.

Although the operations of distillation, reforming and cracking still form the basis of crude oil refining, in common with about 80% of industrial chemical processes, modern refineries are heavily dependent on catalysts. One major challenge facing the oil refinery industry is the cost effective production of ultra-low sulphur transport fuels. A number of new high performance and multifunctional catalysts and processes have been developed to produce petrol containing sulphur at less than 10 parts per million (ppm) from naphtha whilst retaining the olefins that preserve octane value. The use of zeolite catalysts in the catalytic cracking process has increased the yield of petrol per barrel of crude by 50%, and the ability to control pore size and surface functionality of new mesoporous zeolites has allowed chemists to discover new catalytic processes. Catalyst design engines have also been developed, that take advantage of fundamental research into the contributions of each component of the catalyst system, to help design new catalysts for specific market needs, such as hydrogen management in the hydro cracking process.⁷

The sequential processing and separation of molecules by distillation in a conventional refinery has led to the suggestion that the average molecule of refined product is re-boiled and re-condensed an average of thirty-five times. As a consequence it has been estimated that retrofit opportunities in a conventional refinery could save over two-fifths of the fuel at very attractive prices, while designing a new facility from scratch could be made 'many, many' times more efficient.⁸ Membranes have the potential to significantly save energy costs. According to Katzner,⁹ membrane separations could reduce capital and operating costs for the separation of propane and propylene by 50–70%. Savings due to reduced energy costs could amount to roughly half the cost of the propylene.⁹ Process intensification and divided wall distillation columns capable of carrying out more than one operation simultaneously could also significantly increase production efficiency.

It is now possible to produce rigorous dynamic models of the whole refining process. Computers can be used to simulate rapidly the vast majority of process plants and to enable full kinetic studies to be carried out. Research groups have developed algorithms and dynamic simulators that describe basic reactions and physical properties of chemical feedstocks and model the transformations that occur between the molecules themselves. These can be used for process scale-up and for optimising the control of the reaction vessels.¹⁰ On-line sensors and quantitative models of the chemical transformations will allow precise control of the total set of products resulting from one specific process in a production facility (i.e. the product slate) in line with real-time market demand.

5.1.3 Unconventional Oil

Utilising a significant proportion of the unconventional oil reserves represents a number of challenges to innovative chemists in terms of production cost reduction, handling and upgrading.

Many of the estimates of remaining oil reserves assume that a better understanding of the chemistry and physics of reservoirs and petroleum fluids will enable much more oil to be extracted from reservoirs than has been achieved in the past. It is also assumed that the large heavy oil deposits and tar sands of Canada and Venezuela, which are characterised by high density and viscosity, and the large deposits of oil shale in the US,

⁷ UOP Newsletter Spring 2004 (<http://www.uop.com/>).

⁸ C.M. Burns (2003). *RMI and Shell Explore the "Stackless Refinery"* (www.rmi.org).

⁹ J.R. Katzner (2003). *Energy and Transportation*. Washington: US National Academy Press.

¹⁰ see Centre for Process Systems Engineering, Imperial College London (www.cpse.net).

China and Russia will be refined into transport fuels given favourable economics.

Although the reserves of unconventional oil are very large, it is difficult to extract and refine. An integrated approach to the entire chain – from the reservoir to pre-processing, production, transport and upgrading – is required to reduce the costs to levels associated with conventional crudes. Thermal methods are mainly used to mobilise heavy oil in the reservoir. This is achieved either by injecting a hot fluid such as steam into the reservoir or by generating heat *in situ* by burning some of the oil in place (fire-flood). There are several variations of the steam injection technique including cyclic stimulation or ‘huff and puff’. This was discovered accidentally in the 1960s and involves injecting steam for several days, shutting in the well to allow the surrounding rock to warm up and then producing until the production rate declines, when the process is repeated. Although fire-flooding seems attractive and is thermally more efficient than steam, in practice it is difficult to manage. In some cases, CO₂ can be injected into heavy oil reservoirs where thermal methods are not feasible using a process similar to ‘huff and puff’. Other processes rely on the injection of solvents (e.g. propane or naphtha) that mix fully with the residual oil to overcome capillary forces and mobilise the heavy oil.

Once the heavy oil has been produced, there are problems associated with the handling and transport of such viscous semi-solid materials. Oil in water emulsions have been used for some time to transport both heavy oil and, in some cases, coal by pipeline. Using surfactants to form an emulsion of 70% bitumen and 30% water enables bitumen to be used directly as a fuel for power stations in Venezuela.

Technology for the conversion of both coal and natural gas to liquid fuels has been developed, but it is still at an early stage and is consequently expensive. However, if the cost of conventional crude increases, technical improvements in these processes are to be expected. The development of improved catalysts and separation and conversion processes will become increasingly important to the refinery chemists of the future, as the sweet crudes of the past are replaced by heavier, more acidic and higher sulphur feed stocks. Refineries and chemical plants capable of converting a wide range of feedstocks, including crude oil, heavy oil, natural gas, coal and even biomass, to a tailored range of gas and liquid fuels, as well as to chemicals through synthesis gas (syngas) chemistry, may be a feature of the future. Already the concept of a single chemical plant that produces a wide range of both chemicals and fuels from carbonaceous feedstocks *via* a syngas intermediate known as ‘polygeneration’ is being widely discussed as a source of transport fuels for the growing Chinese economy.¹¹

Finally, although only 10% of crude oil is supplied to the petrochemicals industry, the potential recycling of plastics to provide refinery feedstock could become significant.¹² This has the added advantage of reducing the burden on landfill and should attract a government subsidy.

5.2 Coal

Coal use is increasing worldwide but declining somewhat in the UK. Electricity production accounts for most of the UK's coal consumption and this market is sensitive to the balance between coal and gas prices. The main barriers to coal use are the need to achieve a 20% reduction in CO₂ emissions by 2010, growing to 60% by 2050, as well as to comply with the Large Combustion Plant Directive (LCPD) on airborne emissions and the Integrated Pollution Prevention Control (IPPC) Directive on efficiency.

There is a worldwide trend of increasing coal usage to meet the rising global demand for electricity. Coal-fired power stations provided 39% of the world's electricity in 2000 according to figures produced by the International Energy Agency (IEA).¹³ The IEA further predicts that world electricity demand will increase by

¹¹ L. Zheng, N. Weidou, Z. Hongtao and M. Linwei (2003). Polygeneration – coal gasification. *Energy for Sustainable Development*, Volume VII, No 4.

¹² J. Nishimo, M. Itoh, H. Fujiiyoshi, T. Ishinomoni, N. Kubota (2004). Development of a feedstock recycling process for converting waste plastics to petrochemicals. *IHI Engineering Review*, **37**, 2.

¹³ IEA (2002). *World Energy Outlook 2002*. Paris: IEA.

2.4% per annum between 2000 and 2030,¹⁴ and coal consumption is therefore also expected to continue to increase. In 1999, 4.3 billion tonnes of coal were produced,¹⁵ and China and India together currently consume 1.5 billion tonnes per year, mainly for power generation.

This differs from the situation in the UK. Domestic coal production fell from 108 million tonnes to less than 30 million tonnes between 1986 and 2002.¹⁶ However, coal remains a primary energy source. Coal was used for 32% of the United Kingdom's electricity generation in 2002, which represented more than 80% of coal use. Much of the coal consumed in Britain is now imported. In 1992, the amount of coal used for power generation was 78.5 million tonnes, falling sharply to 47 million tonnes by 1997.¹⁷ However, due mainly to increasing gas prices, coal use for power generation rose to 49 million tonnes in 2002,¹⁵ and increased to 52 million tonnes in 2003.¹⁸ There has been a continued downward trend in coal use in the UK's other coal market sectors.¹⁸ Between 1992 and 2003, industrial use fell from 6.6 million tonnes to 0.7 million tonnes, domestic use from 4.2 million tonnes to 0.9 million tonnes and smaller markets from around 1 million tonnes to 400,000 tonnes. Only the use of coal for coke making and subsequent use in the steel industry remains a substantial market and even this fell from 9.0 million tonnes to 5.3 million tonnes over the same period.

5.2.1 Barriers to Coal Use in the UK

Coal-fired power generation plants will come under increasing pressure from EU legislation aimed at reducing emissions resulting from power generation. There will be further pressure to reduce both CO₂ emissions, as a result of Kyoto, and other airborne pollutants, as a result of the Large Combustion Plant Directive (LCPD).¹⁹

The UK's commitment under the Kyoto Protocol to reduce CO₂ emissions by 12.5% below 1990 levels by 2008–2012 has been followed by more demanding domestic targets of 20% by 2010 and 60% by 2050. Were the UK to attempt to meet its 2050 CO₂ target by replacing fossil fuels with biofuels, it would require the UK's electricity grid to undergo a massive expansion to carry power from small producers throughout the UK or conversely would place a huge burden on the infrastructure to build a large number of small generating plants and keep them supplied with fuel all year round. The concomitant increase in electricity costs would also seriously damage the UK manufacturing economy, potentially forcing production to be shifted overseas to countries with less stringent environmental legislation, which is clearly undesirable.

New European Commission Directives, including the LCPD from 2008, Integrated Pollution Prevention Control (IPPC)²⁰ from 2006 and the EU Emissions Trading Scheme (ETS)²¹ from 2005, collectively address conventional pollutants such as SO₂, NO_x and dust, as well as responding to concerns about greenhouse gas emissions by introducing carbon trading. Related to this, there are issues surrounding the quality and classification of ash that affect its saleability or disposal to landfill, which are discussed more fully in Section 8.1. A slump in the wholesale price of electricity since the New Electricity Trading Arrangements (NETA) were introduced in March 2001 has reduced the profitability of generation in the UK, whilst in the last twelve months global coal prices have increased. Consequently, generators are looking in detail at

¹⁴ IEA (2003). *World Energy Investment Outlook – 2003 insights*. Paris: IEA.

¹⁵ WEC (2001). *Survey of Energy Resources 2001*, 19th ed. London: WEC.

¹⁶ US DoE (2004). *United Kingdom Country Analysis Brief*. Washington, DC: US DoE

¹⁷ Minchener and Barnes (1999). *Chemical Variation and End Uses of Coal at the Present and in the Future*. London: HMSO

¹⁸ DTI (2004). *The Digest of the United Kingdom Energy Statistics*. London: HMSO.

¹⁹ European Commission (2001). Directive of the European Parliament and of the Council 2001/80/EC of 23 October 2001 on the Limitation of Emissions of Certain Pollutants into the Air from Large Combustion Plants. *Official Journal of the European Communities*, **L309/1**, 27.11.2001, 1–21.

²⁰ European Commission (1996). Directive of European Parliament and of the Council 1996/61/EC of 24 September 1996 concerning integrated pollution prevention and control. *Official Journal of the European Communities*, **L 257**, 10.10.1996, 26–40

²¹ European Commission (2003). Directive of European Parliament and of the Council 2003/87/EC of 13 October 2003 establishing a scheme for greenhouse gas emission allowance trading within the Community and amending Council Directive 96/61/EC. *Official Journal of the European Communities*, **L275/32**, 25.10.2003

whether to invest in new technologies such as flue gas desulphurisation (FGD). The total FGD capacity of existing plants or those under construction in the UK is 10,000 MWe (= 10 GWe), but even if planning applications submitted for a further 5,000 MWe (= 5 GWe) are approved, it is by no means certain that the necessary plants can be built in time to meet LCPD targets, now that delays in the announcement of how the Directive will be implemented in UK law have been encountered. Continued delays may result in much of the existing UK power station fleet having to be opted out of the LCPD, considerably limiting the lifetime of the plant and creating a lack of generating capacity over the next decade. Similar concerns arise over equipment modifications required to comply with new NO_x emissions limits.

Coal-fired stations can opt out of the expensive equipment modifications needed to comply with the LCPD, providing that they only continue to operate for a limited period. Also, compared with the high capital cost and lengthy planning and construction times applicable to new coal-fired plants, gas-fired plants can be built relatively quickly and inexpensively. Gas is a lower nitrogen-, virtually zero sulphur- and lower carbon-content fuel: these are the three factors mainly affecting compliance with legislation. Consequently, the effect of both EU and national legislation over the next ten years is likely to bring about a reduction in the proportion of coal-fired power generation in the UK in favour of gas. The balance between global prices for gas and coal will determine the extent of the fall in coal use. In the medium term much depends on the level of investment the power sector is prepared to make to comply with new EU legislation and on the technologies available. Government policy will have a significant influence, because it is not yet fully clear how EU legislation will be transcribed into UK law or whether there is likely to be the political will to support the development of clean-coal technologies.

The Government's Energy White Paper,²² published in 2003, focused not only on limiting the environmental impact of energy production and use but also on three other specific targets. These can be summarised as: maintenance of a secure energy supply; promotion of a sustainable energy economy capable of supporting economic growth; and ensuring that every home can be adequately heated at an affordable cost. With the present state of technology it is not possible to meet these objectives and the commitments to reduce CO₂ and other emissions simultaneously. Security of energy supplies is a very important consideration, particularly as the availability of gas cannot be guaranteed as indigenous reserves are becoming scarce. In addition, if there is a need for a further reason to develop clean-coal technologies that goes beyond achieving security of fuel supply in the UK, then it is the huge worldwide market that will open up over the next 20 to 30 years. The UK has been a world-leader in clean production of power, and it is in an ideal position to take advantage of the opportunities that this expanding market will present.

5.2.2 Meeting the Challenges for the Coal Sector in the UK

Coal-fired generation should have a long-term role in providing energy diversity and security, providing ways can be found to reduce CO₂ emissions in the longer term, whilst complying with other short to medium term barriers resulting from tightening environmental constraints.

The main focus of coal research in the UK has for many years been the reduction of emissions and improvement of efficiency in pulverised coal-fired generation plants. Much of this research, though wide-ranging in its engineering applications, draws upon chemistry and applied chemistry for much of the underpinning science. The source for much of the following information is a draft text made available by the Coal Research Forum for use by the RSC.²³ The areas discussed below are divided into short, medium and long-term technical challenges.

²² DTI (2003). Energy White Paper: Our energy future – creating a low carbon economy. London: HMSO. (Available from: www.dti.gov.uk/energy/whitepaper).

²³ Coal Research Forum (2004). Coal Research Needs in the UK, 4th ed (draft).

Short Term Challenges – Power Generation

Short term technical needs in coal-fired power generation relate specifically to control of SO₂, NO_x and carbon in ash. Research should be focused specifically on better materials for plant design, catalysts for emissions control and a better understanding of specific processes such as corrosion and ash deposition. Improved process monitoring and performance prediction tools are also required.

The power generation sector in the UK faces some specific short term technical challenges as a result of the need to comply with LCPD and IPPC²⁰ legislation. The areas of primary concern are gaseous emissions, the need to maximise efficiency and the control of emissions of solid wastes. At the same time, coal must remain competitive and so there is a need to minimise production costs. In the context of the existing fleet of pulverised fuel (PF) power plants in the UK, the areas of overriding concern are control of SO₂, NO_x, dust and carbon in ash.

There is a particular need for the development of better materials of construction for flue gas desulphurisation (FGD) systems to cope with the erosive and corrosive environment within them. For PF plants not equipped with FGD there will continue to be a need to use imported low-sulphur coals in order to comply with SO₂ emission limits. This increases the need for better fuel performance prediction and fuel testing capabilities, which are mentioned in more detail below.

Improved burner designs are needed to maximise burnout whilst minimising NO_x production. The detailed requirements for NO_x control technology developments are discussed in Section 8.1.1.

Emissions of dust and production of carbon in ash are related, because as the efficiency of combustion is reduced electrostatic precipitator (ESP) performance can be impaired, leading to higher dust levels. High carbon in ash also increases the cost of power production as a result of wasted fuel and entails the need to dispose of ash residues to landfill. Several research areas are related to controlling carbon in ash.

- *Milling and feed systems.* PF flow distribution, measurement, control and coal quality effects on milling performance are of concern. Digital imaging techniques are being developed for on-line measurement of PF size distribution and concentration. Computer modelling of flows has been refined based on physical modelling and plant data to aid classifier designs.
- *Coal performance prediction.* Burnout predictors, based on pyrolysis and char combustion models, are being refined with information on char morphology from modern image analysis equipment. Char reactivity measurements have been used to deduce the temperature/time history of coal particles, and a new, easier-to-use and more reliable method of determining reactivity is being developed. The effects of ash properties also need to be assessed. Methods for predicting deposition under low-NO_x firing conditions require investigation, and expert systems for the monitoring of slagging and fouling require further development. The wider range of imported coals and biomass materials now being used prompts the need for better understanding of the chemistry of slagging, fouling, deposition and corrosion in PF boilers.
- *Combustion control.* Combustion flame monitoring, flame behaviour, boiler performance and control are important, not only for obtaining optimum burn-out and boiler efficiency, but also to predict the effects of particle size and performance of alternative coals without having to carry out expensive combustion tests. Investigations of on-line flame characterisation using light scattering may be useful. Systems are also being investigated for real-time monitoring of combustion in PF boilers through video imaging with computer-based analysis. New video techniques have been developed for observing near-burner flame regions to improve computational fluid dynamics (CFD) simulation of burners and furnaces and to study carbon burnout and ash formation. On-line finger printing of flames is being developed to identify the characteristics of fuel burn and obtain better burnout of blends. Three dimensional digital imaging techniques, based on a number of two dimensional images, are being developed to provide a better view of flame geometry and so improve CFD simulations. On-line monitoring of carbon-in-ash is being developed, as ash carbon levels have risen with the introduction of low-NO_x burners.

Short Term Challenges – General and Non-Electricity Sectors

There is a general need for better understanding of coal chemistry that may assist in process and emissions monitoring and equipment design. There are also specific research needs for metallurgical, industrial and domestic applications as well as for the development of advanced coal products.

Coal testing, process modelling and monitoring are areas of more general applicability that require continued development. In some cases many of the developments required are generic and can be applied to both the power sector and other applications. In other cases more specific developments are needed for the metallurgical, industrial and domestic sectors.

Means of readily evaluating coals and of predicting the behaviour of coals and coal blends are of increasing importance as the range of coals imported into the UK grows. Operators of industrial processes need simple screening tests to assess coals at the procurement stage, and technology manufacturers need similar tests to help in providing guarantees of performance for new plant designs. Standard tests need to be defined for simulated process conditions, e.g. true volatile matter measured at realistic heating rates for high temperature processes, tests to predict NO_x emissions, development of reliable cost effective techniques to predict corrosion and ash deposition rates, and tests for predicting the handling characteristics for a wide range of applications.

The development of computational fluid dynamics (CFD), other software tools and powerful computers means that modelling techniques are increasingly being relied upon in process design. CFD modelling needs to be improved to reflect the latest findings in coal science, such as the development of particle structure, pore diffusion and reaction within particles.

Improved techniques for collecting process data are required for many of the processes using coal. Monitoring equipment and systems for on-line detection of various species in coal-utilisation plants need to be developed. Examples include monitors for coal particle size and uniformity of flow, and non-intrusive techniques for monitoring conditions in coal flames. There is also a lack of suitable fast response techniques for monitoring various gaseous species.

In the specific field of metallurgical coke manufacture, for which significant tonnages of coal are still consumed in the UK, studies for reducing emissions from coke ovens and improving coke quality and the efficiency of coke making are of significant importance. The development of an oven charging control system to ensure consistent charge bulk density and the investigation of coke oven blend additives to moderate damaging wall pressures are the main areas of research. Understanding coke behaviour in the hottest zones of blast furnaces is also important. The direct use of coal in blast furnaces is a way of reducing costs and improving efficiency. This also requires development of milling and handling equipment for preparation of coals for injection.

Manufacturers and users of industrial coal-firing equipment, including cement kilns, are engaged in programmes to improve the efficiency, convenience and cleanliness of these systems. In particular, the effects on emissions of co-firing waste materials and biomass are of significant interest. This sector spans a very wide range of equipment types and scales, from small underfeed stokers to large pulverised coal-fired cement kilns. Research is needed on burner design, toxic emissions and expert control systems.

Research work is already being carried out by industry and at academic centres on developing novel materials from the products of carbonisation, including anthracene oil, coal tar pitches and combustion residues. These form the basis of chemical feedstocks, activated carbons, and binders and materials for the construction industry. There is also interest in catalyst developments for hydrocracking of coal-derived liquids.

Research into improved briquetted domestic fuels should be aimed at greater product quality, identifying lower cost alternative feedstocks without detriment to environmental or safety standards and developing new binder systems. This is a significant area for the domestic market but also has a particular application

for developing countries, where coal is the primary energy source in many domestic dwellings and air quality in the home and its impact on health is of particular concern.

Fundamental research into the effects of coal type on reactivity is required, and another area of interest is co-gasification with waste and biomass, including the development of improved designs and mathematical simulation techniques.

Medium Term Challenges

Medium term challenges in the coal industry relate to improved materials for supercritical and advanced gasification plants as well as the development of gasification technologies themselves. Specifically, developments need to be evaluated at the demonstration scale.

Medium term developments are likely to stem from the need to construct newer and more efficient plants. Two parallel approaches can be envisaged. Ultimately, highly efficient plants moving towards potentially zero emission technology will be required. Medium term requirements for this technology are likely to include the development of the underpinning science and the construction of demonstration plants for specific processes. However, if several of the older UK stations opt not to comply with the LCPD, it is possible that new coal-fired plants may need to be constructed to meet UK energy demand. If this happens within the next 10–15 years, it is likely that any new plant would be based on pulverised fuel-fired supercritical technology modified to co-fire biomass. Beyond that period any new plant would be likely to be gasification-based. Therefore a number of areas for the focus of medium term research can be identified.

- *Supercritical plants.* Supercritical plants require developments in the field of high temperature materials. As temperatures are increased for higher efficiencies in supercritical power plants, new alloys and fabrication techniques are required. Co-firing applications also require additional corrosion resistance. The effects of trace metals need to be considered specifically for co-firing applications. Steam turbine related activities, such as the development and characterisation of improved materials, and the development of new designs and methods of reduced cost fabrication will be important for supercritical PF units.
- *Air-blown gasification cycle (ABGC).* R&D on gasification in the UK over the past 15 years has centred on the ABGC. An air blown technology was initially selected as it offered great fuel flexibility with low capital cost and at the same time would enable a very high efficiency cycle by using high temperature gas turbines. Rig tests and char reactivity studies have aided the understanding needed to refine the cycle, but the technology (now owned by Mitsui Babcock Energy Ltd) remains at the point of requiring a demonstration at around 100 MWe.
- *Integrated gasification combined cycle (IGCC).* The main need for R&D activity on IGCC concerns materials, for gasifier refractory linings, syngas coolers and gas turbines. Hot gas path alloys and coatings for blades and vanes for natural gas fired turbines are the subject of continuing development by the manufacturers. Tests on, and modelling of, the deposition from coal-derived gases of particulates and alkali compounds on turbine blades are required. Reliable hot gas clean up (at 500°C and above) would enhance the efficiency of IGCC cycles (as well as the ABGC). IGCC needs to be lower cost and have greater reliability and ease of repair.
- *Additional issues.* Erosion-corrosion resistant coatings need development for circulating fluidised bed combustion (CFBC) systems. CFBC offers a relatively low emission alternative to PF combustion at lower capital cost. However, the chemistry surrounding sulphur removal in fluidised bed and gasification-based processes is complex, and there is scope for improving sorbent efficiency and for developing low-cost technologies for small-scale plants. Trace elements and volatile organic species are also of increasing concern. There is a need to predict trace element mobilisation in combustion and gasification systems from the composition of the coal mineral content. Tests are also needed on the adsorption of chemical species, such as mercury, dioxins and furans, using granular active carbon. Other areas of investigation that are needed are on the effectiveness of the removal of trace elements by electrostatic precipitators and the fate of volatile trace species in IGCC systems.

Long Term Challenges

Longer term challenges relate to developing CO₂ capture and storage technologies and integrating these with combustion and gasification plants. There is also a need to interface various power generation plants with fuel cells and to focus on a move towards zero emission technologies. Initially the underpinning science needs to be developed but ultimately demonstration projects will need to be considered.

Longer term challenges mainly concern reducing greenhouse gas emissions. For PF systems, there have been studies on optimising the performance of amine-based CO₂ scrubbers. However, for the longer term, developments in this area would be better directed towards gasification-based systems, with CO₂ removal from the fuel gas after a shift reaction followed by firing of hydrogen in the gas turbine. Operators have not targeted greenhouse gas emissions from the iron and steel industry so far, although utilisation of process by-product gases is established practice.

In addition to CO₂ removal, CO₂ storage is an area requiring development. See Section 8.2 for a full discussion of CO₂ capture and storage.

5.3 Natural Gas

For future developments of the natural gas energy sector, there will be a high demand for chemists and chemical engineers in areas such as fundamental physical chemistry (e.g. thermodynamics, chemical kinetics, combustion chemistry), analytical chemistry and environmental chemistry.

Natural gas has a higher hydrogen/carbon ratio than oil or coal and emits less CO₂ for a given quantity of energy consumed – clearly its use can help ease a number of environmental concerns. Furthermore, gas leaves virtually no particulate matters after burning, therefore the potential benefits for improving air quality are significant, relative to other fossil fuels.

There will be an on-going requirement for natural gas and the UK gas industry will have to respond to several business drivers. Chemical scientists will have a strategic role to play in upgrading and improving current systems and developing new technologies.

Natural gas met 39% of the UK's energy demands in 2002 - making it the single largest contributor ahead of oil (35%), coal (15%), nuclear (9%) and other primary energy sources (2%).²² It is predicted that by 2006 the UK will be a net importer of gas, with Norway providing a major source in the near term and Russia, the Middle East, North Africa and Latin America in the longer term.²² With the growth in imported gas supplies to the UK, gas composition and quality will vary and combustion systems will have to cope with this variation. As imports of gas increase, thermodynamic studies will be of the utmost importance as a means of improving the understanding of gas properties and developing mixing and blending systems. The development of cost effective gas purification technologies will be important to enable low-quality gas to be produced and utilised. Furthermore, analytical chemistry will be critical for measurements relating to gas quality, 'fingerprinting' gas sources and supporting improvements in metering and efficient use of gas.

Process integration will lead to improved energy resource management. An integrated systems approach to energy conversion and use can boost industry's competitiveness while reducing emissions of greenhouse gases to the atmosphere. Combined cooling, heating and power (CHP) – cogeneration of heat and power – is leading to significant optimisations in generation technologies. Chemistry will contribute to improved methods of processing gas to reduce energy use in these activities and lower parasitic energy losses. Burner developments will contribute to low-emission technologies such as oxy-fuel systems, use of recirculated flue gas and flameless combustion.

Natural gas, like other fossil fuels, will feel the impact of tightening environmental legislation on international (e.g. Kyoto Protocol), European (e.g. Emissions Trading) and UK (e.g. Ofgem's new social and

environmental agenda) levels that will force combustion systems to improve emissions and efficiencies. A sound knowledge of chemical kinetics will be imperative for understanding high temperature chemistry in gas flames for efficient conversion of the fuel and limiting pollutant production. There will be a need for improvements in high temperature materials for enhanced efficiency and high performance, while catalyst development will enable improved combustion for a range of gas types and qualities and for emissions clean-up. Continued developments in combustion chemistry will stimulate new ways to understand emissions production and destruction chemistry with a view to controlling pollutants. Meanwhile progress in sensors and instrumentation will improve control of combustion systems for improved efficiency and reduced emissions. From an environmental impact perspective, water chemistry – either in heating systems (heat exchanger design, water treatments, etc) or in the waste water from gas processing – needs to be strongly supported. Furthermore, environmental chemistry in general will be vital for understanding the impact of certain pollutants on the environment.

5.4 Renewable Energy

Innovation will be central to addressing climate change, through the development and use of low carbon technologies. The scope is considerable for innovative chemistry research in areas such as photochemistry, new materials, feedstock conversion processes, gas separation technologies and coatings, to realise the full potential of renewable energy technology.

Energy efficiency and a shift to non-carbon energy forms could lead to absolute reductions in CO₂ emissions of around 60% by 2050 in the OECD economies. In the longer term, the world can aspire to having its energy needs met with zero greenhouse gas emissions. There is a full range of renewable energy technological options including solar, offshore wind, wave and tidal streams, biomass from crops and wastes and geothermal energy.²⁴ Strong national and international policy commitments have sustained growth rates for wind and solar energy of greater than 20% over the past 10 years, which suggests that renewable energy will make a growing contribution to the energy supply mix during the coming decades. It is estimated that more than \$20 billion was invested in new renewable energy in 2003, up to one sixth of total global investments in power generation equipment. Cumulative investments in renewable energy totalled at least \$100 billion between 1995 and 2003, and markets for new renewable energy are expected to approach \$85 billion annually within the next decade.²⁵

5.4.1 Chemistry Research in Renewable Energy

Whilst perhaps not immediately obvious, the scope for innovative chemistry research in developing the full potential of renewable energy technology is considerable. The conversion of sunlight into electricity by third generation photovoltaic (PV) devices is a field that is likely to expand rapidly, encouraged by the growing market for PV solar cells and the potential for significant reductions in the cost of PV modules. Recycling biological waste from cities and agriculture into useful fuels and combustible gases provides a number of challenges in terms of developing enzymes to break down ligno-cellulose, improving and optimising gasification and thermochemical conversion processes, as well as developing cost effective and environmentally sound gas clean-up technology. Advances in materials science to develop high strength, lightweight materials for turbine blades and towers are also required in order to facilitate the construction and continued operation of large wind and tidal power turbines. Long lasting protective coatings will also be required to reduce maintenance costs and prolong the operating life of wave and tidal energy devices.

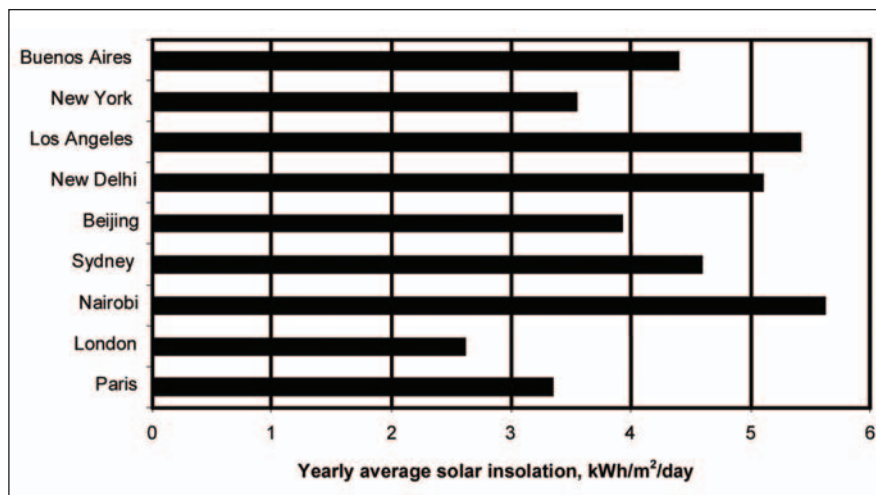
²⁴ See *Assessment of Technological Options to Address Climate Change* – Imperial College Centre for Energy Policy and Transport (<http://www.iccept.ic.ac.uk/pdfs/Tech%20initiative%20ICCEPT%20FINAL.pdf>).

²⁵ Eric Martinot (2004). *Global Renewable Energy Markets and Policies*. New Academy review in *Mainstreaming Renewable Energy* REW Review issue 2004–2005.

5.4.2 Solar Energy

The solar radiation incident on the Earth's surface is between 100 W/m^2 in temperate regions and 300 W/m^2 nearer the equator.²⁶ Figure 3 displays the yearly average solar insolation (the amount of solar radiation incident on the surface of the Earth) for a range of different locations.

Figure 3: Yearly average solar insolation levels (taken from 10 year averages).



Source : Nasa surface metrology and Solar Energy Data Set

This energy can be utilised in at least three different ways: PV technologies, which directly convert light into electrical current; solar-thermal systems; and so-called 'passive solar' technologies, where building design maximises solar lighting and heating. The major area of interest for chemists lies in the development of new photoactive materials that can be used to convert sunlight or artificial light directly into electricity.

PV Technologies

Photovoltaic devices consist of a semi-conducting material, currently most commonly silicon, which convert photons of light into electrical current by means of the photoelectric effect. They were developed in the 1950s to power space satellites, but their potential for providing remote power for telecommunications, water pumping and refrigeration rapidly increased demand for terrestrial applications. The drawbacks of early photovoltaic technology also became obvious, namely cost, low power density and intermittency of operation.

Although prices are coming down, grid connected residential PV systems currently cost around \$7 per Watt whilst stand-alone silicon modules are about half this amount. A number of different technologies are at various stages of development to both reduce the cost of solar modules and to increase their efficiency. Over 80% of modules are currently based on crystalline silicon. Silicon is an excellent material for solar cell production since its technology has become highly developed as a result of the global semiconductor market. In addition, its supply is virtually inexhaustible and it is non-toxic, although its manufacture is currently highly coupled to semiconductor demand. In the late 1970s and early 1980s thin films of inorganic semiconductors made from CdTe, CuInSe₂, amorphous silicon, thin film silicon and TiO₂ were developed as potentially cheaper PV materials. Innovative research on very thin (less than 20 atomic layers), high efficiency silicon devices is now in progress.²⁷

²⁶ M. D. Archer and R. Hill (eds) (2001). *Clean Electricity from Photovoltaics*. London: Imperial College Press.

²⁷ M. A. Green, Centre for Advanced Silicon Photovoltaics and Photonics, University of New South Wales, Sydney, Australia.

One of the factors that keep system costs high for these technologies is the requirement of high temperature processing of the semiconductor material. This and the rapid growth of the organic light emitting diode market have resulted in considerable research on PV materials based on molecular, polymeric and nano-phase materials. Although commercially viable efficiencies have yet to be demonstrated, progress is rapid. In 2004 at least two manufacturers claimed efficiencies of 5% for organic PV materials that can be printed or sprayed on to a thin support, flexible backing film, potentially offering considerable production cost reductions.^{28,29}

The growing number of uses for photovoltaic devices and the considerable improvements in reliability and price have generated a market that is growing at about 25% per annum. However, the cumulative installed capacity of solar PV is currently only just over 2,000 MW. Although PV began by providing power to remote locations that had no grid connection, over 50% of today's world market is for building integrated photovoltaic (BIPV) devices that are incorporated into the roofs and structures of buildings. Providing governments continue to support the installation of BIPV and introduce policies that allow net metering, by which consumers can sell surplus electricity back to the grid, it is likely that the demand for PV will continue to grow. As a result, many independent studies suggest that the costs of PV will continue to fall and that it is plausible to envisage module costs of \$1 per Watt or less by 2020 – this would allow BIPV to provide electricity below today's retail price in sunny areas of the world.³⁰

Useful amounts of electricity can also be generated directly from infrared radiation using a process called thermophotovoltaics.³¹ It is unlikely that the power of the sun will be harnessed directly using this technology, but it is theoretically possible. It is more likely that thermophotovoltaics will be used to generate electricity from waste heat to boost the efficiency of conventional thermal power generation technologies.

5.4.3 Biomass Energy

Strictly speaking solar power and biomass are both ways of utilising energy from the sun. In the case of biomass, plants use solar energy to drive chemical transformations and create complex carbohydrates and lipids.

Biomass energy is a generic term to describe energy in the form of heat, electricity, and liquid and gaseous fuels extracted from agricultural and forest residues, other organic wastes, and specifically grown crops. In common with solar PV, biomass has a low energy density and relatively low conversion efficiency. Unlike solar PV and many other renewable energy resources, biomass has the advantage of being able to store solar energy for use on demand.

Biomass already contributes significantly to the world's primary energy supply, probably accounting for around 12600 TWh a year (9–13% of world energy supply).³² The 1.6 billion people who lack access to modern energy forms and for whom wood, dung and crop residues are the only means of cooking and heating consume most of this.

Modern Biomass for Heat and Electricity

Currently only about 1960 TWh of biomass is consumed to produce electricity, steam and biofuels. However, the use of biomass has expanded considerably in several countries in the last decade, largely as a result of supportive policy frameworks. Modern biomass for heat and electricity production contributes around 4%

²⁸ Siemens researchers achieve a breakthrough in increasing the efficiency of organic solar cells, Siemens press release 7th January 2004.

²⁹ Global Photonic Energy Corporation and Princeton University. Solarbuzz, 19 November 2004.

³⁰ PIU 2001a, WEC/UNDP 2000, IEA 2000.

³¹ T. Coutts and M. Fitzgerald (1998). Thermophotovoltaics. *Scientific American*.

³² United Nations Development Programme (2000). *World Energy Assessment: Energy and the Challenge of Sustainability* (<http://www.undp.org/seed/eap/activities/wea/>)

of primary energy in the US, 11% in Austria, 20% in Finland and 17% in Sweden. Biomass for district heating and CHP is also well established in Denmark and Germany³³.

Most biomass energy is derived from other industries, such as forestry residues and wastes from the wood processing industry in the US and Scandinavian countries. Agricultural residues and paper pulp are widely used in some countries, such as Denmark and The Netherlands. Biomass technologies are under development both for small- and large-scale applications, and experiments with gasification for use in high efficiency combined-cycle power plants are in the demonstration phase. The cost of these plants is expected to be substantially reduced through replication and economies of scale once the plants enter early commercial application.

Much lower costs could be achieved in co-firing applications, where, for example, suitable quantities of biomass are supplied to existing coal plants. The largest potential for cost reduction lies with gasification technologies, in part because of the efficiency gains over combustion plants at capacities typical of biomass electricity plants. Future biomass electricity costs from dedicated plants fuelled with energy crops could be around \$0.05–0.06 per kWh. Short term market growth in biomass energy is likely to be based on the production of heat and electricity using combustion and gasification technology, including co-firing with fossil fuels.²⁴

Biogas is generated when bacteria anaerobically degrade biological material, such as agricultural or municipal waste. It has a lower calorific value and contains higher levels of corrosive components than natural gas, but if properly processed can be made suitable for feeding to natural gas supplies. As with natural gas, CO₂ is the main component that must be removed, either by pressurised water scrubbing, chemical adsorption, pressure swing adsorption, membrane separation or cooling by low temperature phase separation. See Section 8.2 for a more detailed discussion of CO₂ capture and storage.

Current biogas processing costs are so high that it can only compete if there are low biogas production costs. Biogas could become a source of gas for heating and transport if more plants were built and processing costs were reduced. In Germany, for example, production is sufficient to supply 3.7 million m³ per year of biogas to a municipal bus fleet of over 100 vehicles in Linköping.³⁴

Biofuels

Today, modern biomass provides about 20% of Brazil's primary energy supply, with much of this being alcohol fuel, which accounts for about 30% of gasoline demand. In early 2003, the European Commission issued a directive promoting the use of biofuels for transport, setting out two indicative targets for EU member states – 2% biofuels inclusion in the fuel pool by December 2005 and 5.75% by December 2010.

The relatively low conversion efficiency of sunlight into biomass means that large areas of arable land would be required to allow a significant amount of the existing fuel pool to be substituted with biofuels. Scenarios developed for the US and EU indicate that short term targets of up to 6% displacement of fossil fuels with biofuels appear feasible using conventional biofuels. A 5% displacement of gasoline in the EU would require about 5% of available cropland to produce ethanol and 15% to produce diesel (land requirements for diesel are higher than for ethanol because of lower yields of liquid fuel per hectare).³⁵ Kheshgi *et al* estimate that the equivalent of 12% of US cropland would be required to produce enough ethanol to replace the energy content of 10% of the US gasoline consumption in 1990. However, if all the carbon dioxide emissions associated with the production, harvesting, and conversion of corn to ethanol were to be offset, the land area required would be nearer to 50% of available cropland.³⁶

³³ United Nations Development Programme and World Energy Council, 2000. Bauen, 2001.

³⁴ W. Schulz, M. Hille and W. Tenscher (2004). *From Feedstock to Feed-in*. REW.

³⁵ L. Fulton (2004). *Driving ahead – biofuels for transport around the world*, REW Review.

³⁶ H. S. Kheshgi, R. C. Prince and G. Marland (2000). The potential of biomass fuels in the context of global climate change. *Annu. Rev. Energy Environ.*, 25, 199–244.

Biofuels are more expensive than conventional transport fuels, but improved conversion technologies will broaden the range of feedstock. For example, the cost effective hydrolysis of lignocelluloses would considerably increase the source of biomass for bioethanol production to include woody and grass crops as well as bio-waste. Work is underway in a number of countries and in particular the US to reduce the cost of converting cellulose to sugars, although a considerable amount of biomolecular and chemical engineering is required in order to achieve commercially attractive prices. Recent work in this area has led to the concept of a 'bio-refinery' similar to a petroleum refinery, which would use the whole of the biomass feedstock to produce a number of products in addition to biofuels, such as high value chemicals and co-generated electricity. Encouragement by US government and EU funding and targets for inclusion of biofuels in the transport fuel pool should see rapid developments in this area.

Gasification and thermochemical technologies are receiving increased attention as methods of converting biomass into transport fuels. Gasification to syngas enables the production of a variety of fuels including methanol, ethanol, dimethyl ether and synthetic diesel.

The Future for Biomass

Biomass is a versatile and important fuel and also a rich feedstock for the chemical industry. The potential for increased exploitation of biomass resources is very large. In spite of the apparent high land requirement for the production of significant quantities of biofuel using current technology, many estimate that the total solid biomass potential is about 25% of total projected global energy demand in 2050.

There are significant opportunities associated with the development of energy crops, such as the management, development and commercialisation of biomass conversion technologies and the implementation of biomass energy projects. However, the challenges are considerable and will require novel conversion technologies as well as a deeper understanding of the chemistry of biomass production and the potential environmental issues related to water demand and biological diversity.

5.4.4 Wind

Wind energy has grown rapidly over the last decade, with 40,000 MW current capacity providing nearly 0.5% of the world's electricity supply. Most forecasts show the capacity of wind generation continuing to grow. The German Wind Energy Institute estimates that wind generation capacity could increase fourfold by 2012, with 110,000 MW of new capacity boosting capital expenditure by €130 billion.³⁷ There has been a step change in the design of wind turbines allowing the construction of much larger machines than the 0.5 MW turbines familiar in the large onshore wind farms that provide 1% of California's electricity. Average installed capacity is now close to 1MW per turbine, and massive 4–5 MW machines are on the drawing boards for offshore projects – GE Wind Energy took the lead by erecting a 3.6 MW prototype in 2002. Materials science will clearly play an important role in developing the lightweight, high strength materials necessary for the construction of turbine blades and towers. There is also scope to develop new insulating materials for the high voltage cables required to bring electricity to shore. Corrosion will also be a problem for offshore turbines exposed to salt, air pollution and UV radiation. Wind turbines are expected to last for 20–25 years, and developing and providing coatings for their protection is already a strongly competitive and growing business.³⁸

5.4.5 Geothermal

Energy from the Earth's core is used around the world mainly for electricity generation and heating, whilst in some cases the steam is used directly in chemical process plants. The CO₂ emissions from high-temperature geothermal fields is far lower than the emissions from conventional fossil fuel plants,

³⁷ Wind Energy Study (2004). *Assessment of the Wind Energy Market until 2012*. DEWI.

³⁸ K. Muhlberg (2004). *Keeping your coat on by REW*.

but small quantities of undesirable gases such as hydrogen sulphide are often produced. The world's geothermal installed capacity is 15,580 MWth for direct heat applications and 8227 MWe of electrical generating capacity. Some experts predict that this could eventually grow to between 65,000 and 138,000 MWe, enough to supply about 17% of the world's population. Again the challenge for chemists is to develop materials or surface coatings that can withstand the corrosive environments associated with handling geothermal fluids and gas separation technology to deal with toxic gas emissions.

5.4.6 Ocean Energy

The oceans cover more than two thirds of the planet's surface and represent an energy resource that is theoretically far larger than we need. The most developed ocean technologies are tidal barrages, with the largest being the 240 MW facility at La Rance in France. However, the last decade has seen a renewal of interest in ocean power, and there is a degree of competition to become the global leaders in wave and tidal stream technology. Consequently, there are several devices with capacities of 0.1 MW to 2 MW which exhibit different design features currently on test around the world. These range from tidal current turbines to large pistons that cause rising waves to force a column of air through a turbine.

Other less developed technologies rely on ocean thermal energy conversion (OTEC), salinity gradient/osmotic energy and marine biomass. Although a number OTEC devices and schemes have been proposed to use a heat engine to extract power from the temperature differences between the surface and deeper layers of the sea the technical challenges are considerable. Similarly, whilst the energy released when a river reaches the salinity of the sea is very large, it is a very diffuse energy resource. Nevertheless it is a resource that remains untapped and which could potentially form a challenging research topic.

5.5 Nuclear

Nuclear power represents a carbon-free energy pathway and is an important component of the energy mix. It is likely that the future will see a return to favour of nuclear power in the UK. A key priority for the nuclear industry is therefore to redress the run down in nuclear fission research and education skills in UK universities. One of the greatest challenges for nuclear fusion is the development of high performance structural materials capable of withstanding extreme operating conditions.

5.5.1 Nuclear Fission

The UK currently has 31 operating nuclear reactors at 14 power stations, which provide around 25% of the electricity in the UK. Nuclear power supplies a larger proportion of energy than its proportion of capacity, reflecting its use in base load operation.

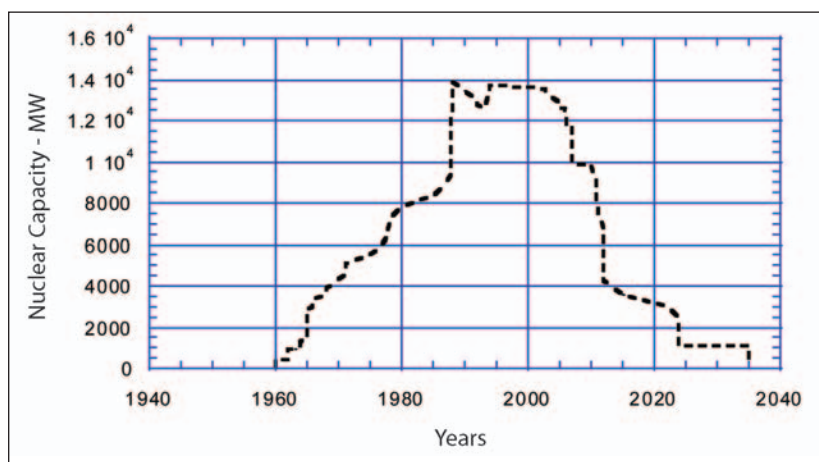
Over the period to 2010, some fourteen Magnox reactors (the first generation of nuclear reactors in Britain) and one advanced gas-cooled reactor (AGR) station are scheduled for closure. This will total 3572 MW of capacity. Between 2010 and 2020 most of the AGR stations and many large coal-fired plants are scheduled for closure.

A unique aspect of the UK's nuclear position, in comparison with other countries, is that only the UK needs to start replacing its nuclear reactors in the short-term just to maintain its nuclear generation capability. Other countries can afford to wait for up to a couple of decades because their reactors are mainly light water reactors (LWRs) whose lifetime can realistically be extended to 60 years. Many countries (e.g. France and Japan) also benefit from having a very much younger population of reactors, which again gives a longer timeframe. In contrast, the expected operational lifetimes for the UK's gas cooled reactors have very little leeway (a matter of no more than two or three years) rather than the decades for LWRs, so the UK projected decline curve as shown in Figure 4 is real.

³⁹ Dickson and Fanelli Istituto di Geoscienze e Georisorse, CNR (2003). The Earth's own powerhouse – power and heat from geothermal energy. *REW Review*, 2003.

At the moment no new reactors are planned in the UK. If that situation persists the nuclear generation capacity in the UK will decrease to zero before the mid-century. The rate of decrease may well be moderated by extensions of reactor lifetimes, but the overall shape of the curve will not change significantly.

Figure 4: UK nuclear generating capacity in the absence of new build



The importance of nuclear energy to the UK and within the EU can be seen from the following Eurostat figures.

- In the UK, 23% of electrical energy came from nuclear in 2000.
- The overall average across all EU countries in 2000 was 21% of installed generation capacity and 33% of electricity production (but Foratom say 35%).
- Nuclear energy electricity production grew by 6.6% between 1995 and 2000. However, electricity production in total grew by 10.7%.

Nuclear power provides about 16% of the world's electricity demand. Around the world, 63 new reactors are proposed, but there are some heavy caveats on these figures. For example, the data includes some Russian units, even though the status of these is very uncertain. In addition, other developments include, for example, numerous power reactors in Belgium, Finland, Germany, Spain, Sweden, Switzerland and the USA. The Netherlands, a new parliamentary committee on technology issues has been created with a mandate to include issues related to nuclear energy.

This worldwide activity indicates that the nuclear option is being retained by other nations. Security of electricity supplies at stable and competitive market prices are the major attractions of nuclear energy. In addition, in view of present government environmental ambitions, nuclear offers an emission free solution to power generation.

UK Skills Shortage

Despite this worldwide activity there is now a serious shortage of skills in the nuclear industry in the UK, as there is in other industries. The lack of activity over the past years, since the last nuclear stations were designed and built, has led to a significant loss of trained manpower and with the stock of scientific and engineering skills from universities being inadequate, it would probably be difficult to licence new build. Furthermore, for decommissioning tasks engineers and scientists have to be brought back from retirement. In short, when manufacturing capability losses are also considered, this energy option, based on UK resources alone, is not available other than on a project management basis using imported technology. The level of activity being carried out elsewhere in the world, however, indicates that nuclear technology is accessible and that nuclear energy is seen in other countries as a viable solution to electrical power supply.

Whatever the short to medium term future for nuclear power in the UK, the observation by the European Commission is relevant inasmuch as 'in the longer-term beyond 2010 the long lead-in time for energy technology means that it is essential to maintain long-term research, partly to find a solution to nuclear waste and partly to hand down nuclear expertise to future generations'. Section 8.3 includes a discussion of the challenges facing the handling and disposal of nuclear waste.

Next Generation Nuclear Energy Systems

Nuclear systems that are currently available, such as the BNFL/ Westinghouse AP1000 system, have been designed with modern liberalised energy markets, such as those emerging in the EU, in mind. For example, the AP1000 embodies passive safety features that utilise the forces of nature to bring the reactor to a safe condition in the event of any unexpected incident. These features are coupled with proven operating experience for the systems and components that make up the reactor, as well as a shortened construction schedule (36 months), which helps to make the concept more attractive to potential investors. This design also generates reduced waste volumes in comparison to previous reactor concepts and is well on the way to being licensed in the US (following on from the AP600, which achieved US Design Certification in 1999).

Whilst the AP1000 represents an attractive option for deployment in the near term, requirements in the medium to longer term may dictate that other concepts need to be addressed, such as the emerging hydrogen economy. It has been recognised that High Temperature Reactors (HTRs) such as the Pebble Bed Modular Reactor (PBMR) are ideally suited to the large-scale production of hydrogen without associated CO₂ emissions, due to the high temperature process heat that these systems generate. HTRs potentially have a major role to play in the development of a successful hydrogen economy, both in countries that already have nuclear power and in many that do not. It is pleasing to note that a good deal of valuable work in support of HTR development came from the EU Framework 5 programme.

In the longer term, new system concepts, such as those being developed under the banner of international programmes like Generation IV and INPRO, have the potential either to deliver step-change benefits in terms of performance, non-proliferation or economics, or else are suited to deployment in geographies or market conditions where conventional large-scale plants are unsuitable. It is notable that all of these longer-term developments (PBMR, Generation IV, INPRO) are collaborative ventures, largely due to the size and timescales of such projects and the need to draw upon a wide range of expertise and experience.

5.5.2 Nuclear Fusion

The UK has long been a strong supporter of nuclear fusion research since its early development days at Harwell in the 1950s. Although fusion is still at the development stage there has been great progress over the last 50 years. There have been two main streams of fusion research: inertial confinement and magnetic confinement. In the former, very small spheres of deuterium and tritium are uniformly compressed by powerful lasers in pico-second time ranges. In magnetic confinement fusion, plasmas of deuterium and tritium or other isotopes in a toroidal vessel are bound by magnetic fields and heated until fusion conditions are reached. In both techniques the combination of maintaining high temperature, density and confinement time can yield fusion. The goal of the research is to push these conditions further until more energy is created through fusion than is delivered externally to heat the system. Progress in fusion over the past decade can be demonstrated by a number of experiments where conditions have been created such that more energy is generated through fusion than is put in.

The challenges in fusion research are now to prolong these conditions from seconds to continuous duration and to extract the energy in a useful form; both are required for an industrial scale energy source.

The UK has hosted the JET nuclear fusion experiment, which is one of world's largest experimental magnetic fusion devices, over the past 25 years. JET has had a number of very successful campaigns that have extended the conditions for fusion. It also has demonstrated the ability to operate with deuterium-

tritium plasmas, which bring greater challenges associated with radiation, such as the activation of the device and the management of tritium.

Whilst JET has been very successful its usage is limited, in that a larger geometry is needed to improve confinement and explore fusion plasma conditions, such as sustained alpha-particle heating. The cost of developing the next generation of device is prohibitively expensive for any single nation (greater than \$10 billion). Over the past decade the main countries supporting fusion development (US, EU, Japan, China, Russia) have agreed to build the International Thermonuclear Experimental Reactor (ITER), which will be sufficiently large to explore fusion plasma conditions close to those in a commercial scale power generator. However, it will still be an experimental device and will not generate power that can be utilised. ITER may well be the last experimental device needed before progressing towards the first demonstration commercial power plant. To date the engineering design of ITER has been completed, and the next step is to agree where the device will be constructed. There have been prolonged negotiations between countries, with the two remaining contenders being Japan and France. It is hoped that these negotiations can be resolved and construction started within the next year. It has been reported that if a decision on the ITER was made in 2005, the first plasma should be possible in ITER by 2015.⁴⁰

Apart from the continued research into plasma physics, magnetics, instrumentation and remote handling, one of the greatest challenges in fusion is materials research. Selecting the right materials is a research programme in its own right: materials must withstand high power loadings, have low atomic number, must be non-magnetic and resist radiation damage from intense gamma-ray and high energy neutron fields. To support the research in materials, a device to support ITER has been proposed, which is referred to as the International Fusion Material Irradiation Facility. This will be dedicated to studying the effects of high radiation fields on materials over long periods of time.

⁴⁰ See <http://www.iter.org/>

6. Energy Distribution and Storage

This chapter concentrates on those aspects of energy distribution where chemistry will play a key role. It focuses particularly on hydrogen as an energy vector and energy storage.

6.1 Transition to a Hydrogen Economy

Hydrogen, coupled with fuel cell technology, offers an alternative to our current reliance on fossil fuels for transport and power generation. Hydrogen can, in principle, be produced by a wide range of processes, many of them renewable. However, many of these routes are in early stages of development, and significant research is still required before they will become competitive with conventional processes.

The move to a hydrogen economy will take many decades. In the early stages of the transition significant challenges need to be tackled in the development of better materials for fuel cells and for on-board storage of hydrogen. As demand for hydrogen grows, carbon capture on small and large-scale will become an important issue. For a true hydrogen economy, large-scale hydrogen production processes using renewable or low-carbon energy sources will need to be developed and commercialised.

The hydrogen economy is the name given to an economy based on hydrogen rather than carbon-based fuels. The transition to a hydrogen economy may be the biggest infrastructure project of the 21st century. Whilst R&D has already delivered astounding advances in materials, catalysts and systems for hydrogen production, distribution, storage and conversion, significant challenges remain.

The socio-economic and environmental benefits of a hydrogen economy could be dramatic which justifies the investment of resources and capital. Although the transition to hydrogen can deliver significant environmental benefits from the start (e.g. reductions in urban pollution), it is in the later stages that hydrogen offers a means to transform global energy networks.

6.1.1 The Attractiveness of Hydrogen

As has already been described, concern is growing over greenhouse gas emissions, over finite oil and gas reserves (and, more immediately, over an increased dependence on unstable supplies) and over local pollution from burning fossil fuels. In response, most leading economies in both the developed and developing world have adopted policies aimed at stimulating the adoption of hydrogen as the clean energy choice for the future. As a sign of the global importance of this issue, and of the need for action worldwide, an unprecedented, collaborative partnership of these leading economies was formed in 2003 to co-ordinate activities in this area.⁴¹

When used in fuel cells, hydrogen generates no emissions other than water at the point of use, and very low emissions when burned conventionally. The combination of renewably-generated hydrogen and fuel cells offers a long-term solution to the world's developing energy and environmental crisis. In the short and medium term, the introduction of hydrogen will help reduce overall carbon emissions and will open up new energy pathways to manage the dependence on traditional fossil fuels.

One of the key attractions of hydrogen is the wide variety of routes and feedstocks available for its production on both a large- and small-scale. The different routes for producing hydrogen are discussed in Section 6.1.4. Currently, most hydrogen is produced from the steam reforming of fossil fuels (especially oil and natural gas) but hydrogen can be extracted from most materials of organic origin, either by reforming, gasification or through other chemical or biochemical routes. The extraction of hydrogen from water through electrolysis and thermochemical or photochemical dissociation is also possible. When the energy required for these transformations is supplied from solar, geothermally or biomass sources, then these routes represent truly green and sustainable energy pathways.

⁴¹ International Partnership for a Hydrogen Economy – made up of the ministerial representatives of governments of fifteen of the world's leading economies. See www.usea.org/iphe.htm for further information.

6.1.2 Barriers to Hydrogen

Despite the advantages associated with hydrogen power, significant technical challenges exist to finding a simple and cheap way of producing and storing hydrogen, converting it to electricity and supplying it safely and efficiently to customers. These challenges must be addressed more or less simultaneously before delivering a hydrogen economy.

Production

Energy is required to produce hydrogen, therefore hydrogen as a fuel is only as clean as the process that produces it in the first place. The most common way of producing hydrogen is steam reforming of natural gas in a two-step catalytic process to produce H_2 and CO_2 . Primary concerns surround the efficiency of this process (current steam reformers are only 70 to 80% efficient) and the release of CO_2 . It has been estimated that it costs \$5 to produce the amount of hydrogen *via* steam reforming that releases as much energy as a gallon of gasoline.⁴²

Hydrogen production from fossil fuels, with CO_2 capture and storage, is likely to provide the bulk of hydrogen over the next 30 to 50 years until more cost effective sustainable solutions are developed. Consequently, it will be imperative to develop economically and technically feasible means of capturing and sequestering the CO_2 that is released (see Section 8.2).

The long-term goal is renewably produced hydrogen. Solar power and wind energy can provide 'clean' electricity to split water, but these routes are currently even more uneconomic than steam reforming. Other possible production routes involving biomass gasification and thermochemical cycles using heat are still highly uneconomic but may yield viable alternatives for the future. Whilst production costs have been coming down and innovative solutions are being put forward, there are considerable obstacles that need to be overcome before hydrogen production becomes both technically and economically feasible.

Whilst hydrogen combustion produces zero emissions of CO, CO_2 , NO_x or SO_x , some recent work has raised concerns about the release of molecular hydrogen to the atmosphere. Hydrogen released into the lower atmosphere has the potential to perturb the levels of $\cdot OH$ (the main atmospheric oxidant). Since $\cdot OH$ is the primary atmospheric sink for CH_4 (a potent greenhouse gas), increasing concentrations of H_2 could preferentially remove $\cdot OH$ and indirectly increase the levels of CH_4 in the atmosphere.⁴³ These predictions will ultimately depend on the amount of H_2 that is released into the atmosphere should hydrogen power become a predominant form of energy; there is much speculation surrounding H_2 leakage rates and the expected rise in H_2 levels in a hydrogen economy.

Transportation issues

On-board storage of hydrogen is also posing significant obstacles to delivering hydrogen-powered vehicles. Hydrogen is the lightest element and will occupy a larger volume than other fuels. It therefore needs to be liquefied, compressed or stored in some other advanced storage system to have enough on-board to travel a reasonable distance. Nearly all of today's prototype hydrogen vehicles use compressed gas, but this is relatively bulky. Liquid hydrogen could provide an ideal way to transport hydrogen, but the boiling point of hydrogen at $-253^\circ C$ means that this storage method would be extremely energy intensive, requiring considerable energy to keep and maintain such low temperatures. Other advanced storage materials are being developed, such as carbon based adsorbents (carbon nanotubes) and metal hydrides. However, the high temperatures and pressures required to liberate H_2 and slow- H_2 release are posing serious obstacles to these storage materials.

⁴² R.F. Service (2004). The Hydrogen Backlash. *Science*, **305**, 958–961.

⁴³ A. Ananthaswamy (2003). Reality bites for the dream of a hydrogen economy. *New Scientist*, 15 November 2003.

There are also significant economic considerations surrounding the cost of fuel cells *versus* the internal combustion engine, with the latter typically costing \$30 for each kilowatt of power it produces while fuel cells cost a hundred times more. Technical challenges such as making fuel cells rugged enough to withstand the stress of driving, reducing their size and weight while increasing power density and fuel flexibility also still exist. In the interim, while fuel cell technology is preparing for mass commercialisation, it is likely that more and more hybrid electric vehicles will be deployed, offering significant improvement in terms of energy use and significant reductions in carbon emissions in comparison to the conventional internal combustion engine.

6.1.3 Introduction and Transition

The replacement of carbon-based fuels by hydrogen will take many decades, requiring massive changes to supply, distribution and delivery infrastructure in the entire energy network. The introduction and subsequent expansion of hydrogen into an additional energy vector, as well as a more widely used transport fuel, in the global energy market will thus be a gradual and incremental process. At each stage in the process there will be significant challenges and issues to be overcome. The nature and scale of these issues will change during the transition decades and appropriate solutions to them may also change over time.

Introduction Phase (Current–2015)

At first, it is likely that hydrogen production will be demand led, as requirements for initial supplies are driven by demand for hydrogen as a transport fuel, mainly for fuel-cell vehicles but also for hydrogen powered internal combustion engines. Fuel cells will initially be trialled in buses and fleet vehicles, but penetration is likely to grow with the development of hydrogen fuelling infrastructure. Development of better on-board hydrogen storage systems and further cost reductions in fuel cells could result in their uptake for use in passenger cars, taking advantage of the higher efficiency and enhanced driveability of this new technology.

Establishing a cost effective hydrogen distribution network and identifying better hydrogen storage solutions will therefore be key projects in this phase. Whilst the initial distribution network will be mainly an investment issue (with the development of a full refuelling infrastructure occurring in phases over twenty years or more) the necessary advances in hydrogen storage materials, as well as in improved materials for fuel cell construction, are important current challenges for the chemical sciences community.

Given the low absolute demand for hydrogen (relative to conventional hydrocarbon fuels) the energy efficiency of the production pathway will initially be of secondary importance. Even the most optimistic scenarios for hydrogen fuel forecast that demand in the early years can be satisfied from existing, centralised production capacity. Reforming of hydrocarbons is thus likely to satisfy most demand for hydrogen in the early years. The higher conversion efficiencies make hydrogen, when used in fuel cells, a greener option than petrol or diesel internal combustion engines, even when produced from non-renewable sources.

Continued development of effective renewable or carbon-neutral processes on a production scale will, however, remain an important objective so that these new pathways are ready for later years.

Early Transition Phase (2015–2035)

As intermittent renewable, and potentially nuclear, power generation increases, a need for energy storage using hydrogen is likely to develop. Hydrogen production, *via* electrolysis or thermochemical routes (using heat from nuclear reactors), could start to become more supply driven as hydrogen develops into a true energy vector, as well as being used as a transport fuel.

It is likely that there will be a greater focus on the efficiency and emissions generated during hydrogen production and throughout the energy cycle as growing volumes of hydrogen are produced and demand for hydrogen as a transport fuel increases. Reforming of hydrocarbons, without carbon capture, may

become less attractive as other production routes based on renewables or carbon-neutral pathways are introduced.

For the same reasons, the high energy consumption of compression or liquefaction will focus attention on alternatives to these storage methods in the distribution of growing amounts of hydrogen.⁴⁴ Large-scale, solid-state hydrogen stores using similar materials to on-board stores may provide a solution. Development of processes using materials that can be reversibly hydrogenated (e.g. the reversible conversion of benzene to cyclohexane) offer a further option for hydrogen transport. Catalysis and material stability will be important factors in any such process.

Distributed generation of hydrogen, in smaller 'forecourt reformers' or through improved electrolyzers, will increase should demand grow and if further production capacity is required. Although neither of these offer zero-carbon, or carbon-neutral hydrogen, the energy and costs involved in transporting hydrogen may make these processes attractive in some cases.

Late Transition Phase (2035–onwards)

In later decades the focus of activity is likely to move towards the replacement of hydrocarbon-based production processes by new pathways to hydrogen. Advances in photochemical, enzymatic and high temperature thermochemical cycles may bring costs down to levels that are competitive with increasing oil and gas prices. Hydrogen production from coal, coupled with carbon capture, may also become an important route. These processes are in the early stages of development and much work will be required to provide feasible production processes.

6.1.4 Hydrogen Production

Reforming

Today almost all hydrogen is produced from the steam reforming of fossil fuels (typically naphtha or natural gas). This process, in which the hydrocarbon is reacted with steam at high temperatures over a base metal catalyst, is well developed and is efficiently carried out at industrial scales (US production of hydrogen is around 9 million tonnes annually)⁴⁵. Efficiencies for large-scale processes are in the 70 to 80% range however a non-renewable feedstock is needed as a source of hydrogen (as well as for the additional energy required in the production process).

With typical energy efficiencies in the region of 90% for gasoline refining, the use of hydrogen, produced from reforming hydrocarbons, as a transport fuel is less efficient on a well-to-tank basis (i.e. not considering the efficiency of how the fuel is used). Burning the hydrogen in an internal combustion engine does provide a zero-emission vehicle (addressing urban pollution issues) but consumes more energy overall than a petrol or diesel engine.

When supplied to a fuel cell, however, the improved efficiency of energy conversion, relative to gasoline or diesel engines, means that even steam reformed hydrogen delivers a reduction in greenhouse gas emissions of around 50%, on a well-to-wheels basis, compared with conventional technology.⁴⁶

Further development of the large-scale steam reforming process continues to produce incremental improvements in efficiencies and costs. Reforming on a small-scale (often using autothermal or partial oxidation reforming as well as steam reforming) has been the subject of intense effort. Prototypes of

⁴⁴ With current technology, additional energy, equivalent to approximately 10% of the energy content of the hydrogen (HHV), is required to compress the gas to 350 bar (typically used in first generation on-board tanks). Current liquefaction processes require around 40% of the energy delivered by the hydrogen.

⁴⁵ TMG/The Management Group (2003). *The Hydrogen Report*.

⁴⁶ *Well to Wheels Analysis of Future Alternative Fuels and Powertrains in the European Context*. EUCAR EU Joint Research Centre, November 2003, Fig 8.4.1–2b.

compact and efficient units to generate hydrogen-rich 'reformat' gas for supply to fuel cells have been developed. Although on-board reforming is unlikely to be the solution for transport applications, the use of local (or internal) reforming of natural gas is emerging as the preferred route to generate hydrogen for use in fuel cells for stationary CHP applications.

Gasification

Traditionally, gasification of coal or oil residues has been employed to generate syngas, a mixture of CO and hydrogen, for further use in energy production or as a chemical feedstock. There are many process variants but they typically require high temperatures (1,100 to 1400°C) and usually an air separation unit (to avoid the later separation of nitrogen from the hydrogen).⁴⁷

There are many reviews of exciting and future applications of gasification to a wide range of other feedstocks, including biogas, biomatter and biomatter residues.⁴⁸ Shell has demonstrated the use of mixture of coal and dried chicken waste (25%) in a large-scale gasification process.⁴⁹ Although not yet demonstrated on a large-scale, the use of biomatter as sole feedstock for a gasification plant would generate hydrogen with no net release of CO₂.

Electrolysis

Production of hydrogen from water using renewably generated electricity is highly attractive, as the process is clean, relatively maintenance-free and is amenable to being operated on a large- or small-scale. When coupled with suitable bulk storage of the hydrogen, generated electrolysis provides the means to decouple variable energy demand from an intermittent supply. Electrolyser efficiency varies from 60–90%, significantly affected by electrolyser configuration and electrode activation.

Most water electrolyzers are of a conventional type, using concentrated potassium hydroxide solution to transport electrons between electrodes. However new designs of electrolyser, modelled on a fuel cell configuration, use a solid polymer membrane to separate the two reactions and to perform charge transfer. These Membrane Electrode Assembly configurations are particularly well suited to handling variable current densities, as would be expected from some renewable energy sources.⁵⁰

Further work is needed to develop improved electrode surfaces for both types of electrolyzers.

Thermochemical Water Splitting

Thermochemical water-splitting converts water into hydrogen and oxygen by a series of thermally driven reactions. The next generation of fission reactors could provide the high temperatures needed for these reactions. Careful selection of materials and development of new materials will be necessary to meet the required stability conditions. Understanding the fundamental high temperature kinetics and thermodynamics of these processes will be essential. This production route is viewed as a long term option, which will produce hydrogen in a well established hydrogen economy.

Biochemical Hydrogen Generation

Certain photosynthetic microbes namely green algae and cyanobacteria, produce hydrogen as part of their natural metabolic activities using light energy. By employing catalysts and engineered systems, hydrogen production efficiency could reach 24%. Photobiological technology holds great promise, but because oxygen is produced along with the hydrogen the technology must overcome the limitation

⁴⁷ *Hydrogen Supply: Cost Estimate for Hydrogen Pathways*, NREL, July 2002.

⁴⁸ R. L. Bain (2004). *Current and Potential Energy products from Biomass*. NREL, Jan 2004.

⁴⁹ *Overview of Worldwide Gasification Developments*. Paper presented by Shell at 2003 Gasification Technologies Council Conference.

⁵⁰ M. Newborough (2004). A Report on Electrolysers. *Future Markets and Prospects*.

of oxygen sensitivity in hydrogen-evolving enzyme systems. In addition, the hydrogen production rate from photosynthetic microorganisms is currently too low for commercial viability. Breakthroughs will lie in finding naturally occurring organisms that are more tolerant of oxygen and by creating new genetic forms of the organisms that can sustain hydrogen production in the presence of oxygen.

Unlike cyanobacteria or algae, photosynthetic bacteria do not oxidise water. They do, however, evolve hydrogen from biomass (previously generated from sunlight, water, and carbon dioxide), using several different enzymatic mechanisms with near term potential for commercial hydrogen production. One mechanism in particular looks promising for application as a biological conditioning agent for upgrading thermally generated fuel gases to a level where they can be directly injected into hydrogen fuel cells. This same system has potential to subsequently evolve into a photobiological method to produce hydrogen directly from water.

Photocatalytic Water Electrolysis

Photolytic hydrogen production technologies use the energy from sunlight to split water into hydrogen and oxygen. Two basic criteria must be met: the light harvesting system must have suitable energetics to drive the electrolysis reaction and the system must be stable and durable in an aqueous environment. R&D is focused on these two areas.

6.2 Energy Storage

Challenges for chemists in relation to electricity storage and battery technology include new advances in materials for batteries (lithium-ion and redox flow batteries) and supercapacitors. Innovations in lithium-ion batteries for hybrid and electric vehicles will also require the expertise of chemists to develop new electrode materials and new electrolytes that are tailored for these applications.

The requirement to store electrical energy from traditional power generation has been limited mainly to hydroelectricity. However, the need for storage will increase by orders of magnitude as the energy landscape changes to include a much greater proportion of renewables. All the new energy sources are either intermittent in their supply (photovoltaics, wind, wave) or operate best at or near constant output. Such energy sources are also, in general, smaller and more widely geographically distributed than conventional power stations. Energy storage is not only an imperative to balance intermittent supply and consumer demand, it also has an important role in energy trading (arbitrage), since energy may be stored and then returned to the grid at a higher value. Other important issues are security and quality of supply; both are more challenging as the proportion of renewable generation increases. It is also important to note that there will be more off-grid generation, which in turn demands a greater use of storage to ensure continuous supply. A summary of the various uses of storage is given in Table 1. All this means that storage will be central to securing future energy supplies.

Table 1: Added value of electricity storage in the case of on-grid and off-grid generation.

	On-grid	Off-grid
Inter-temporal arbitrage	×	
Balancing of the system	×	
Grid losses avoidance	×	
Grid investment avoidance/deferral	×	
Reserve capacity – emergency supply	×	×
Voltage/frequency support	×	
Black start	×	
Seasonal/day-night renewable (D G) energy storage	×	×
Uninterruptible Power Supply (UPS)	×	×
Power Quality Management	×	

Source: A. F. Wals and R. H. Hendriks (2004). *Economics of Energy Storage*.

It is evident that energy storage must be seen in the context of the evolving nature of energy generation. It is convenient to divide energy storage into static and transport applications.

6.2.1 Static Energy Storage

Technologies will change with time so it is necessary to consider short to medium term and longer term storage options separately.

2005–2025

Over this period it is likely that renewable energy sources will increase significantly. Renewable energy sources are likely to be dominated by wind and wave power, since these technologies are already available. To bridge the ever-increasing gap between supply and demand whilst minimising the use of fossil fuels, it is important to store the renewable energy when generation is at a maximum (lower cost) and then supply it to the consumer in response to demand (higher value). Storage is especially important for off-grid generation, where there is no back up from the grid.

Over the next 20 years, there will be a great need for electrical energy storage that is cost effective, safe, distributed in nature so that storage is located close to the end-user and that minimises environmental impact. The following summarises the technologies that are likely to make an impact.

Batteries

Rechargeable batteries offer the most direct means of storing electrical energy and as a result are highly efficient. The following represent some of the main contenders:

- polysulphide bromide flow battery;
- vanadium redox flow battery;
- zinc bromide flow battery;
- sodium-sulphur or zebra battery;
- lithium-ion battery;
- lead-acid battery.

Lead-acid is the most mature technology and will continue to evolve, delivering increasing energy density. However, the inherent nature of the lead-acid battery means that the maximum energy density possible remains relatively low. There is also the issue of public acceptability of lead in a greener energy landscape.

The redox flow battery contains two compartments, one for the negative and the other for the positive electrode, separated by a membrane. Solutions containing suitable redox couples are pumped into each compartment and the couples reduced and oxidised. The redox processes are reversed on discharge. The polysulphide/bromide flow battery works at room temperature with a net efficiency of around 75% and has been developed to test-rig level. This technology is now owned by the Canadian company VRB Power Systems, which is conducting further commercial development. The technology is particularly suited to larger-scale applications, given the infrastructure needed to store and circulate the redox couples.

The sodium-sulphur battery has been developed over 30 years. Its most practical implementation is in the form of a zebra battery, where the sulphur is replaced by a metal chloride. The battery uses a solid ceramic electrolyte to separate the sodium and metal chloride and operates at an elevated temperature to maintain molten sodium.

Lithium-ion batteries represent the most important development in rechargeable battery technology for a hundred years. They have three times the energy density of conventional rechargeable batteries and have had a major impact in consumer electronics. A lithium-ion battery occupying some 10 m³ could store 4.5 MWh of energy and with a charge/discharge efficiency of over 99.9%. This technology is already the storage solution of choice in a number of energy research centres around the world.

Although all the batteries present challenges, lithium-ion presents one of the greatest challenges for chemists. Scale up to larger batteries requires:

- fundamental advances in new cheaper, safer electrode and solid polymer electrolyte materials with better performance;
- new non-flammable liquid electrolytes or ionic liquids.

A further possible driver for the development of novel battery technology at the smaller scale end of battery technology is regulation. In the EU, measures have already been taken to limit the mercury content of batteries. Further regulation will aim to reduce other heavy metals, including cadmium, nickel and lead. Also options for disposal of batteries will be limited to encourage collection and recycling.

Flywheels

Flywheels offer a solution that is based on well-developed mechanical engineering, in which energy is stored in a spinning mass.

Chemical science challenges include the need for new lightweight composite materials e.g. polymer/carbon fibre based materials, in order to operate at higher speeds.

Superconductors

In superconducting magnetic energy storage devices (SMES), energy is stored in the magnetic field of a coil within which a current flows. The device consists of a superconducting coil, typically made of niobium with titanium or tin, in a copper matrix, a power conditioning system (PCS), a refrigeration system for cooling the coil and a cryostat vacuum vessel. Efficiency losses are mainly due to the cryogenic system, which has to keep the coil below the critical superconducting temperature of around -268°C .

Chemists are needed to address the identification and development of new superconducting materials with higher critical temperatures, preferably room temperature, and with suitable mechanical properties for processing into coils and wires.

2025–2050

Predicting the energy landscape beyond 2025 is difficult. However, it is clear that over this time period fossil fuels will contribute even less to the energy supply than in 2005–2025 and the dominant energy sources will be intermittent or operate best at constant output. The need for storage will therefore continue to grow, since balancing supply and demand will be even more difficult without fossil fuel power stations.

Major changes will probably come from a move towards the hydrogen economy, which is more likely to be achieved in this time period. Advances in the efficiency of photovoltaic devices as well as the direct photochemical conversion of sunlight to electrical energy can also be expected. Nuclear fusion holds considerable promise as a source of electrical energy in this period.

Photovoltaic and photoelectrochemical electricity generation are, like wind and wave, intermittent; hence energy storage will be a critical requirement for effective use of these technologies. Nuclear generation is likely to prove most efficient if operated at or near constant output, which will also necessitate storage.

Chemical science challenges include the need for:

- continued innovation in lithium-ion, and redox flow batteries;
- new advanced batteries;
- superconductors.

6.2.2 Transport

Again, progress in transport developments necessitate separate considerations of short to medium term and longer term prospects.

2005–2025

Transport currently accounts for some 30% of CO_2 emissions and with the phenomenal growth in vehicle usage in countries such as China and India this contribution is expected to rise substantially. The dominant technology over the next 20 years is likely to be hybrid vehicles: first generation systems are already in the market place. They combine a petrol engine with a conventional nickel and metal hydride battery. There is a great need to replace the nickel and metal hydride battery with lithium-ion, which has superior energy density. It also takes up less space and weighs less, since having two power sources adds weight and occupies valuable space.

Chemical science challenges for lithium-ion batteries (hybrids) include the need for:

- new electrode materials that reduce the cost of the battery, increase safety, are of low toxicity and support high power (charge/discharge rates);
- new electrolytes that are safer, less flammable, less toxic and of high conductivity;
- ionic liquids and solid polymers as new electrolytes.

All-electric vehicles will also make a significant impact. Although the range of electric vehicles is currently limited by battery technology, advances will increase this substantially. However, it is unlikely that electric vehicles will be able to offer the range or performance of hybrid vehicles. For all-electric vehicles, the sodium-sulphur or zebra battery, as well as the lithium-ion battery, offer possible solutions.

Chemical science challenges for lithium-ion batteries (pure electric) include the need for:

- lithium-ion battery electrodes that are safe, cheap, low toxicity and high energy density (compared with hybrid applications, high energy density is important but rate is less of an issue);
- new electrolytes that are safe, of low flammability and high conductivity;
- new advanced batteries;
- better understanding of fundamental battery electrochemistry.

6.2.3 Supercapacitors

Supercapacitors, like batteries, are electrochemical devices, but they differ from batteries in that supercapacitors are optimised for power rather than energy storage. Conventional supercapacitors employ high surface area carbon electrodes and aqueous based electrolytes. However, recent innovations have included the replacement of one carbon electrode with a lithium intercalation compound such as $\text{Li}_4\text{Ti}_5\text{O}_{12}$, the use of non-aqueous electrolytes allowing higher voltages and the use of nanomaterials. These devices can act as important power buffers, absorbing energy at a high rate, then transferring it to devices such as batteries or flywheels. They are particularly attractive technologies in hybrid vehicles or direct electric traction.

Chemical science challenges need to address:

- new electrode materials;
- new non-aqueous electrolytes;
- better understanding of fundamental mechanisms.

Rail transport

As well as the use of a hybrid technology for private transportation, lorries and buses, it is likely that increasing use of such technology will be made in rail transportation. Further electrification in the UK would be expensive, but a combined diesel/battery hybrid power train could have significant advantages. It would allow diesel engines to operate under optimal conditions and therefore minimise emissions, while regenerative braking and acceleration can be supplied from the battery.

The storage technologies developed for transport in the 2005–2025 period are likely to continue beyond 2025 and will require further step changes to keep pace with demands for performance and efficiency.

2025–2050

The major change in this period beyond 2025 is likely to be the introduction of the hydrogen economy. In transportation this will involve a move to fuel cell powered vehicles: such vehicles will be hybrids in which a solid oxide or polymer fuel cell will be coupled to a battery and/or supercapacitor combination. The supercapacitor/battery will provide regenerative braking, rapid acceleration, and start-up, permitting the fuel cell to operate under optimal conditions.

Chemical science challenges in this period are expected to be similar to those described in the earlier time period, with hydrogen storage being a key issue in the context of its use in vehicles.

7. The Efficient Use of Energy

Major opportunities exist for improvements in the conversion of primary energy in transport, distribution of energy and in end-use technologies. Innovation in these sectors will be underpinned by chemistry (e.g. developments in materials, new strides in corrosion chemistry, high performance catalysts).

One of the key aims of any sustainable energy policy must be to promote efficiency. The two underlying objectives of promoting efficiency are to preserve natural resources and to minimise damage to the environment. Natural resources can refer to both raw materials and the energy sources consumed in their processing. Environmental damage can occur from emissions produced during the manufacturing of products, the generation of power needed for processing, the disposal of wastes and the disruption of the natural environment that surrounds a major development.

This section discusses issues related specifically to energy use, but at the outset it should be stated that energy efficiency cannot be considered in isolation from efficient use of raw materials and the environmental effects of waste disposal. A process that is in itself more energy efficient but which consumes a particularly rare and valuable resource or produces an especially hazardous waste might be less preferable to a process that is less efficient. The reverse can also often be the case, where the impact of complex recycling schemes on the conservation of natural resources has to be considered in the context of the energy used and compared with a process generating an equivalent product from new materials. The best overall approach for assessment is to apply resources efficiency Life Cycle Assessment, which was developed in the UK as part of ISO14001.⁵¹ There are undoubtedly developments in materials use and processing where the chemical sciences can play an important part in the more efficient use of energy and which might indirectly lead to improved cycle efficiency, but this is too broad a topic to be discussed here.

For large industry, legislation on energy efficiency is encompassed within the IPPC Directive²⁰, which came into effect in October 1999 and places a greater emphasis on energy efficiency, waste management and reducing natural resource consumption. Established activities have to be compliant with the Directive by October 2007 and compliance is achieved through Best Available Techniques (BAT), which are summarised in BAT Reference (Bref) documents issued by the EC. A key change is that previously legislation was based on the BATNEEC principle ('Not Exceeding Excessive Cost'), which implies a cost-benefit weighting of various options. Despite the absence of the NEEC qualification, the concept of avoiding excessive costs is encompassed in the IPPC definition of availability. This is important, since any energy policy must take a balanced view of energy-economy-environment interactions and also must include a social cost-benefit analysis in order for the policy to be sustainable. Nevertheless, within the existing legislation, any improvement that produces an overall cost reduction or is cost neutral in terms of the overall process is likely to be a requirement, whatever the cost of the environmental component.

Within this framework, future requirements for research and development related to efficient use of energy and natural resources can be identified. It is important that priorities for energy efficiency R&D be developed in conjunction with industry, as one of the objectives should be to develop export markets. This approach was suggested by the Irish Government in its 'Green Paper for Sustainable Energy'.⁵² According to the Green Paper, four priority areas require significant development, namely industrial energy use, transport, construction and domestic energy use. The same categories are considered here and many of the suggestions in the Green Paper are included in the discussion that follows. Some policy issues are also outlined.

⁵¹ ISO 14001 (1996). *Environmental Management Systems*.

⁵² Irish Department of Public Enterprise (1999). *Green Paper on Sustainable Energy*.

7.1 Transport

Oil derived liquids are at present the most cost effective transport fuels and the most efficient energy storage materials available to us. Whilst estimates of the ultimate global reserves of petroleum reserves vary, it makes sense to recover, convert and use the remaining liquid crude oil as efficiently as possible. Much of value in the crude oil is currently lost because of an inadequate understanding of the processes involved at the molecular level.

Changes in vehicle design are being driven by the need to improve efficiency and reduce emissions. Chemists, engineers and material scientists must be encouraged to work together to develop the next generation of fuels and lightweight hybrid vehicles capable of two or threefold improvements in fuel economy. New lightweight materials for the air transport sector will also yield improved efficiency.

In spite of current concerns about the constrained oil supply and high cost, most scenarios for the next 20 to 50 years suggest that the world's growing demand for energy will be primarily supplied by fossil fuels. Currently, about 74 million barrels of oil are consumed every day, mostly as transport fuels, which is the sector where oil is most suited as the primary energy carrier, and where substitution is arguably most difficult. By 2020 this is predicted to have increased to about 110 million barrels per day (bpd),⁵³ although production actually declined slightly during the years 2000–2002.⁵⁴ The demand for oil for transportation in the Asia Pacific countries is growing at 3.5% per annum from a current demand of about 18 million bpd compared to growth in Europe of just 0.5% from a demand of about 15 million bpd.

Changes in vehicle design are being driven by the need to increase efficiency and reduce CO₂ emissions. In 1997 there were 600 million vehicles on the world's roads, with engines operating at efficiencies of 10–25% for petrol and 15–35% for diesels. Transmission, road and other losses reduce efficiency significantly for the overall vehicle. Vehicle engineers around the world are currently chasing every lead with a view to achieving the goal of improved fuel efficiency coupled with reliability and affordability. It is generally accepted that the customer is unprepared to compromise his or her expectation of vehicle performance, reliability or cost, so technological improvements are necessary alongside environmental developments.

Multidisciplinary teams including chemists and chemical engineers have already achieved significant improvements in the operation of the internal combustion engine by developing direct injection spark ignition systems and small diesels with more efficient turbo chargers. Efforts to improve engine efficiency by variable valve timing, cylinder deactivation, to reduce engine displacement during normal driving, reductions in engine friction and accessory loads, and sophisticated engine management systems all show promise.⁵⁵ Significant improvements have already been made to the fuel and exhaust system by introducing unleaded petrol, detergent additives and oxygenated fuels and catalytic converters.

Vehicle performance can also be considerably improved by reducing weight through the use of lighter construction materials. The past 20 years has seen a steady decrease in the amount of iron and steel in a typical family car with a corresponding increase in the amount of polymer composites, aluminium and even magnesium. Increased attention to the various bulk, surface and compositional chemistry aspects of the forming, joining and recycling of these materials, to reduce manufacturing, design and assembly costs without compromising safety, will greatly enhance the use of lightweight materials in vehicle construction. This will require polymer and synthetic chemists to create new structural materials and designs to radically reduce vehicle weight without compromising safety.

In the past few years some vehicle manufacturers have introduced hybrid drive trains into the market place. Various arrangements are possible but the combination of a smaller gasoline or diesel engine coupled to electric batteries and electric drive motors, together with recovery of the vehicles momentum through regenerative braking, have led to dramatic increases in energy efficiency. Further improvements

⁵³ *World Economics and Energy Outlook*. Presentation by ExxonMobil at the Oil & Money Conference, November 2003.

⁵⁴ *BP Statistical Energy Review 2003*.

⁵⁵ World Business Council for Sustainable Development (2001). *Mobility 2001*. (www.wbcscdmobility.org)

in this approach will require lightweight construction materials and technology, efficient low emission engines and improved battery or alternative energy storage technology. Introduction of hydrogen fuel cells, alone or in hybrid configuration with a battery, offer the possibility of removing the car from the environmental debate, as well as allowing the use of renewable and sustainable fuels.

A further fruitful area of research might be to consider personal mobility as a systems engineering problem consisting of the engine and fuel, the transmission system, the vehicle itself including the wheels, the road surface and construction, the refuelling infrastructure and the eventual recycling of the components. Much of this will require a deep understanding of the chemistry and chemical engineering aspects of the fuels, their combustion characteristics, the engine and vehicle shell materials, the control systems and sensors required, transmission and energy storage and the re-use of the component materials. The task of creating a sustainable transport system when 'cars will continue to be the preferred means of personal mobility in the urbanised regions of the developed world'⁵⁶ is considerable and will require the ingenuity of chemists as well as engineers.

Air transport is receiving increasing attention because of environmental concerns linked to CO₂ emissions, air quality and noise. Continuing atmospheric chemistry research into the impact of aircraft emissions in the upper troposphere (extends from about 14 to 18 km) and lower stratosphere (extends from the troposphere to about 50 km) is required. To reduce emissions, designs with reduced weight will benefit fuel economy and efficiency. Embedded sensors and controls (in intelligent gas turbine engines) could reduce noise, emissions and costs through more effective diagnosis and maintenance processes.⁵⁵ New materials are required (e.g. low-cost composites, corrosion-resistant, damage-tolerant alloys and smart materials) to reduce manufacturing, life-cycle costs and reduce travel time,⁵⁷ whilst advanced coatings for the next generation of gas turbine engines are required for improved fuel efficiencies and emission reductions. There is a real need for innovative work in this area. Multidisciplinary teams of chemists and engineers are needed to develop viable solutions.

7.2 Industrial Energy Use

Research chemists should be encouraged to consider alternative energy sources such as photochemical, microwave and ultrasonic energy sources for chemical reactions, as these may offer advantages over other more conventional energy sources.

Research chemists often have little alternative to using conventional round-bottomed flasks and heating mantles, or oil-heated steel autoclaves when developing new products and processes. Unfortunately the ready availability of such equipment limits creative thinking about the most energy efficient way to carry out a reaction. As the process is scaled-up so is the mechanism for providing the required energy. Hence, for most chemical processes use thermal sources of energy originating from fossil (or nuclear) fuels, which are used to produce steam or heat oil. The mechanism of heat transfer is often through an external jacket with an internal agitator being used to provide both heat and mass transfer. Solvents are often added to the reaction to reduce viscosity to enable the heat and mass transfer to occur. The energy input to such processes is non-specific i.e. it is not directly targeted at the chemical bond or even the molecules undergoing reaction. Much of the energy is 'wasted' in heating up reactors, solvent and even the general environment. For some processes alternative, more specific forms of energy, such as photochemical and microwave energy, may be beneficially applied. Whilst use of such alternative forms of energy is not new, due to the increasing cost of energy they are currently being considered as viable options by manufacturing industries.

Some of the advantages of using other forms of energy input are briefly explored below. However in order to make a real difference to the energy consumed by industry these alternative energy sources must become much more widely available to the typical research chemist. University courses should also cover energy efficiency and the important role that chemists can play, both individually and as part of a

⁵⁶ World Business Council for Sustainable Development (2001). *Mobility 2001*. www.wbcscdmobility.org

⁵⁷ Commission on Engineering and Technical Systems (1998). *Maintaining US Leadership in Aeronautics: Breakthrough Technologies to Meet Future Air and Space Transportation Needs and Goals*.

multi-disciplinary team. Photochemical, microwave and ultrasonic reactors should be taught as having a valuable contribution to make towards energy efficiency and not just as a specialist technique for specific reactions.

7.2.1 Photochemical Reactions

Photochemically initiated reactions offer a range of advantages. Photons are absorbed by specific molecules, hence energy can be focused into the actual reactants rather than at the system as a whole. A photo-initiated process has potential advantages in saving energy involved in the purification of products, since photons are very clean reagents. Since the energy is more directed, reaction temperatures are generally lower, which may give higher selectivities, reduce by-product formation from competing reactions and save energy associated with purification.

Although academic research on photochemistry dates back many years, its uptake by industry has been limited. This is, in part, a result of there being many unsolved inherent problems. Significant challenges still exist in overcoming problems such as reactor fouling, a fairly common problem in chemical manufacturing. Unless very severe it is often only a minor inconvenience in thermal processes, with the main effect being a slight reduction in heat transfer efficiency. In photochemical processes even small amounts of fouling on the photochemical window or reactor wall, through which the light has to pass, can completely prevent the reaction from occurring. In thermal processes fouling can often be minimised through selection of reactor materials e.g. glass, stainless steel, Inconel, PTFE. However, in photochemical processes there is little flexibility in choice of 'window' material due to the requirement for transparency at a particular wavelength.

Radiation of a particular wavelength (monochromatic) is required to initiate a specific electronic transition. However, most UV and visible light sources are polychromatic. For example, common mercury arc lamps emit around 50% of their energy at wavelengths between 405nm and 578nm range. For most processes well over half of the electrical energy supplied to the lamp is wasted, reducing the overall energy efficiency and increasing process costs. In addition, some lamps also emit some of their energy as heat, which is again wasteful of energy and necessitates installing a cooling device (frequently circulating cold water).

Furthermore, light sources are often expensive, especially if made of thick-walled quartz, as in high-pressure mercury lamps, hence equipment costs may be high compared to thermal processes. In addition, since the power of transmitted light drops off as the square of the distance from the light, for efficient reaction and energy usage the reactants must be as close as possible to the light source. This has practical implications for design of industrial reactors.

Photochemical reactions are likely to be used in niche applications for improved economics and to give 'cleaner' reaction conditions. Unless there is a major breakthrough in reactor and lamp design, very widespread use of this technology is unlikely in the short term. Perhaps the best hope of producing high intensity monochromatic sources of radiation rests with lasers, but current equipment costs are too high to justify their use for commercial chemical production.

7.2.2. Microwaves

Photochemistry, at least in principle, offers the possibility of targeting energy at a particular bond in a molecule. Other sources of energy have less specific targeting but go some way to achieving this goal. It is well known that a microwave oven will heat certain substances up extremely quickly whilst others take much longer.

Microwaves may be considered a more efficient source of heating than conventional steam or oil heated vessels, since the energy is directly imparted to the reaction medium rather than through the walls of a reaction vessel. For heterogeneous reactions microwave energy may provide selective input.

In recent years there has been a large increase in reactions carried out using microwaves. With a heating rate of 10°C per second being achievable, it is easy to see how the overall reaction time can be

considerably shortened. Although there are examples of improved reaction selectivities and yields using microwave heating, any specific microwave effects, other than can be obtained by rapid heating, have not been conclusively proven. However, it has been postulated that microwave induced reactions follow the most polar pathway possible.

Although well designed industrial single-mode ovens are now available, most microwave experiments have been carried out in domestic multi-mode ovens that have poor control. This has led to several explosions occurring due to over-heating of organic solvents. Safety aspects, coupled with the natural limitations on solvents imposed by microwave heating, has led to many reactions being carried out in water or, more commonly, under solvent-free conditions. This has obvious benefits for energy efficiency, with energy only being imparted into the reactants.

7.2.3 Ultrasound

Ultrasound refers to sound waves with frequencies higher than those detectable by the human ear i.e. around 18 kHz. The terminology has become common knowledge due to widespread use of ultrasound scanning equipment in medical applications. Here high frequency waves in the range 3 to 10 MHz are pulsed at low power levels and the scattering pattern as they 'hit' various body parts and echo back are analysed and reconstructed into an image. The ultrasound frequencies of interest for chemical reactions (typically 20 to 100 kHz) are much lower than used for medical applications, but the power used is higher. Ultrasound initiated reactions usually (but not always) offer the advantages of following predicted pathways. Reaction rates are often higher, whilst bulk reaction temperature remains low, which is indicative of good energy efficiency.

7.3 Buildings

There is considerable scope for chemists' involvement in developing safer and more environmentally benign alternatives to current insulating material.

The efficient use of energy in buildings is one of the fundamental sustainability issues. It is critical when promoting energy efficiency in building design that attention is paid to cooling and ventilating buildings, which should take precedent over concerns about heating. Current modelling of climate change would suggest that, within the next twenty to thirty years in southern England, modern, highly insulated buildings with low thermal mass will become insufferably hot in summer. Excessive energy will have to be consumed to provide mechanical cooling if these buildings are to remain in summertime use.

The remaining problem in building design that concerns energy efficiency is maintaining temperature and relative humidity inside a building within the range at which we continue to feel comfortable. This is a wide range, but it is far narrower than the range of equivalent conditions in ambient air, even in a temperate climate such as that of the UK. Applied chemistry may benefit the process of making insulation requirements ever more stringent,⁵⁸ but its principles should first be directed toward critical study of the insulation materials available at the moment. All insulators work by confining air to such a degree that its movement is stopped. Convection currents distribute heat effectively away from warm surfaces towards colder ones. If air is confined, its very poor thermal conductivity slows down heat loss to a point at which it almost ceases. In general, insulation material that has the smallest and most closely centred air cells has the greatest thermal resistance, provided that the substance enclosing the cells is also a very poor heat conductor. The best performing insulation products are made of foamed plastic: these can be thermo-plastic, such as extruded/expanded polystyrene, or thermo-setting plastic, such as polyisocyanurate.

Even a cursory study of the chemistry of these materials invites questions about our growing reliance on them. Without exception, their embodied energy is high, because the raw materials are all derived from

⁵⁸ Building Regulations under Part L.

petrochemicals. In fact, the lowest figure for embodied energy in a commonplace inorganic insulation product is 17.3 MJ/kg. This is not a foamed plastic, but a mineral fibre, Rockwool, made by boiling volcanic rock at 1500°C using coke as the heating fuel. Thermo-plastic materials can, in theory, be recycled. In practice, the present UK waste management industry has no effective systems in place to retrieve these plastics from the waste stream, to sort them and to send them for recycling into new plastic. Thermo-sets cannot be recycled. In practice, these very light, air entraining materials are being consigned to land-fill on reaching the end of their service life, a practise that is clearly unsustainable. Burning the time-expired plastic in a power station fuelled by household rubbish is the only environmentally responsible disposal route available at present, but even this discharges CO₂.

The main concern with foamed plastic, however, must be focused on blowing agents. Most of the fluorinated gases formerly used for this purpose are now banned, both by the Montreal Protocol and by subsequent EU legislation. Despite these regulations, ozone layer depletion will still occur because the earlier generation of plastic that was foamed with these gases is still present in buildings. When the insulation is crushed or broken open during the buildings' eventual demolition, the fluorinated gas is released. HFC, a gas that has 3,400 times the arthropagic property of CO₂, is still used to foam at least one phenolic insulation product. The insulation industry has responded to the challenge posed by the adverse properties of fluorinated blowing agents by switching, almost *en masse*, to the use of pentane. By exploiting pentane's high vapour pressure, plastic can be foamed effectively to make thermally efficient, closed cell insulation. Unfortunately, pentane is highly inflammable. The gas remains within the micro-cells of the foamed insulation because these cells are completely enclosed by an impermeable plastic wall. Manufacturers claim that they have taken measures to avoid any increased fire risk, but this has still to be verified. Until there are reliable independent fire testing data, there remains some scepticism about the fire safety of these pentane-foamed products. Furthermore, the nature of the products of combustion when pentane burns is a cause for concern. In an oxygen-rich environment, the reaction produces large quantities of CO₂. In an oxygen-depleted environment, the reaction produces CO, which clearly presents health and safety concerns in the event of a pentane-filled insulation board catching fire in a confined space. These are considerable challenges that need to be overcome and will involve chemists and other science disciplines. Chemists will play a pivotal role in the innovation needed to develop safer and more environmentally benign alternatives to fluorinated blowing agents and pentane blowing agents.

There is considerable scope for chemists' involvement in developing insulating materials in the environmentally friendliest way. Organic insulation products are not only sustainable and disposable at the end of use without environmental penalty but they are also inherently hygroscopic. Water forming as condensation on the outside of the insulation layer can be absorbed and held in the organic material until conditions warm sufficiently to promote its loss by evaporation. Since organic insulation readily absorbs moisture from the atmosphere, it can offer significant advantages in controlling humidity within a building.

Another material receiving attention is bio-fibre, which is now used as insulation but has a venerable history as an insulating textile when made into clothing. Wool has impressive elastic properties and an equally impressive capability to recover when extensively stretched. What is less well known, however, is its affinity with water. Within its keratinous outer sheath, wool has a cellular core that can absorb water vapour and chemically convert it into stored liquid water. The great advantage of the chemistry is its reversibility. More awareness of these properties is needed in order to exploit them for building construction. Fortunately, awareness is growing and there are several woollen insulation materials now available for building purposes. One prominent brand, Thermafleece, is made from the wool of moorland sheep, for which there is no other ready market because it contains water resistant fibres (kemp) that will not take dye. The salient issue is that wool has a cooling capability to complement its known effectiveness as a cold weather insulation material. Faced with a future in which sweltering summers might become far more frequent, this dual performance may confer great benefits.

All bio-fibres will decay in the presence of water and oxygen, meaning that end of life disposal is easy and harmless. However, if an insulating material were to bio-degrade inside a building before the end of its serviceable life, it is unlikely to be specified thereafter. All organic materials will not only burn, but will also support combustion. There are relatively benign chemicals, such as boracic salts, that will inhibit decay and increase fire resistance. These are added as protection for the ligno-cellulosic granule insulation material. There are obvious problems that need to be overcome to balance the need to achieve long service life and reasonable fire-resistance without compromising the environmental advantages inherent in organic insulation.

7.4 Domestic Applications

The research objectives in the domestic sector should focus on deployment of innovative products and services, integrated packages for fuel consumption and energy conservation, efficient ventilation and heating systems, and strategies for waste minimisation and recycling. More advanced developments might include heat recovery and localised electricity production from solar power or from small-scale CHP systems.

High efficiency organic light emitting diodes (OLEDs) are likely to become common in the visual displays for mobile phones, personal organisers, computers and TVs and are likely to find increasing use in lighting systems, thereby reducing electricity demand. The market is projected to grow by a factor of 150 between 2003 and 2006.⁵⁹ At least one petrochemical company is developing in-house technology for OLED production and many other chemical companies are entering into strategic collaborations in this area. This market is likely to increase demand for speciality polymers and chemicals from the petrochemical industry.

⁵⁹ OLEDs set to glow. *Chemistry in Britain*, January 2003.

8. Products – Waste – Recycling

8.1 Emissions from Combustion

An improved understanding of the fundamental chemistry underpinning the release of gaseous and solid emissions from combustion processes is required before minimising emissions and developing appropriate pollution control technologies. Improved catalytic systems and new exhaust clean-up technologies are needed to simultaneously reduce emissions of a range of pollutants from vehicles.

8.1.1 Gaseous Emissions from Stationary Sources

Gaseous emissions from combustion processes can be classified into the following main groups of species.

- Oxides of nitrogen – formed from all fuels.
- SO₂ – formed from most fuels other than natural gas.
- CO₂ – formed from all carbon-containing fuels (although biomass fuels are considered to be carbon neutral).
- Volatile trace metals – mainly from coal and oil.
- Volatile organic compounds (VOCs) – can be formed from most fuels.

Chemistry is specifically applicable to the measurement and control of these species. In some cases the fundamental chemistry is well understood, such as that associated with SO₂ formation. For others less is known about the precise mechanisms and the influence of process conditions or the impact of specific fuel properties, as is the case for the release of some toxic organic species during combustion.

NO_x emissions from stationary sources are a particular concern at the present time because of the impact of the Large Combustion Plant Directive (LCPD)¹⁹. This particularly affects power generation plants, but most energy-intensive processes that are combustion-based produce NO_x emissions as a result of the combination of molecular nitrogen and oxygen in the process gases at high temperature. NO_x is a constituent of acid rain and a contributor to photochemical smog. One form of the nitrogen oxides, N₂O, is also a greenhouse gas. Control of NO_x generally requires the development of technology that permits operation at lower temperatures. For combustion, this means wider use of equipment such as fluidised beds or the use of gasification-based rather than combustion-based technologies. However, in the UK the predominant technology used for power generation is pulverised fuel combustion and high temperatures are integral to this process. Here, the situation is made more complex because a large proportion of electricity is produced from nitrogen-containing fuels, such as coal and biomass, which give much higher levels of NO_x and do so with fuel-specific chemical kinetics.

Means of reducing NO_x through refinement of combustors and air staging require further development, while new NO_x emission modelling concepts for future and on-line prediction of emissions provide a potential means to minimise emissions. Optimised equipment designs are also required. In particular, the effects of interactions between burners in multi-burner boilers would benefit from the development of improved computer models to simulate interacting flows. Laboratory investigations have been carried out to establish NO_x formation mechanisms and the effect of coal quality, but faster and more reliable screening techniques are required. Technologies such as coal-over-coal re-burning and NO_x reduction through selective catalytic reduction (SCR) are expensive, but improved variants of the less capital-intensive selective non-catalytic reduction (SNCR) is of significant interest.

SO₂ emissions are only of significant concern for the combustion of coal. Improvements in flue gas desulphurisation technology, especially materials of construction, are required. This is discussed more fully in Section 5.2.2.

CO₂ is the main product of combustion for all carboniferous fuels and is the subject of a multi-national agreement signed in 1997 at Kyoto to limit the effects of global warming. CO₂ capture and storage is discussed in detail in Section 8.2.

Coal and oil contain toxic metals that are released during combustion. The main volatile metal is mercury, although cadmium and selenium are also volatile to some degree and are released in volatile form initially, condensing onto suspended particulates as the combustion gases cool. Most toxic metals are, however, released in solid form and the issues surrounding toxic metals release are therefore discussed in Section 8.1.2.

Many classes of volatile organic compounds are produced by the incomplete combustion of fuels. They comprise a complex range of chemicals some of which, although emitted in very small quantities, are highly toxic or carcinogenic. VOCs are also important because of the role they play in the photochemical formation of ozone in the atmosphere. Compounds in this category include PAHs (polyaromatic hydrocarbons), PCBs (polychlorinated biphenyls), dioxins and furans. At present, legislation covers ambient concentrations of these species and emissions are not monitored continuously. In part this is because of the complexity of analysing for many of these species and because continuous analysis is unreliable or not possible at all. Better methods of analysis are required and the maintenance of more complete inventories of emissions would lead to a better understanding of the process conditions that give rise to their formation. Better combustion monitoring and control systems represent a simple way of limiting emissions. Many of these species are emitted as particulates and better particulate control and capture technology would produce a reduction in the release of these species.

8.1.2 Particulates and Solid Wastes

Particulates and solid wastes are unintentional by-products of combustion. The term solid wastes is used here to refer to inorganic, non-combustible material that remains in solid form during and after the combustion process, whereas particulates refers to solid material in the form of small particles that are airborne and exit the combustion process with the gaseous products. Solid residues are derived from solid and liquid fuels, such as ash from coal and biomass combustion. Particulates such as soot and volatile organic species that become associated with soot particles, or which are formed in condensing post-combustion gases, can be derived from most fuels, even gaseous ones. However, particulates from coal and oil are liable to contain heavy metal species making them more of an environmental hazard.

Dust is usually controlled by electrostatic precipitators or by bag filters, which form a physical barrier to the release of small particles. These processes are generally well understood and for many years the main concern has been the reduced efficiency of dust capture that can arise as a result of the effect of carbon in ash which has been discussed in Section 5.2.2. However, concerns in recent years have switched to the release of very small particles, such as PM10s (below 10µm) and even PM2.5s (below 2.5µm). These materials represent the greatest risk to human health as they represent a sizeable proportion of particulates emitted, can be more easily inhaled into the lungs where they may enter the bloodstream and are the most difficult to capture. There is a need for better equipment to monitor emissions of these particles and for the development of better ways to reduce the soot particles formed during combustion. In the longer term it is likely that even greater reductions in emissions of SO₂ and NO_x will be required because these gases can react in the atmosphere to form aerosol particles, referred to as “secondary” fine particulates, and they can add to overall PM2.5 levels in the atmosphere.

Coal, biomass materials and heavy fuel oils used in power generation and industrial and commercial heating applications all contain significant quantities of ash. The composition of the ash varies from fuel to fuel, and the species present may have a significant effect on corrosion and, for coal and biomass, on ash deposition within a combustion plant. This has been discussed in Section 5.2.2. However, an increasingly significant problem is the disposal of solid residues from combustion.

The costs associated with disposal of high carbon-in-ash residues are already high because of the quantities of ash involved. Morris and Read report that under the UK 1996 Landfill Tax Regulations, ash qualifies as an inert material allowing it to attract a lower disposal cost of £2 per tonne.⁶⁰ The current cost might therefore be expected to be £400 per MWe of capacity, with additional costs being incurred for handling. However, the recent Landfill Directive aims to reduce the environmental impact of landfill by limiting the quantities of waste disposed of in this way.⁶¹ Currently, ash is classified as a by-product and not a waste, but the Directive delegates the classification of materials to environmental authorities in individual EU Member States. Reclassification as a waste could bring about an increase in disposal costs to £15 per tonne.

Ideally, ashes from large combustion processes should find commercial applications rather than presenting environmental disposal issues, but this is dependent on ash quality, the variability of this quality and economic factors such as marketable value considered against refinement and transportation cost. Typical applications include the following.

- Structural fill and stabilisation: used to improve compressible and poor load bearing ground or for landscaping.
- Grouting: used for filling cavities and controlling the ingress of water.
- Cement and concrete: relies on the pozzolanic reactions of ash with calcium hydroxide to form cements either with or in place of Portland cement or in the manufacture of pre-cast concrete units.
- Lightweight aggregates: the pozzolanic nature of ash may contribute to the strength of aggregates for use in masonry units and structural concrete.
- Bricks and tiles: when mixed with clay, ash may offer durability and enhanced appearance as well as possibly reducing energy costs.
- Fillers: hollow cenospheres find high value applications as fillers in paints, plastics, varnishes and refractories.
- Neutralising agent for waste acids: a use for ash with high pH.
- Mineral extraction: can be used as a direct feedstock, e.g. as a source of magnetite.

The suitability of ash for any particular application depends on the product quality. This may include the particle size distribution of the material or may also include chemical composition. Applications where components may leach out into potable water supplies have strict chemical composition constraints and compliance is usually assessed through leaching tests. There have been very few studies of trace metals due to difficulty in the accurate determination of trace metal concentrations and limited understanding of the speciation of trace metals in aqueous and solid phases. Improved methods for determining the speciation of trace metals in solution and solid phases should be developed as well as a better understanding of the transition of species from solid to aqueous phases. The effect of coal and ash properties and the relationship between these and plant operating conditions should also be developed. Together these developments would significantly improve the environmental impact of coal combustion, whether the solid residues are utilised in specific applications or disposed of to landfill.

The carbon content of ash is a particular issue since, although small amounts may enhance the colour of a product, larger amounts reduce pozzolanic performance. Combustion processes are primarily focused on cost effective heat or power production, but increasingly it will be necessary to consider the implications for ash disposal. Improvements are needed in the control of product quality and research to find a wider range of uses for by-products is important. One particular area being studied at present is that of applications for carbon-rich components of fly ash as activated carbons, catalyst supports and sorbents for gaseous and airborne pollutants, such as carbon dioxide and volatile trace metals, or even as a medium for the storage of hydrogen.

⁶⁰ J. R. Morris and A. D. Read (2002). The UK Landfill Tax and the Landfill Tax Credit Scheme: Operational Weaknesses. *Resources, Conservation and Recycling*, **32**, 375–387.

⁶¹ European Commission (1999). Directive of the European Parliament and of the Council 1999/31/EC of 26 April 1999 on the Landfill of Waste. *Official Journal of the European Communities*, **L 182**, 16.07.1999, 1–19.

8.1.3 Emissions from Transport

Traffic pollution problems from motor vehicles are worsening worldwide, but problems are particularly severe in developing countries due to rapid growth in vehicle numbers, poor infrastructure, limited implementation of engine management and emission control technologies, and lack of a framework for vehicle regulation. Emissions from motor vehicles are regulated in most Western countries, but the control of non-stationary emissions is more difficult, because complex dedicated emissions control technologies cannot be easily applied at small-scale and at an affordable cost.

For petrol- and diesel-engine vehicles, engine management systems, catalytic convertors and the introduction of lead-free and low sulphur fuels have improved vehicle efficiency and emissions performance significantly in recent years but there will need to be further developments in the future if traffic volumes continue to rise.

The control of combustion in motor vehicles is an area for improvement. The simplest way to improve emissions from vehicles is to improve efficiency. Lean-burn engines go some way towards achieving this by burning fuel with a small excess of air. Such combustion achieves increased energy efficiency and reduced emissions of greenhouse gases, such as CO₂. However, in spite of higher efficiency, lean-burn emissions continue to be a problem because clean-up technologies are not available for lean exhaust. Conventional catalytic converters are unable to simultaneously reduce the nitrogen oxides, carbon monoxide, hydrocarbons, and particulates from lean-burn engines to required levels and so improved catalytic systems are required. Catalyst limitations also impede the control of emissions from diesel vehicles. Improvements in systems that absorb emissions during cold-start operations and clean them up as they desorb onto a warm catalyst or traps capable of reducing NO_x, as well as oxidising particulates, would significantly improve emissions from diesel vehicles.

Sulphur content is still a key issue, particularly for diesel. In order to operate engine systems effectively and cleanly, lean mixtures and complex after-treatment systems are required, and these require the use of low sulphur fuels. Such fuels must be widely available everywhere if they are to have a significant impact on the environment. Catalysts are needed for low-sulphur fuels to be improved and produced economically.

Attention is turning to emissions of a wider range of species from transport. Petrol- and diesel-engine motor vehicles emit a variety of VOCs either as unburned fuels or as combustion products. VOCs are also emitted by the evaporation of solvents and motor fuels. Benzene and 1,3-butadiene are of particular concern, as they are known carcinogens. Petrol vehicles account for 70% of total emissions of benzene, whilst the refining, distribution and evaporation of petrol from vehicles accounts for approximately a further 10% of total emissions. Petrol and diesel vehicles also emit 1,3-butadiene; however, unlike benzene, it is not a constituent of the fuel but is produced by the combustion of olefins. Other than in the vicinity of synthetic chemical plants, the dominant source of 1,3-butadiene in the atmosphere is the motor vehicle. Again the development of new exhaust clean-up technologies or catalysts would be of benefit.

There is also increasing concern about emissions from air transport. Improvements in gas turbine design have improved efficiency and reduced emissions of species such as NO_x but progress is likely to be slow until emissions reductions are driven forward by legislation. In 2004 this issue was recognised at international level when the British and German governments agreed to investigate what could be done to address this issue.

There is relatively little that can be done to limit CO₂ emissions from the combustion technologies used in transport. Capture and storage at the micro-scale is unlikely to be a viable option. Also, there are limits to what can be done to restrict emissions from petrol and diesel storage and transportation. Ultimately, vehicles powered by fuel cells are likely to be the only option. This technology is improving all the time. The use of fuel cells and of hydrogen as a means of energy distribution are discussed in detail in Section 6.1.

8.2 CO₂ Capture and Storage

In CO₂ capture and storage, capture technologies constitute a critical component of zero emission power generation schemes. The major thrust of research is in the optimisation of solvent absorption systems, development of new separation systems and a move to achieving more concentrated gas streams by way of, for example, pre-combustion decarbonisation or flue gas recirculation with oxygen addition ('oxyfuel').

CO₂ storage in North Sea oil and gas fields must be addressed now, as this sector moves into the decline phase, to avail of this storage mechanism. Areas which will warrant further attention include collaborative research by chemists, geologists and engineers into: corrosion of well completions and long-term sealing; geochemical and geomechanical impact on the reservoir cap rock and overlying seals (long-term integrity); maximising storage potential and surveillance and monitoring.

8.2.1 State of the art

This section summarises the state of the art and discusses those gaps in technology that should be addressed to encourage greater deployment of CO₂ capture and storage (CCS). Much of the following is based on discussions and documented outputs of the CO₂NET thematic network on carbon capture and storage, sponsored by the EU Framework Programme and published in more detail at www.co2net.com.

Capture

CO₂ capture is a well-known technology in different sectors to separate CO₂ from flue gas, natural gas and hydrogen (in syngas). Captured CO₂ is vented, used for enhanced oil recovery or purified to produce high-purity CO₂ for niche market applications (e.g. the food and beverage industry). Three process routes are available:

- pre-combustion;
- post-combustion;
- oxyfuel combustion.

Pre-combustion capture

In pre-combustion capture, CO₂ is captured from a gas mixture which is produced by partial oxidation of natural gas, coal oil residuals or biomass. This gas mixture contains predominantly H₂ gas and CO₂ (15–40%) at a high pressure (15–40 bar). Separating CO₂ from H₂ is the main task in pre-combustion capture. Physical absorption is the leading option (when partial pressure is sufficiently high), but membranes and cryogenics might become interesting alternatives in the future.

Post-combustion capture

In post-combustion capture, CO₂ is captured at low pressure and low CO₂ content from flue gas by separation from N₂ and O₂. This technology can be applied to large power plants such as pulverized coal plants and natural gas turbine fired combined cycles, cement kilns and industrial boilers and furnaces. The leading technology in post-combustion capture is chemical absorption using monoethanolamine. Alternative options to capture CO₂ from flue gasses are adsorption, cryogenics and membranes, but these options are still relatively expensive.

Pre-combustion capture is considered to be a key technology for the production of hydrogen from fossil fuels, especially in integrated coal gasification combined cycle plants, where CO₂ capture could be cheaper and more efficient compared to capture at pulverized coal plants.

Oxyfuel combustion

A concentrated stream of carbon dioxide can be produced by the exclusion of nitrogen before or during the combustion/conversion process. The difference with previous process routes is that here the separation is targeted to produce oxygen from air (i.e. separation of oxygen from mainly nitrogen), thereby avoiding the need for CO₂ separation. Cryogenic separation is the conventional technology to

produce pure oxygen, separating air into liquid oxygen and gaseous nitrogen, argon (which can be sold) and some trace components. Fossil fuels are then burned in an atmosphere of pure or enriched oxygen. A part of the flue gas, which consists mainly of CO₂ and H₂O, is recycled to the combustion chamber to enhance the CO₂ content for subsequent removal. This also helps to control the flame temperature, since current materials applied in the power industry cannot handle such high temperatures. Finally, water is condensed from the flue gas that is not recycled and CO₂ is removed by compression. Since the volume of inert gas in the boiler is lower than conventional systems, the boiler efficiency is increased. This technology has already been applied in some glass, steel and iron industries but has yet to be widely deployed due to the high costs and the energy requirements of the oxygen separation technologies.

Biological Capture and Mineralisation

About 90 gigatonnes of carbon are exchanged between the ocean and the atmosphere each year with a net uptake by the ocean of 2.2 gigatonnes. The upper warmer ocean layer contains about 1030 gigatonnes of carbon whereas the deeper ocean stores around 38,100 gigatonnes, drawing 1.7 gigatonnes from the surface layer each year.⁶² Acceleration of mineral formation from dissolved CO₂ in a controlled manner would enhance the capacity of the ocean as a CO₂ sink without the potentially damaging ecological impacts of elevated CO₂ concentrations. Wright has suggested that microbial consortia mediate precipitation of a range of carbonates including dolomite and magnetite in ephemeral, highly saline lakes that occur in arid parts of the world.^{63,64} The way in which iron reducing bacteria convert atmospheric carbon dioxide to calcite, aragonite and siderite in ash collection ponds is being examined by Oak Ridge under US DOE funding as a means of sequestering CO₂. This has the added advantage of stabilising fly ash into a stable mineral. Several claims are made for this research including combination with agricultural and food processing waste treatment to provide energy for microbial growth.⁶⁵

Direct Capture of CO₂ from the Atmosphere

In 2001, Lackner, Grimes and Ziock argued that it is technically feasible to capture CO₂ from natural airflow at a rate that far exceeds natural photosynthesis.⁶⁶ Their idea is based on the construction of many 300 metre tall, 115 metre diameter convection towers, where a down draft is created by cold water pumped to the top of the tower. Air flowing out of the bottom of the tower would pass 9,500 tonnes of CO₂ per day through a Ca(OH)₂ absorbent. The absorbent would then be regenerated to release a concentrated stream of CO₂ for disposal. The authors estimate that the process would cost \$10–15 per tonne of CO₂. The focus of their paper is to suggest a viable and cost effective alternative to changing the transportation infrastructure to non-carbonaceous fuels and they conclude that all of the CO₂ produced by the consumption of transportation fossil fuels could be captured for \$0.09–0.14 per gallon of gasoline. Additional costs would be incurred to store or sequester the captured CO₂.

Storage

An example of CO₂ storage is the Sleipner West natural gas field production operated by Statoil, in the Norwegian sector of the North Sea. In order to meet market specifications, the CO₂ content in the natural gas has to be reduced from 9 % to 2.5 %. Rather than emit this CO₂ to the atmosphere, as is a normal practice, Statoil decided to store the CO₂ underground. Since 1996, Statoil have been storing approximately 1 megatonne of CO₂ per year in a saline aquifer. The saline aquifer is similar to a sandstone reservoir, that contains oil and/or gas, but contains saline porewater instead.

⁶² The Intergovernmental Panel on Climate Change assessment (IPCC 1966).

⁶³ D. T. Wright (1997) An organogenic origin for widespread dolomite in the Cambrian eilean dubh formation, NW Scotland. *Journal of Sedimentary Research*, **67**, 54–64.

⁶⁴ D. T. Wright (1999). The role of sulphate-reducing bacteria and cyanobacteria in dolomite formation in distal ephemeral lakes of the Coorong region in Southern Australia *Sedimentary Geology*, **126**, 147–157.

⁶⁵ R. J. Lauf and T. J. Phelps (2001). *Bio-mineralisation for Carbon Sequestration Fossil*. Energy Programme, Oak Ridge

⁶⁶ K. S. Lackner et al (2001). *Capturing Carbon Dioxide from Air*. US 1st National Conference on Carbon Sequestration, Washington.

Another example is the Weyburn oilfield in Saskatchewan, Canada. Here, Encana, the field operator, is injecting CO₂ to enhance oil recovery (EOR). CO₂ is a good solvent for oil that allows the oil to move more easily through the reservoir, aided by a slight increase in the oil volume and improved sweep efficiency of the CO₂. The CO₂ for this EOR operation is supplied from flue gas from the Dakota Gasification Company in North Dakota. At the end of the EOR operation the CO₂ will be left behind in the reservoir.

The oil industry, especially in the onshore oilfields of Texas, has been using CO₂ for EOR for several decades. Hence the technologies and experience of injecting CO₂ underground are already well established.

There are three broad options for CO₂ storage: depleted oil and gas fields; deep saline aquifers; and unmineable coal seams. The potential for storage in unmineable coal seams is very small in the UK and will not be considered further in this document. Depleted oil and gas fields offer the advantages of having, by definition, a proven trapping mechanism (though some fields do allow hydrocarbons to migrate out of the main reservoir, occasionally to the surface). Also, due to the exploration and production history, much is known about these traps in terms of their geology, size, storage capacity, sealing caprocks etc. In contrast, saline aquifers have not been studied previously and although their theoretical storage capacity is very large, geologists have not had opportunities to establish this absolutely.

8.2.2 R&D Issues

Capture

Amine scrubbing is currently the most widely used process for CO₂ capture and has been used, for example, in the Sleipner plant since 1996 to remove CO₂ from natural gas. Considerable technical experience exists with respect to generation of relatively small amounts of food-grade CO₂ and for relatively low volume industrial purposes such as cooling and fire fighting equipment. However, the process is costly and inefficient when used with the dilute streams of CO₂ found in the stack gases from the current generation of fossil fuel power plants. It accounts for more than 80% of the overall cost of the carbon capture and storage (CCS) chain. The development of other more cost effective methods of CO₂ capture is one of the key issues relating to CCS (along with public acceptance of geological storage). Other methods are under examination (e.g. membrane or cryogenic separation), but the major thrust of research is aimed at achieving more concentrated gas streams by way of, for example, pre-combustion decarbonisation or 'oxyfuel' i.e. use of a low nitrogen, high carbon dioxide gas stream for combustion.

More specifically, further research is needed into post-combustion decarbonisation technologies, with a view to validation of absorption technologies in integrated pilot plants and development of novel chemical solvents and associated process technologies with significantly reduced capture costs and energy consumption. Other separation processes to be investigated include membranes, adsorption, high temperature solid sorbents, as well as cryogenic approaches.

Similarly, within the field of pre-combustion decarbonisation there is a need for validation of absorption technologies in integrated pilot plants as well as the development of novel reactor concepts for H₂/CO₂ separation (e.g. membrane, adsorption and absorption for the enhanced reforming/ gasification process). Some concepts for generation of multiple products, including CO₂ capture, warrant further study.

Validation of de-nitrogenation/oxyfuel technologies in integrated pilot plants is also essential, as are novel concepts for oxygen production or oxygen transfer. Further development of fuel conversion technologies should focus on drastic improvements in capture processes or avoidance of separation processes.

Capture technologies constitute a critical component of zero emission power generation schemes. It is necessary to work on the development and validation of new integrated processes providing near-complete CO₂ capture, while at the same time trying to achieve higher energy efficiencies and/or lower costs. This could also include incorporation of biomass co-combustion and partial CO₂ capture as well as multi-pollutant removal concepts addressing, for example, sulphur components, NO_x and trace metals.

It is essential that the development of capture processes is properly integrated into complete CO₂ mitigation chains, providing enhanced uptake through:

- integration with improved combustion technologies;
- and synergistic approaches for CO₂ capture and CO₂ storage.

Storage in Oil and Gas Fields

The CO₂ storage capacity of old and current oil and gas fields in Western Europe amounts to approximately 37 billion tonnes. Although this is only a few percent of the estimated storage capacity of aquifers, these fields offer a potentially useful test bed and niche market for larger-scale commercial sequestration. If the injection of CO₂ into such reservoirs can generate a marketable by-product, through EOR, the net costs of CO₂ sequestration could be reduced and this might encourage oil companies with substantial prior experience to participate in the programme. Additional information gained with this type of application will also be relevant for the more general aquifer storage of CO₂. Regulatory issues are also likely to be simpler and potential sites could become available earlier than for aquifers.

Most experience of CO₂ EOR has been gained onshore in the US and Canada. Operating offshore in the North Sea is a more difficult proposition, though much of the on-shore experience is still relevant. There is, however, an issue of timing. Already many of the large early discoveries in the North Sea are in the decline phase, as is the entire British offshore sector, and the Norwegian and Danish North Sea sectors are predicted to move into the decline phase within a few years. A concern is that older oil and gas fields may be decommissioned before CO₂ EOR and enhanced gas recovery (ERG) projects can be implemented.

Many of the major international oil companies, needing a rate of return of 12%, are moving their interests to lower risk areas elsewhere in the world and leaving the North Sea to smaller independent operators. These low cost operators can operate at the end of the maturity line of a field, by operating at a rate of return of 8%, but this leaves little tolerance on such tight margins for new technology in the North Sea. Small operators cannot afford or risk using new technology, as the major operators could. The window of opportunity is therefore shortening.

Issues for which further R&D is either necessary or desirable to optimise storage potential as opposed to the present norm of minimising CO₂ generation include the following:

- Corrosion of well completions and long term sealing;
- Geochemical and geomechanical impacts on the reservoir cap rock and overlying seals (long-term integrity);
- Maximising storage potential;
- Surveillance and monitoring;
- Technology transfer.

Aquifer Storage

Deep saline aquifers constitute by far the greatest potential for geological storage of CO₂, being capable, in principle, of storing several hundred years' worth of Europe's power plant-derived CO₂. Suitable aquifers are, however, unevenly distributed throughout Europe, with the majority of the theoretical storage potential located in the North Sea, far away from the main power plants and other major emission points. It should be noted that the UK has one of the largest capacities in Europe for offshore CO₂ storage in aquifers. Very considerable aquifer potential does still exist onshore and near-shore, but detailed assessment of the aquifer potential at any given location is a prerequisite to understanding the regional, national or local storage capacity. The information available about saline aquifers is often scant and considerable effort is required to assess the capacity and suitability of various aquifers.

Although a number of technical issues dealing with storage safety, monitoring and longevity are still outstanding, the public acceptance of geological storage is probably the overriding issue. To address public acceptance, it is important to carry out a number of onshore geological storage pilot projects, selected to represent a geographical spread and a range of geological conditions. The European Commission's 6th Framework Programme will provide the first such small scale demonstration. Following these projects, there will be a need for several other small projects, as well as a few concerted projects at greater scale, bringing European policies and the main players together in one or just a few activities. The rolling out of geological storage demonstrations across Europe is perceived to constitute the main scientific bottleneck to the successful deployment of CCS. In other words, it does not matter how much CO₂ can be captured, and at what cost, if geological storage cannot obtain public acceptance as a safe, long term CO₂ abatement method.

With respect to subsurface processes, further research requirements include laboratory experiments to improve knowledge of the behaviour and physical properties of CO₂ as part of the reservoir and the effects on sealing capacities of overlying caprocks and the presence of other fluids. In conjunction with the improved knowledge at the small-scale, it is essential that *in-situ* field experiments are conducted. These should aim to elucidate the effects of different geological settings, geological variance, CO₂ migration and long term processes using and integrating natural analogues and laboratory experiments, as well as identifying suitable sites for demonstrations.

In addition, research should focus on the potential impacts on both offshore and onshore ecosystems of spatially restricted but very high concentration CO₂ leaks, thereby helping to define site performance and safety criteria. Methodologies and protocols should be developed for long term performance assessment of storage sites. These will integrate much of the disparate research needs and knowledge described above into long-term predictions of probable risks and potential impacts of CO₂ leaks.

In the field of material and equipment development, the utilisation of aquifers requires further development of corrosion resistant material (e.g. pipes, pumps, cements) and cheap, long-life measuring sensors for down-hole (e.g. leak detection, pressure and temperature gauges) as well as surface uses (e.g. gas sniffers, seismology and compaction sensors). There is also a need for the further development of new cheap, high resolution CO₂ plume monitoring methodologies.

8.3 Nuclear Waste

Nuclear waste research spans waste management, waste storage and dispersal, decommissioning and contaminated land management. Environmental chemistry (including hydro-geochemistry, radio-biogeochemistry and biosphere science) and wasteform chemistry (which includes the fundamental science of materials used in the immobilisation of nuclear waste materials) will have a pivotal role to play in providing solutions to nuclear waste management.

Research into radioactive waste management aims to ensure that the treatment of the waste effectively separates the active and non-active constituents, with near to zero discharges, and that the final waste containment is as failsafe as possible. Safe industrial solutions have already been found for the permanent disposal of low-level waste and for packaging and above surface storage of high-level or long-lived waste. Regarding the ultimate disposal of high-level waste, most research has been conducted on deep geological disposal in both saturated and very dry atmospheres. Good progress has been made in countries such as Finland, Sweden and the US. It is, however, necessary that each country addresses its own options and preferred solutions because each country has differences in the geological sub-strata and fuel designs. Hence there is a need for continuing research.

Many countries have also built up waste inventories from early pioneering research on nuclear energy. These wastes were generated in an era when environmental impact, safety and pollution controls were less stringent. Many of these waste inventories need supporting research to cover the aspects outlined below.

8.3.1 Waste Management

Research requirements include:

- Improved techniques to physically characterise the waste and establish a detailed materials inventory analysis.
- Separation of the wasteforms, both physically and chemically. The research targets include novel waste matrices for special waste types and future fuel cycles and abatement technologies for the removal of specific radionuclides.
- Treating nuclear waste can result in additional radioactive effluence and a key goal is to develop novel technologies for effluent abatement, initially reducing and ultimately leading to zero discharges.

8.3.2 Waste Storage and Dispersal

Development requirements include:

- The design and engineering of deep underground storage repositories and containment vessels.
- Predicting the environmental impact of disposing of high-level waste and intermediate-level waste.
- Development of repository concepts aimed at containment rather than dispersal, including technologies such as reactive backfill materials to trap contaminants (i.e. salt, bentonite).
- Generic research into the environmental fate of contaminants.
- Sensors and instruments to measure the integrity of the repository and waste integrity, particularly for longer term monitoring once the repository is complete.

8.3.3 Decommissioning

Having removed and treated the waste, it is then necessary to dismantle the original storage buildings.

The key goal again is to avoid unnecessary additional waste, and current research is aimed at:

- Novel technologies for decontamination to reduce waste volumes, including effluent free decontamination systems.
- Novel technologies for effluent free cutting and dismantlement processes (such as dry plasma).

8.3.4 Contaminated Land Management

The need to establish a 'green site' sometimes requires the treatment of contaminated land, and research is required to:

- reduce the uncertainty in modelling arising from lack of data (i.e. source term, geology, hydrogeology, contaminant transport);
- improve site survey techniques to map contaminant pathways;
- predict the effect of climate change/coastal erosion on nuclear sites.

Given the exotic nature of some wastes there is a need for substantial investment in underpinning research and technology.

Research is also focusing on the treatment of spent fuel to reduce the radioactive waste volume and separate out recyclable fuel feedstock. In some cases long-lived transuranic elements can be partitioned and potentially transmuted into less long-lived elements or burnt in advanced reactors. A means of reducing the stockpile of separated plutonium involves incineration in reactors.

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Mr John Hutchinson	Feilden + Mawson
Dr Mike Lancaster	Chemical Industries Association

Appendix I

UNITS OF POWER	
Watts (W) Kilowatts (kW) Megawatts (MW) Gigawatts (GW)	A Watt is a standard unit of power Kilowatt = 1000 Watts, Megawatt = 1000 kW, Gigawatt = 1000 MW
Megawatt thermal (MWth) Gigawatt thermal (GWth)	A unit of power specifying the thermal output.
Megawatt electric (MWe) Gigawatt electric (GWe)	A unit of power specifying the electric output (as distinct from the heat output).
UNITS OF ENERGY	
Kilowatt-hour (kWh) Megawatt-hour (MWh) Gigawatt-hour (GWh) Terawatt-hour (TWh)	Energy = power × time. Thus a kilowatt-hour is the energy of a 1kW device running for 1 hour. Megawatt-hour = 1000 kWh, Gigawatt-hour = 1000 MWh. Commonly used to show energy consumption (e.g. an average home would use about 4000 – 4500 kWh of electricity per year) or to show how much energy would be produced by an energy technology.

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