IPTS Cleaner Pathways Workshop

Institute for Prospective Technological Studies

The Institute for Prospective Technological Studies (IPTS), which is part of the European Commission's Joint Research Centre, recently held a workshop on June 24–25 in Seville, Spain, on 'Strategies to facilitate the use of cleaner pathways for the production of substances and materials'. The IPTS is one of the eight institutes of the Joint Research Centre. Its role is the observation and follow-up of technological change; in order to get a better understanding of the links between technology, economy and society and to provide techno-economic intelligence to the European Commission. Under its environment work programme IPTS is assessing the socio-economic impact that development of clean processes, products and services will have.

Towards the end of 1998, IPTS carried out an 'expert inquiry' survey into sustainable technologies for the chemical industry with the aim of identifying innovation options which would both provide the European chemical industry with competitive advantage and provide environmental benefits. The findings from this survey are still being analysed and currently remain confidential. In addition to this survey this workshop aimed to improve IPTS' understanding of how clean technology can be developed and taken up by the chemical industry, with particular focus on how future EU policies could help. The workshop was arranged around particular themes, which are briefly summarised.

Efficiency of carbon use and clean production examples

The next two papers concentrated on improving the efficiency or carbon use. Martin Patel from the Fraunhofer Institute for systems and innovation research presented a flow model for the manufacture, use and waste management of synthetic carbon products within Germany. The study indicated that the total primary energy related to the life-cycle of synthetic organic materials in Germany is approximately 1700 PJ with CO_2 emissions around 57 million tonnes, however relative to the economy this is equivalent to 12% of the energy used and only 6% of CO_2 emissions. The share of carbon based materials produced by recycling is less than 10% of the total domestic consumption, indicating grounds for significant improvement. The study also indicated that potential savings achievable by 2005 amounted to 15% of energy used and 28% of the CO_2 emitted, most of these savings could be made by using waste as a resource.

Michele Aresta from the METEA Research Centre stressed the importance of life cycle analysis in determining how sustainable a product or process actually is. He then went on to demonstrate the potential role of carbon dioxide in chemical synthesis. Use of carbon dioxide as a raw material would not only help preserve fossil fuel carbon, it can be the source of many cleaner synthetic routes than currently employed. Amongst the examples quoted was the potential for replacing phosgene in the synthesis of carbonates and carbamates (Figure 1). Should these processes become economically viable it will be a significant improvement on the current preferred commercial routes involving reaction of phosgene with alcohols or amines, not only due to the problems associated with use of phosgene but also due to the production of HCl.

Examples of how commercial organic synthesis pathways had been 'greened' were given by Bjorn Akermark from the Swedish Royal Institute of Technology. An interesting example is the case of acetic acid, originally made by fermentation of ethanol. This is one of several biotechnology processes which may be considered green because of their use of renewable resources but which in fact produce copious amounts of waste. This process was later replaced by conventional organic processes which did not offer any real environmental advantages; these included production of acetic acid *via* acetylene made from calcium carbide and the Wacker process using ethene as starting material. It was not until the Monsanto methanol carbonylation process came on stream that acetic acid production could be considered to be clean.

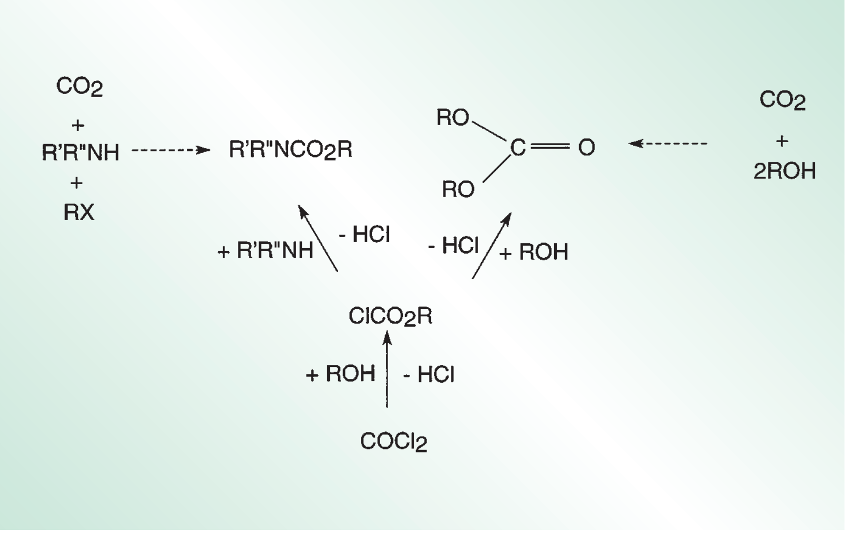

Figure 1

Green Chemistry programmes

The next session discussed some of the green chemistry movements within Europe. Kurt Wagermann from Dechema, whose organisation is sponsored by the German Federal Ministry, the chemical industry, Allcheme and universities, is pulling together the sustainable chemistry movement in Germany. There is a current working party discussing how best to incorporate the ideas of sustainability into the education curriculum, school and university education being seen as key to the future of clean chemical production. Dechema are also coordinating a R&D programme on inherently safer chemical products, solvent free processes and chemicals from renewable feedstocks. One of the debates currently going on is whether government funded programmes should be under one 'sustainable manufacturing' umbrella or whether the ideas on sustainability should be included in all programmes.

Pietro Tundo representing INCA described the origins of the green chemistry movement in the US and the various definitions and principles of Green Chemistry. Recommendations from the 1998 OECD workshop on sustainable chemistry were discussed, these included proposals for sustainable chemistry awards, the call for member countries to undertake R&D programmes into sustainable chemistry and for OECD to promote the incorporation of sustainable chemistry concepts in education. INCA itself is a consortium of Italian universities with a common interest in Green Chemistry, which is supported by government. The consortium is currently looking at several thematic areas including clean chemical processes transformation within the environment and advanced analytical methodologies. The consortium also run an annual EU sponsored summer school on Green Chemistry for young graduates, this year's was held in Venice in September.

Mike Lancaster from the Royal Society of Chemistry's Green Chemistry Network explained the networks activities in promoting Green Chemistry in education and industry in the UK. The drivers enabling industry to adopt cleaner technologies were discussed and case studies presented. As chemists become more skilled in financial workings of companies and accounting procedures become more focused on individual processes it is becoming easier for companies to appreciate the effect clean technology can have on the bottom line. An excellent example of this is the recent conversion of Hickson & Welch's optical brighteners process to use water in place of volatile organic solvents. The Hickson's process was becoming uncompetitive due to high raw materials cost and increasing cost of waste disposal and regulation compliance. This is a classic case of a company turning to clean technology to save money—in this case £300,000 p.a. Although many of the tools Green Chemists require are available they are not readily accessible and the philosophy and culture of Green Chemistry has not yet percolated through industry and educational establishments. Networks such as the GCN have significant roles to play facilitating the 'greening' of both education and industry.

Jacques Calzia from CEFIC described the Sustech programme under which the European chemical industry is undertaking collaborative research into sustainable technologies. Through Sustech the industry is demonstrating its willingness to respond to public concern, and to be a willing partner with government on moving towards cleaner technologies. The R&D projects being undertaken are all designed to produce cost savings and include areas such as bioprocess engineering, contaminated land remediation, separation technology and design. Through these programmes CEFIC aim to influence EU policy, enhance the public reputation of the chemical industry and have a greater influence on university research.

Gerard Riviere presented the role of COST in encouraging a multidisciplinary approach to research and sharing of best practice. The 28 members of cost are working on 20 scientific areas, the chemistry section of which is a fairly recent development. The programmes are funded by individual countries' research councils but endorsement by COST helps to ensure that grants are available.

History of Clean Technology Development and the Role of Government

Luitgard Marschall from Münchner Zentrum für Wissenschafts und Technikgeschichte provided a fascinating account of the development of the German chemical and biotechnology industries in the 20th century. At the beginning of the century both industries were of comparable importance but due to the shortage of agricultural crops and government policy after the First World War the chemical industry began to grow at the expense of the biotechnology companies. This situation continued for the next 50 years, Germany losing most of its biotechnology expertise along the way. From the seventies onwards Government policy has tried to resurrect the biotechnology industry but this has been difficult in light of competition from Sweden, Japan and the US who never lost expertise in this area. The lesson for the Clean Technology movement is that all disciplines, including chemistry, biotechnology and engineering, have an important role to play and EU policy should reflect this need and encourage interdisciplinary research.

Mahshid Sotoudeh from the Austrian Academy of Science discussed the demand for cleaner technologies, highlighting some of the problem areas and barriers. One of the areas of concern was the focusing of R&D on the production process with little attention being paid to the end use, waste generation and recycling. There is a need for greater understanding of eco-efficiency concepts in product life cycle. She concluded that one of the main barriers to adoption of cleaner processes was lack of communication between and inertia of interested parties (industry, customers, universities, policy makers and environmental activists) and called for structural changes and more discussion.

Klaus Jacob (Free University of Berlin) presented a study on the link between legislation and the decline in production of chemicals. The main conclusion were that the major drop in production of hazardous chemicals came before any regulation, indicating industry does respond to environmental pressure. He advocated government setting targets to develop clean technology but not rigorous legislation.

Gerald Petit (EU Commission DGIII) addressed issues of the global competitiveness of the chemical industry and how the EU wishes to integrate internal market, environmental, health & safety and employment issues with sustainable development. Any EU industry regulation would need to take these factors into account. DGIII is hoping to work more closely with organisations such as CEFIC to develop industry co-operation through benchmarking and initiatives to improve training and education.

The workshop concluded with groups presenting their views on the problems and solutions to industry becoming more sustainable with ideas on how policy should be developed to encourage this process. Examples include:

- Development of a readily accessible clean technology toolkit
- Encouragement for education establishment to incorporate sustainable concepts
- Tax incentives for development of clean products and processes
- Awards to encourage clean production and R&D
- Greater company openness in environmental accounting
- Development of methodologies which will define what a sustainable product is
- Easier access to risk capital for eco-friendly developments

The workshop demonstrated the wide interest in clean, green, sustainable chemistry in Europe and by pulling all the various strings together hopefully IPTS will be able to propose a policy approach which encourages both industry and educationalists to become more green whilst maintaining industry competitiveness.

Mike Lancaster,
Green Chemistry Network

Ionic liquids at the RSC Congress

The use of ionic liquids as solvents for organic reactions was a major theme of the 1999 summer meeting of the Molten Salts Discussion Group, held as part of the RSC Annual Congress at Heriot-Watt University in Edinburgh, Scotland (6–7 September). Ionic liquids are seen as potentially green replacements for conventional organic solvents and are currently the subject of a great deal of interest from both industry and academia.

Dr Tom Welton from Imperial College, London, gave the opening talk of the meeting, entitled 'Molten Salts as Reaction Media for Organic Solvents'. This gave a general introduction to those physical properties of molten salts which make them attractive for organic synthesis. He explained that, at normal working temperatures, ionic liquids have no vapour pressure and so do not evaporate: this is an important property from a clean technology point of view as solvent evaporation is a major source of VOC emissions. It also gives the additional advantages that the solvent may be handled in a vacuum, and that volatile solutes are readily removed by distillation. Ionic liquids are highly polar, but poorly nucleophilic, making them good solvents for polar and ionic compounds, without coordinating strongly to metal centres. The combination of these two properties makes ionic liquids particularly suitable for reactions involving transition metal catalysts.

Dr Welton explained how the use of large anions and bulky organic cations reduces the coulombic interactions and so reduces the melting point; for example, $[EtNH_3]^+NO_3^-$ has a melting point of only 12 ºC. Many of the most recently developed ionic liquids are based on the 1,3-dialkylimidazolium cation. Several of the physical properties of the ionic liquid, including the melting point, miscibility, viscosity, and even the selectivity of the chemical reaction may be controlled simply by altering the length of the alkyl groups and the nature of the anion. For example, in Diels–Alder reactions, the ratio of *endo* to *exo* product is sensitive to the structure of the ionic liquid used. Some other examples of successful reactions performed in ionic liquids were given, including alkene dimerisation, and rhodium-catalysed hydrogenations. In the latter case, the turnover frequencies and product yields were higher those seen for polar solvents such as acetone or acetonitrile.

Dr Paul Dyson from the University of York, UK, who is involved in a collaborative project with Dr Welton, talked about the applications of ionic liquids for hydrogenation catalysis using a liquid biphase approach. At low temperatures, ionic liquids are immiscible with water but, on warming past a critical temperature, form a single phase in which the reaction occurs. Upon completion, the reaction is cooled and phase separation occurs; the water soluble products are now in the aqueous phase and can easily be recovered, whilst the catalyst remains in the ionic liquid ready for reuse. This combines the reactivity advantages of homogeneous catalysis with the separation advantages of a heterogeneous system. In principle, this is similar to fluorous biphase catalysis, but has the advantage of not requiring any special fluorinated ligands: many 'off-the-shelf' catalysts may be used. 1-Octyl-3-methylimidazolium tetrafluoroborate was found to be a particularly useful ionic liquid for these applications, as phase mixing occurs at a convenient 58 ºC. This liquid biphase approach has been used successfully for the hydrogenation of butynediol using a rhodium phosphine complex catalyst. This biphasic approach also works with mixtures of ionic liquids and organic solvents, and a ruthenium complex catalysed hydrogenation of benzene to cyclohexane was found to proceed in a molten salt–neat substrate system at a rate of 500 turnovers per hour.

Dr Rob Thied of BNFL, UK, introduced QUILL, the Queen's University Ionic Liquids Laboratories, which is a collaboration between academia and industry, and includes 17 industrial members. QUILL is based at Queen's University in Belfast, Ireland, and will be the first international research centre to focus on ionic liquids (see *Green Chemistry*, 1999, **1**(3), G58). QUILL's objectives were described as: pooling of resources and the 'gearing' of funding; collection and sharing of fundamental data; advancing the understanding of ionic liquids; development of applications of ionic liquids technology; solving engineering challenges whilst minimising risk; gathering of IPR (intellectual property rights) where appropriate; and development of industry–industry and industry–academic liaisons. The research conducted at QUILL will be industrially relevant, pre-competitive and interdisciplinary, and will address the measurement of physical parameters critical to the use of ionic liquids on an industrial scale, including specific heat capacities, corrosiveness, recyclability, long term chemical stability, and disposal after its useful lifetime. Dr Thied's talk was followed by a lively discussion after it was revealed that QUILL will not be sharing the results of their measurements of fundamental properties with non-consortium members, until they are sure that IPR will not be compromised. Dr Thied said that this was to protect the investment of the consortium companies, and could not estimate when the data might become available. This was met with disappointment by at least one member of the audience, who pointed out that public money was involved, and felt that such important information should not be kept secret.

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