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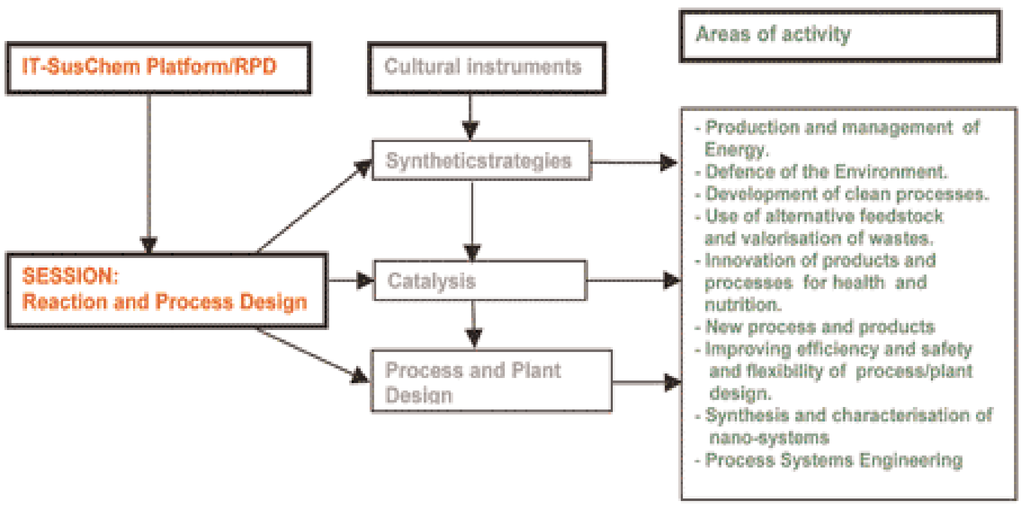

Fig. 1 - Scheme of the "Reaction and Process Design" session of the Italian Vision of the Technology Platform for Sustainable Chemistry (IT-SusChem)

THE PROGRAM OF IT-SUSCHEM PLATFORM/RPD

The Italian Vision draft document of the Technology Platform for Sustainable Chemistry has been launched at Bologna October 23rd, 2006 and now is still in elaboration with the support of all the scientific and industrial community. The draft document related to the Session "Reaction and Process Design" has been elaborated by considering, first of all, the necessity to achieve significant progress in three different cultural ambits that are: synthetic strategies, catalysis, process and plant design.

The document related to the Session "Reaction and Process Design" has been elaborated along the general lines reported in Fig. 1. Therefore, the document is a general overview of the potentialities offered by the mentioned cultural instruments in relation to the activities that can be regarded as Sustainable Chemistry. The goals of this Session though completely in agreement with the European Platform SusChem (see Fig. 2) are to some extent more focused on some Italian peculiarities that are: (i) Italian chemical industries are of small or medium size and their activity lies mainly in the field of fine chemicals, pharmaceutical intermediates and specialties or formulated products; (ii) our Country imports all kinds of energetic sources and fuels (petroleum, natural gas and coal) and there is a strong Italian interest in developing new sources of energy and fuels. The main areas of activity for the Reaction and Process Design Session of the Italian Technology Platform for Sustainable Chemistry are the followings:

1) Products and technologies for the energy management derived from sources alternative to petroleum, such as, for example, renewable sources;
2) Products and technologies for a better protection of the environment;
3) Development of clean processes;
4) Use of alternative feedstock, in particular renewable feedstock, and valorisation of wastes as source for new products;
5) Improvement of active products delivery strategies for health nutrition;
6) New products, new synthetic pathways, new processes and new technologies for the production of fine chemicals, pharmaceutical active principles, active ingredients for new materials and formulated products. Commodities must also be considered with the aim to study more efficient and environmentally friendly technologies;
7) Improvement of the efficiency of energy and water use in processes and of the safety and flexibility of processes and plants;

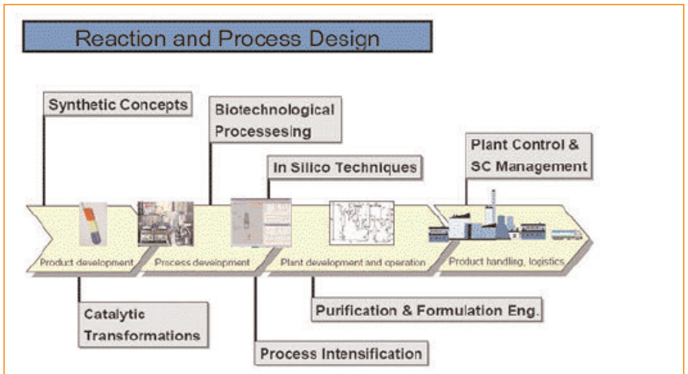

Fig. 2 - Scheme of the Reaction and Process Design reported by the European Platform SusChem

8) Synthesis and characterisation of nanostructurated systems;
9) Improvement of Process System Engineering.

The different steps which are necessary for developing innovative products and processes increasing efficiency and for saving energy require new synthetic concepts, new catalytic transformations, process intensification, in silico techniques development, and new formulation methods. All these aspects are opportunely deepened in the document.

The complementary approaches of chemical synthesis, process design and engineering will be considered in any relevant step from the laboratory to the process plant with the aim at introducing innovation, where possible, and at achieving a sustainable development. This needs the collaboration of chemists with organic, inorganic, analytical and physicochemical skills, working together with industrial chemists and chemical engineers.

Synthetic strategies

"Sustainable Chemistry" has the main objective to save and improve the positive aspects of chemistry, reducing or eliminating the negative ones. This requires the obtainment of new products, new synthetic strategies and processes and new technologies, more environmentally benign and addressing the human needs. To this aim there is in the chemical sciences a need to develop benign synthetic pathways which, in addition to being high yielding, are simple and exhibit high atom efficiency, hence a reduced number of steps and no waste, are safe and environmentally acceptable. Moreover another important step is to optimize resources. The main features of an ideal synthesis are shown in Fig. 3.

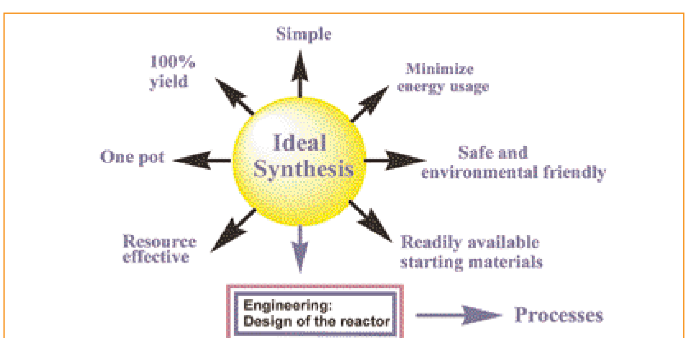

Fig. 3 - Features of the "ideal synthesis"

Removing conventional organic solvents in chemical syntheses is also important in the drive towards benign chemical technologies. Organic solvents are often high on the list of toxic or otherwise damaging compounds because of the large volumes used in industry, and difficulties in containing volatile compounds. Nowadays replacement reaction media may include (Fig. 4) ionic liquids (ILS), supercritical CO_2, water, fluorous solvents, polyethylene and polypropylene glycol. A paradigm away from using solvents in synthesis as solventless reactions, can lead to improved outcomes and more benign synthetic procedures. Beyond many other advantages regarding issues like selectivity, yield, waste, ease of recycling, these unconventional media will certainly boost clean extraction/reaction processes as in the case of the association of ILS with other green solvents.

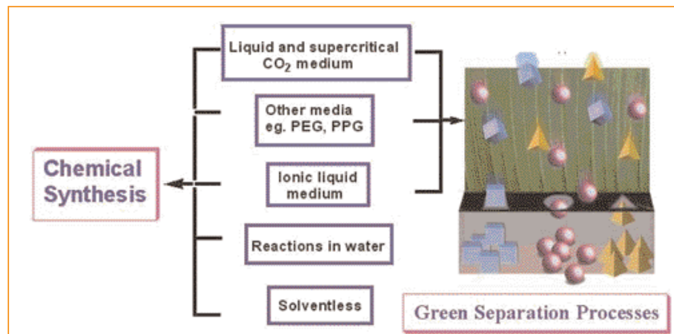

Fig. 4 - Unconventional media pool for sustainable synthesis (Partly taken from: *Green Separation Processes*, Wiley-VCH, 2005)

Moreover several reactions of traditional organic chemistry require reagents which lead to large quantities of waste disposal materials in the reaction or are highly toxic and aggressive. Trivial but fitting examples in this sense are represented by the use of allylic bromide, of conventional Lewis acids, dangerous oxidants and phosgene. The search for new substrates and/or reagents to support development of new processes/products by intelligent and cost-effective testing methods/strategies, remains a major target of sustainable chemistry but evaluation of potential toxic effects is necessary, with particular attention to priority issues as defined in REACH.

Breakthroughs in the synthetic strategies addressed towards sustainable chemistry can provide valuable alternatives to conventional methodologies. The generation of substances by joining small units together with heteroatom links with the goal of developing powerful, selective and modular "blocks" that work reliably in both small- and

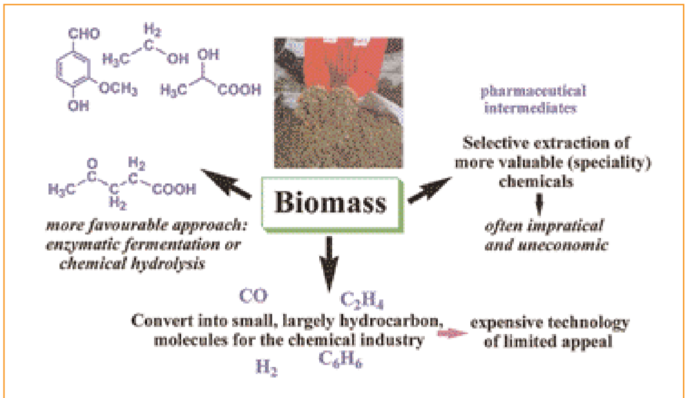

Fig. 5 - Current methods of exploiting biomasses for the production of chemicals

large-scale applications ('click' chemistry), and multicomponent reactions (MCRs), convergent reactions in which three or more starting materials react to form a product where basically all or most of atoms contribute to the newly formed molecule, are representative examples. Within the field of special syntheses of relevant interest would be in particular the development of novel synthetic protocols and processes that, while providing a convenient access to functional materials for advanced applications, are also modular, wide in scope, give very high yields, and generate by-products that can be easily removed by non-chromatographic methods. These processes based on the use of a multistep/one-pot synthetic strategy are also characterised by a "modular approach" concept, since are forming materials including backbones composed of regularly alternating (different) modules with the interplaying role of impressing mechanical and functional properties.

Renewable feedstocks

Great amounts of energy are consumed by the chemical industries (about 20% of the energy consumed by all the manufacturing industries). Nowadays, all this energy in Italy is mostly imported, sometimes from politically unstable countries. The Italian chemical industries have a great interest in the development of energy saving technologies. Besides, these new technologies could find application also in other industries and chemistry might play a leading role in a more rational production, storage and use of the energy. Therefore, all the efforts aiming at reducing the energy consumption and at decreasing the dependence from oil and other non-renewable fossil sources of chemical production, are further strategic issues which will be substantiated by searching alternative feedstocks based on natural resources to replace fossil fuels. Efforts are being directed to implement the methods of exploitation of biomasses (Fig. 5).

Plant biomass is nowadays the only alternative sustainable source of carbon based energy, fuels, chemicals (Fig. 5) and materials. New and more efficient processes are necessary to convert a broader variety of biomasses into biofuels (Fig. 6). Technologies available to transform biomasses include: pyrolysis, bio-oil refinement, gasification and Fischer-Tropsch conversion.

Catalysis

In the development of *Sustainable Chemistry*, catalysis plays a pivotal role as more than 80% of all products of chemical industries are produced through catalytic processes (Fig. 7). Topical problems concerning all of the issues proper of *Sustainable Chemistry* have not yet been resolved and many conceptual advancement and technological improvements are needed to achieve better selectivity, efficiency and economy of the known processes and to design new catalytic cycles. A revolution in the catalytic performances is expected from the application of nanotechnologies to the catalysts preparation. Very important is also to find new synthetic routes for converting classical stoichiometric processes into catalytic ones, for obtaining useful products from

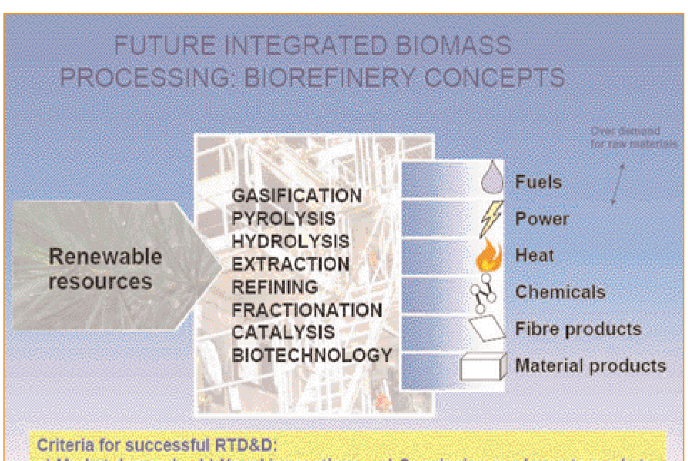

Fig. 6 - New processes and products from renewable feedstocks

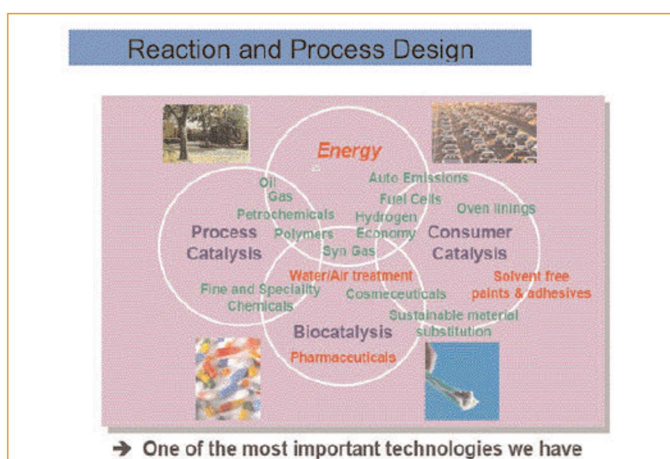

Fig. 7 - Role of catalysis in the realization of new products and new processes

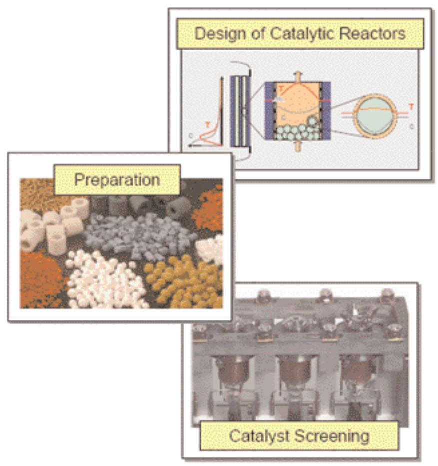

Fig. 8 - New catalysts for new catalytic processes

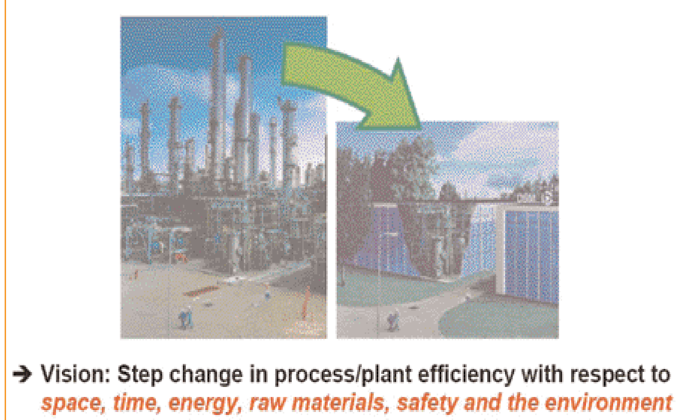

Fig. 9 - New concepts in Plant Design (from: *Klaus Sommer*, Bayer Technology Group)

industrial waste materials. Sustainable chemistry needs new and more efficient catalysts (homogeneous, heterogeneous and heterogenized) for new reactions and new products. It is, then, interesting to observe that the features of the catalysts employed together with the existence of multiphase systems, can strongly affect the type of reactor to be used and the modality of the conduction.

Research priorities for catalytic transformation are: zero emission processes requiring 100% selectivity, use of alternative and/or renewable feedstocks, use of non conventional energy sources (light, microwaves), catalysis for protecting the environment (catalytic technologies aimed at reducing greenhouse gas emission, solving water and air issues etc.), new catalysts and new catalytic concepts for improving health and quality of life (catalytic smart sensors, self cleaning materials, organocatalysis, etc.).

Starting from new feedstocks, the development of a new generation of zero emission catalysts, the design and the production of nanoscale catalytic particles for new catalytic processes, and the realization of new reactors suitable for the new generation of catalysts (see Fig. 8) are therefore exciting challenges to face out in a near future.

However, any new idea coming from catalysis and synthetic strategy needs to be developed at the industrial level by using chemical engineering science, in order to improve the efficiency of the existing processes, of plant equipment and of the overall production systems by promoting innovation through the development and use of more sophisticated techniques of simulation, optimisation, automation and intensification. A completely new approach to chemical plant design must be developed to obtain more efficient, safer and more flexible devices (Fig. 9). At this purpose, when convenient, the miniaturisation of plant unit operations would be realised transforming batch multipurpose systems in continuous multipurpose ones.

Catalytic processes operating within fuel cells, especially concerning the efficiency of the conversion, the fuel versatility, the resistance to poisons, the transport within the cell, the lifetime of the device and the economics of fuel cell manufacture, must be strongly improved for achieving a large commercial availability of these devices (Fig. 10).

One of the main scope of "Sustainable Chemistry" is to minimise waste and the environmental impact. These objectives can be reached, first of all, by envisaging more selective catalysts and realizing more and more "clean processes".

However we need new process technologies for removal to the maximum extent of any possible pollutant from the waste streams, including waste process water and flue gases, automobile exhausts and sewage effluents. This will include methods combining catalytic and separation techniques. A valorisation of waste streams that contain organic pollutants is also to be attempted for example through the development of photocatalytic processes which enable the contemporary production of hydrogen and the removal of the organics.

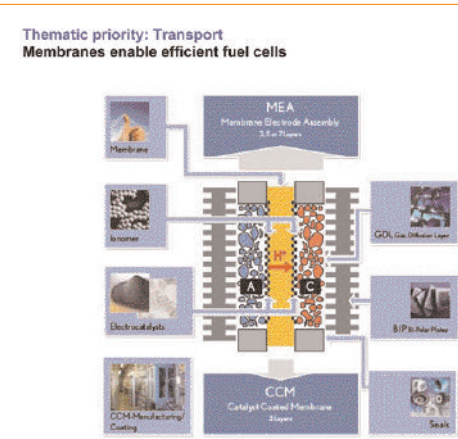

Fig. 10 - Improving Fuel Cells performances