

Seamless chemical engineering science: The emerging paradigm*

R. A. Mashelkar

I consider it to be a matter of great honour that I have been asked to deliver the ninth P. V. Danckwerts Memorial Lecture. Danckwerts' contributions to the evolution of Chemical Engineering Science (CES) are monumental. He set the pace and the tone and defined the features of CES in the early fifties through his path-breaking and incisive contributions. His work has continued to inspire generations of chemical engineering scientists (CE scientists). I certainly happen to be one of them. It is, therefore, a special privilege that I have this opportunity to pay my own tribute to Danckwerts. Today I wish to speak to you on an emerging paradigm – the seamless chemical engineering science.

How did Danckwerts himself view CES? I searched and found a statement in his presidential address delivered to the Institution of Chemical Engineers almost three decades ago. He said: 'I shall use the phrase Chemical Engineering Science to mean the aspects of science developed by chemical engineers for their own purposes in fields not covered by other branches of technology'¹. He also went on to alert us: 'It will be a great mistake to think of the content of chemical engineering science as permanently fixed. It is likely to alter greatly over the years in response to the changing requirements of industry and to new scientific discoveries and ideas for their application'. He was absolutely right. I wish to refer to those explosive advances in science which are reshaping our lives. I also wish to emphasize how these advances in adjacent sciences will force us to reconceptualize CES of tomorrow. I particularly want to focus on the merging boundaries between CES and the adjacent sciences and also on the need to build new bridges with our neighbours.

We look around and see that discrete boundaries no longer exist between various natural sciences such as physics, chemistry, biology, mathematics, etc. Let us remember that the 1985 Nobel Prize for chemistry was actually awarded to two mathematicians! Take even subdisciplines such as inorganic chemistry, biological

chemistry, organic chemistry and physical chemistry. The conceptual boundaries between these disciplines have already vanished. The Nobel Prize winning work of Lehn² was a testimony to this realization.

Is only science going borderless? Of course not. The borderless world has already dawned on us. Borderless organizations are here to stay too. I wish to quote from the speech by Jack Welch, the Chairman and Chief Executive Officer of General Electric (GE), whom we all respect for his dynamism and vision. In his lecture on 'Global Competitiveness' delivered last month, he talked about GE's strong commitment to the boundaryless behaviour and said, 'Boundaryless is the language, the behaviour definer, the culture, the soul of a true global enterprise. It ignores geography, borders, accents, currencies, and unites people of all cultures'. When asked about what happens to those GE people who did not accept this boundaryless behaviour, he responded by saying, '(we) tell them they have to change, or else if they don't change, they have to part company with us. And we do have them part company – lots of them over the question of boundaryless behaviour, of being open'. Strong words indeed – but it shows the way it works in industry. Why does it do so? Let me answer this.

Successful commercialization of modern scientific discovery today demands cross-disciplinary collaboration between scientists and engineers from different disciplines. Advances are generally the sum total of numerous creative ideas and interdisciplinary cooperation. In industry, individuals with diverse scientific and technical backgrounds tend to work together in a mission mode. The driving force for industry is continuous innovation to displace one's own product by oneself – with the well-known fear of someone else displacing it otherwise for them. The concept of interdisciplinary research and development has not gained as much ground in academia as one would have wished. And this is really sad because innovation is not a unidimensional process. It is comparable to the intermeshing gears of a clock. The challenge before us is to make this intermeshing happen.

Why did I decide to speak on this topic? I find myself in an interesting situation. I head the National Chemical Laboratory (NCL) in India. I have to deal with multidisciplinary teams of over 500 research scientists and engineers. I find myself communicating with physical

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chemists, organic chemists, inorganic chemists, etc. I deal with molecular biologists, biochemists, bio-organic chemists too. I also deal with materials scientists, applied mathematicians, NMR experts and so on. Our CES group is placed amidst all these groups and it has to interact with all these disciplines. This interaction is crucial to meet NCL's charter, which is to develop globally competitive products, processes and technologies. Interestingly, we have found that we succeed in this only when we come together as a team, leaving aside all the conceptual and cultural barriers between different disciplines. But I must also honestly admit that I have found it to be a hard act to put together. I thought I would share the agony and ecstasy that I have experienced during all these years of going 'boundaryless' with you.

But before I begin to address the principal issues, I must put the role of an engineering scientist, as I see it, in perspective. I would like to give an analogy with the medical school. We have there basic scientists, who generate new knowledge, but it is knowledge for its own sake. Then we have the hard-core practising clinicians, who use the established tools in their everyday practice. But in between these two communities, there are those academic clinicians. They are the ones who understand the language of the basic scientists and they are the ones who know the demands of the profession, as reflected by practising clinicians. What these academic clinicians do is to use the methods of science to develop new tools and new paradigms that the practitioners would find most helpful. They also communicate the needs of these practitioners to the scientists. The academic clinicians thus play this great role of facilitators. To my mind, a CE scientist is like an academic clinician, a facilitator. His task is to look at the continuous advances that take place in basic sciences such as chemistry, biology, physics, etc. He would harness this knowledge to develop new tools, which hard-core chemical engineers would put to use. The richness of our chemical engineering profession, therefore, depends very critically on the vitality of the CE scientists and also on the rich variety of skills, tools, etc., that they bring into the profession.

I will give my personal perceptions about the following issues. What is the emerging relationship between CES and adjacent disciplines? What driving force is shaping this relationship? How do we respond to the explosion of knowledge in adjacent sciences? What will be the new role of a CE scientist *vis-à-vis* chemical engineering and other disciplines of engineering and sciences? What new tools and techniques can we adopt from other disciplines and, in turn, what could we give to other disciplines? Danckwerts practically defines Chemical Engineering Science as 'applying methods of science to distinctive chemical engineering problems'. Is this definition valid anymore? What should be the new definition?

A word about how I have organized my lecture may be in order. This is certainly not a lecture on 'new frontiers in CES', since these frontiers have been widely discussed and elaborately defined by the Amundson report³. I am also not getting involved in a discussion of the 'core' vs 'frontiers' issue, which has again been dealt with by some of our very best scholars and thinkers^{4,5}. I am also not speaking about the future of fields such as mass transfer, reaction engineering, applied thermodynamics and so on. Furthermore, although I want to deal with the issue of merging boundaries with other disciplines, I am not going to create distinct boxes such as CES-physics interface, CES-biology interface, etc. To me, the boundaries between other disciplines have already vanished. I will, therefore, deal with only some 'generic issues' that should be of concern to us.

This lecture is admittedly a narrow view from a window. I also have the inescapable personal bias, which might show through the examples and the illustrations that I have chosen to give, and also the recommendations that I have dared to make despite my limitations. However, I thought it is worth putting these thoughts on record, since this is the time to do it. Tomorrow might be too late!

Nonlinear dynamics – New interdisciplinary challenges

Complexity and nonlinearity reside in much that a chemical engineer encounters. His ability to acquire new tools and knowledge by exploiting the contemporary advances in physics has undergone a sea change in recent years. A wide variety of features ranging from steady state to multiple steady states to oscillations to chaotic dynamics and spatiotemporal patterns^{6,7} have become more commonplace observations. The advent of increasingly sophisticated experimental tools to detect and analyse microscopic events, new methods of mathematical analysis and computational advances have further accelerated the development in this area.

The discovery of dynamical chaos has opened up many exciting possibilities with wide-ranging implications in natural sciences and engineering sciences, CES being no exception. The usefulness of chaos comes from the fact that it is a collection of many sets of orderly behaviour, none of which dominates under normal circumstances. At first sight an engineer shies away from chaos, because he finds it unreliable, uncontrollable and, therefore, unwanted. However, the challenge for an engineer is to control chaos and make it manageable, exploitable and, in fact, invaluable.

We ought to recognize that the special problems encountered in CES have to be viewed within a grand universal framework. Indeed, forms of quantitative universality have been found to occur in chaos so that it

now seems that studies on a case-by-case basis may not really be necessary. Thus, for example, the routes to chaos by the system when a control parameter is varied follow specific mechanisms like period-doubling, intermittency or crisis. In each of these cases the onset has a typical diagnostic measure. For instance, in the case of period-doubling bifurcation, the ratio of successive bifurcation points tends to converge to a universal constant, now popularly referred to as the Feigenbaum number. The realization that the behaviour of complicated physical systems can be analysed on the basis of very simple nonlinear equations indeed suggests that the complexities of the real world may arise from underlying simple causes. Furthermore, for a system exhibiting chaotic dynamics, an important property is its sensitivity to its initial conditions. Even an infinitesimally small difference in specifying initial conditions accurately may lead to a catastrophic growth in the error. This means that one can make near-accurate short-term predictions about the system behaviour but certainly not long-term. This has profound significance in many CE systems that we deal with.

Multidimensionality, intermittency and coupling are conditions that are frequently met in many CE systems. Therefore, such systems become serious candidates for exhibiting chaotic behaviour. The subtleties brought out by the chaos theory pervade a number of situations, covering complex reactions in a CSTR, bubbling from a submerged orifice, mixing and so on. Let me illustrate the point further by giving some illustrations.

Chemical systems provide excellent prototype systems for studying nonlinear behaviour, since they offer a variety of convenient settings ranging from the simple to the more complex⁸. In this context, an open, well-stirred system (CSTR) following nonlinear kinetics and involving a few chemical species forms a good basis for the study of low-dimensional nonlinear dynamics and steady-state behaviour. Common examples of systems with nonlinear kinetics involve reaction mechanisms with autocatalytic or nonisothermal feedback features⁹. It is interesting that an early experimental observation of chaotic dynamics was reported by Schmitz *et al.*¹⁰ for the now famous Belousov–Zhabotinskii oxidation reaction scheme. Continued theoretical and experimental investigations have revealed newer and newer nonlinear dynamical and bifurcation patterns. Attention continues to be given to analysing the behavioural patterns of systems of interest to chemical engineers, say, for example a nonisothermal consecutive reaction $A \rightarrow B \rightarrow C$ occurring in a CSTR^{11,12}.

Open systems operating far from equilibrium produce a very rich behaviour. Advances in modern instrumental methods such as photoelectron, field electron and field ion microscopy reveal the ensuing structures with higher and higher resolution power. Oscillatory, chaotic and spatiotemporal concentration patterns of the adsorbed

species for carbon monoxide oxidation on platinum surfaces for various types of catalysts, including supported wires and foils, are available¹³. Specific domains of the catalysts show synchronization as a result of heat conduction through the supporting material or even through the gas phase. Propagating reaction–diffusion fronts (diffusion coupling) also leads to such synchronization. The important keywords are, therefore, coupling and synchronization.

Due to the coupling between complex kinetics and transport processes in CE systems, a wide range of dynamic behaviours can be observed. Possibility of dynamic pattern formation by coupling at a larger scale was demonstrated by Arce and Ramakrishna¹⁴. The dynamic behaviour and the stability of such systems and its linkage to the understanding of formation and propagation of long-range dynamic patterns (including travelling waves in reactors) is obviously a hot topic for study. True CE culture is entering into the field; the contributions by Fox and Villermux¹⁵ on the role of micromixing (a typical CE paradigm) in controlling the existence and nature of oscillatory patterns is a good example.

The development and study of nonlinear systems has been confined to study of low-dimensional systems so far. But a CE scientist has to look far beyond this. He has to deal with systems involving time delays (something that an electrical engineer may not experience in his systems) or those that are modelled by a set of partial differential equations. The time delay elements, for instance, are inherent in many CE operations, such as in feedback loops of well-mixed processes. The effect of their presence in the observed dynamics of a nonlinear system can be quite dramatic and they require attention.

Consider the classical problem of bubbling. We have been looking at this problem for decades. But suddenly a potentially new way of looking at it has emerged. Tritton and Egde¹⁶ found that bubbling from a submerged orifice is sometimes regular and sometimes irregular. They observed a period-doubling sequence leading to chaotic behaviour. Subsequently, intermittency of varying degrees and period-3 patterns were observed. Examples such as this suggest that such new tools can lead us to look at dispersion science in a very different way.

Consider another classical problem of mixing. Recent experimental studies and the merging of kinematics with dynamical systems and chaos are providing a paradigm for analysing mixing from a universal viewpoint. This is as well, since there is a large spectrum of problems studied in various disciplines in which mixing assumes importance (Figure 1). A universal framework can be used for analysis in different disciplines, whether it is mixing in a screw extruder or mixing in the mantle of the earth¹⁷.

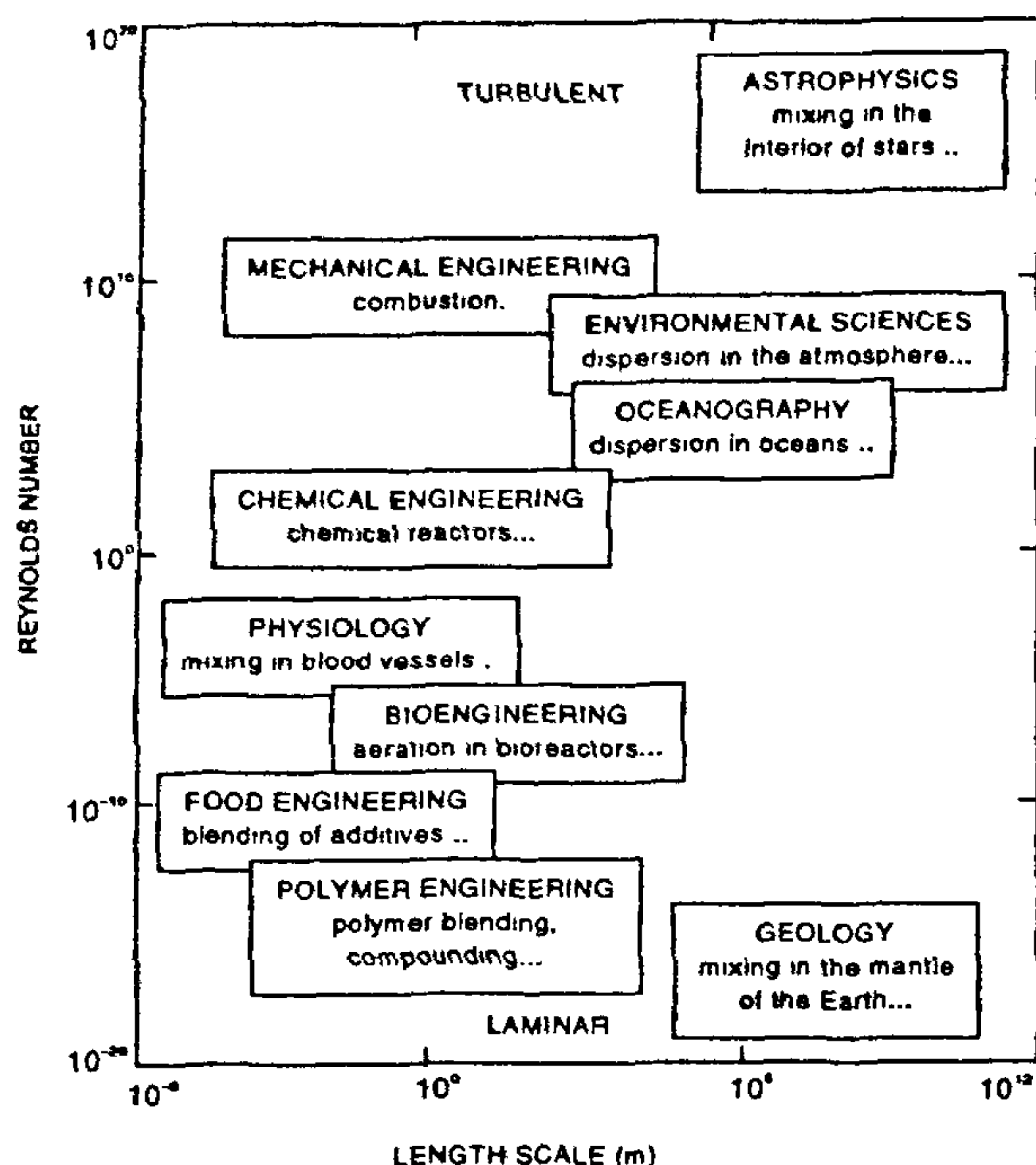


Figure 1. Mixing phenomena studied in diverse disciplines.

The real excitement lies in the potential of achieving laminar mixing of viscous fluids in a regime of deterministic chaos produced by intermittent change of initial conditions¹⁸⁻²¹. Here mixing results from a fundamental kinematic property. In such chaotic processes, mixing efficiency is not directly related to energy dissipation. The prospect of devising entirely new mixing devices based on these new principles is truly exciting. The recent work by Howes *et al.*²² is interesting from this angle.

The examples I cited are typically those that are at the heart of chemical engineering. But let me move on and tell you about a more complex system, which combines the synergistic efforts from diverse disciplines being interpreted using the theory of chaos, which leads to new ways of taste detection. Let us consider membranes with biological activity. The central question concerns the interrelationship between the microscopic and macroscopic membrane properties. Properties such as the action potential, spontaneous firing and chaotic behaviour can be viewed now from a system-dynamical viewpoint. Thus, for example, the mechanism of oscillatory electrical potential of dioleoyl phosphate millipore filter membrane placed between two solutions of different electrolyte concentration can be related to the macroscopic behaviour of interfaces generated due to chemically driven surface tension effects²³. The system, when subjected to sinusoidal alternating current, synchronizes

with the forcing frequency and also desynchronizes for changing initial conditions. Aperiodic behaviour in the form of chaos appears in the regime²⁴. The appearance of chaos follows the route of quasiperiodicity and analysis of dynamic chaos enables us to use it as a sensor for detecting taste. The simple philosophy followed here is that the substances as received by biological membranes change the membrane potential, leading to sustained oscillation and spatiotemporal firing patterns of the neurons, which when transmitted to the cortex and the brain recognize the taste. It is thus possible to use an artificial lipid membrane to convert chemical information to electric currents and construct sensors that identify the taste. The prowess of the synergy of diverse disciplines is at once obvious here. A CE scientist should simply relish the idea of exploring, analysing and exploiting analogous phenomena and enriching the profession.

Fractals is another concept that has excited the physics community over the past two decades. Fractals are scale-invariant geometric objects with the property that when a small piece is magnified it resembles the whole object statistically. Many physical processes produce phenomena that show self-similarity over a wide range of scales. The methods of fractal geometry have been extensively used in diverse disciplines, ranging from atmospheric sciences to modelling of earthquakes and also in miniature systems in cell biology. Aspects of fractals in chemical engineering problems that we deal with, be they porous electrodes, catalytic surfaces, membranes and so on, have been dealt with very elegantly by Villiermaux⁵. A lack of quantitative connection between the measured value of the fractal dimension and the underlying physics of the process has many times led to a scepticism about its meaningfulness. If one comes out with a fractal dimension after a lot of sweat and hard work, we often have someone saying, 'so what?'. Fractals are not merely physical objects but are strange attractors of the nonlinear systems, which make them all the more beautiful, while being all-pervading at the same time. The connection of physical and mathematical fractals is, however, important, since it links the nonlinear system dynamics to fractal geometry.

The methods of fractal geometry when applied to data obtained from mathematical model, while providing an insight into the behaviour of these nonlinear systems, are grossly inadequate for the measured experimental time series data. Also the presence of noise in the experimental data seriously distorts the results. Clearly, there exists a need for efficient noise reduction methods for dynamically sensitive systems, which need to be tested possibly on model examples first and then on real experimental systems. As more CE scientists get attracted to fractals, these words of caution may be useful.

CE scientist as a molecular information engineer

Molecular chemistry that a chemical engineer conventionally learns is that of a covalent bond. However, it is supramolecular chemistry that is holding the centrestage now. Supramolecular chemistry is the *designed* chemistry of the intermolecular bond^{25,26}. It deals with chemical species that are held together and organized by means of intermolecular (noncovalent) binding interactions. The chemical, physical and biological features of these chemical species constitute the essence of this highly interdisciplinary field. It involves the organic synthetic techniques of receptor construction, metal-ion-ligand complexes involving coordination chemistry, studies of interactions involving physical chemistry and finally biological processes involving substrate binding and recognition. Its location at the intersection of chemistry, biology and physics makes it a unique one and it also offers great challenges to a CE scientist.

Designing systems for storing information in the structural (and eventually temporal) features of molecules and supermolecules constitute the real essence of supramolecular science and engineering. Supramolecular science deals with the process of molecular recognition. The essence of molecular recognition is that the molecular information is stored in the interacting partners. Chemical ingenuity is used to design receptors possessing steric and electronic features. These are designed to be complementary to those of the binding substrate. Further molecular manipulation provides a balance between the rigidity and the flexibility suitable for the function to be performed. Such subtle organization of molecular, structural and dynamical features forms the basis of *molecular information engineering*.

Why should a CE scientist get involved with this field? This is because *molecular information engineering* will be finally concerned with the design of molecular devices and of systems displaying higher forms of molecular and supramolecular behaviour such as self-organization, regulation, cooperativity, communication and replication. Let me explain this a little further.

We know that an interplay between molecular self-organization and molecular recognition of individual constituents leads to the construction of natural supramolecular systems. Such systems combine order and mobility. Their functioning depends on the organization. If CE scientists abandon the limits of their classical thinking, they can start conceiving the development of new materials, which simulate natural supramolecular systems, where their functioning will be governed by their organization. The connecting links between apparently separated disciplines of materials science and life science bringing in the central theme of supramolecular systems is demonstrated in Figure 2.

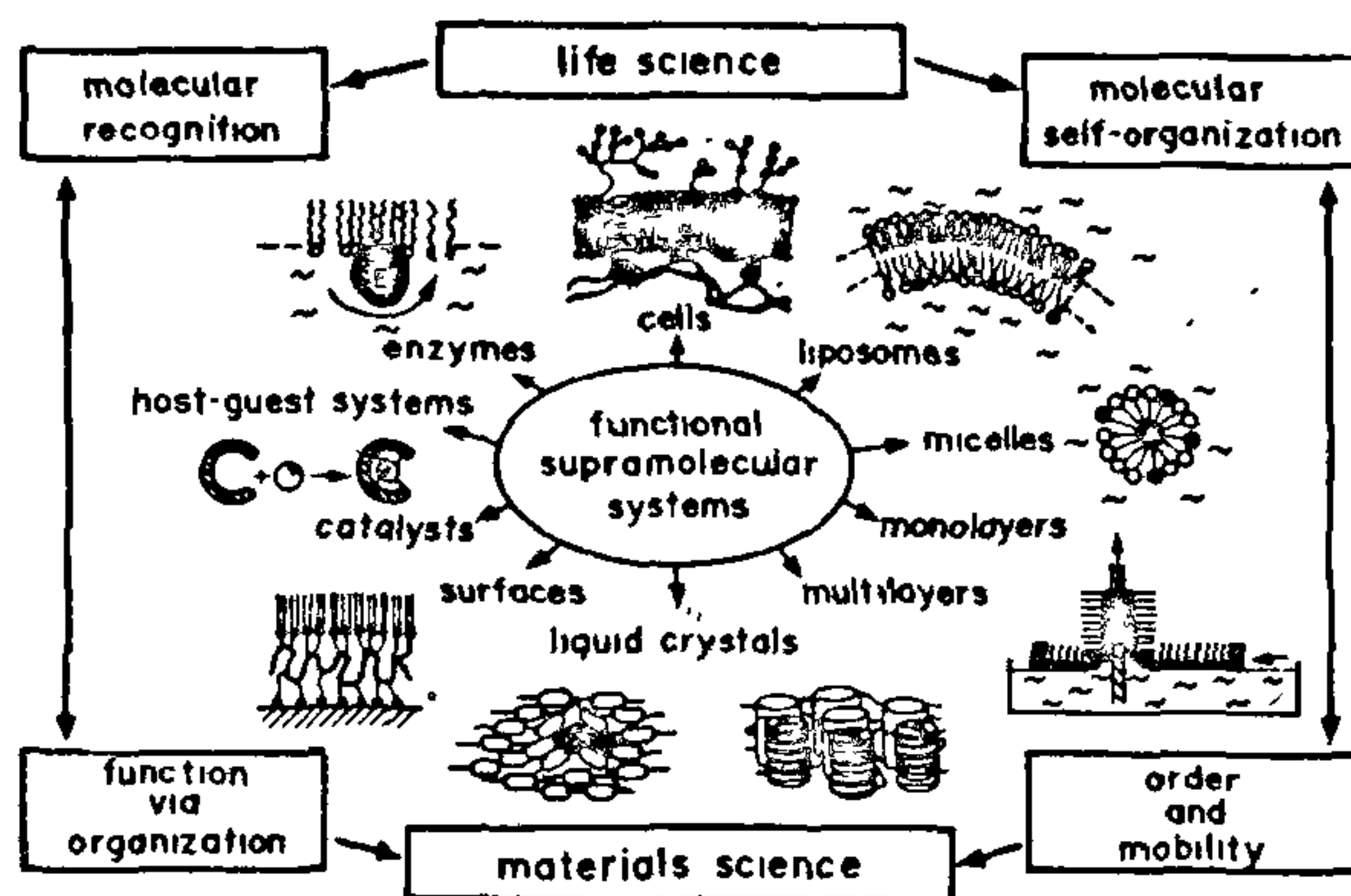


Figure 2. The connecting link between life science and materials science – the role of functional supramolecular systems.

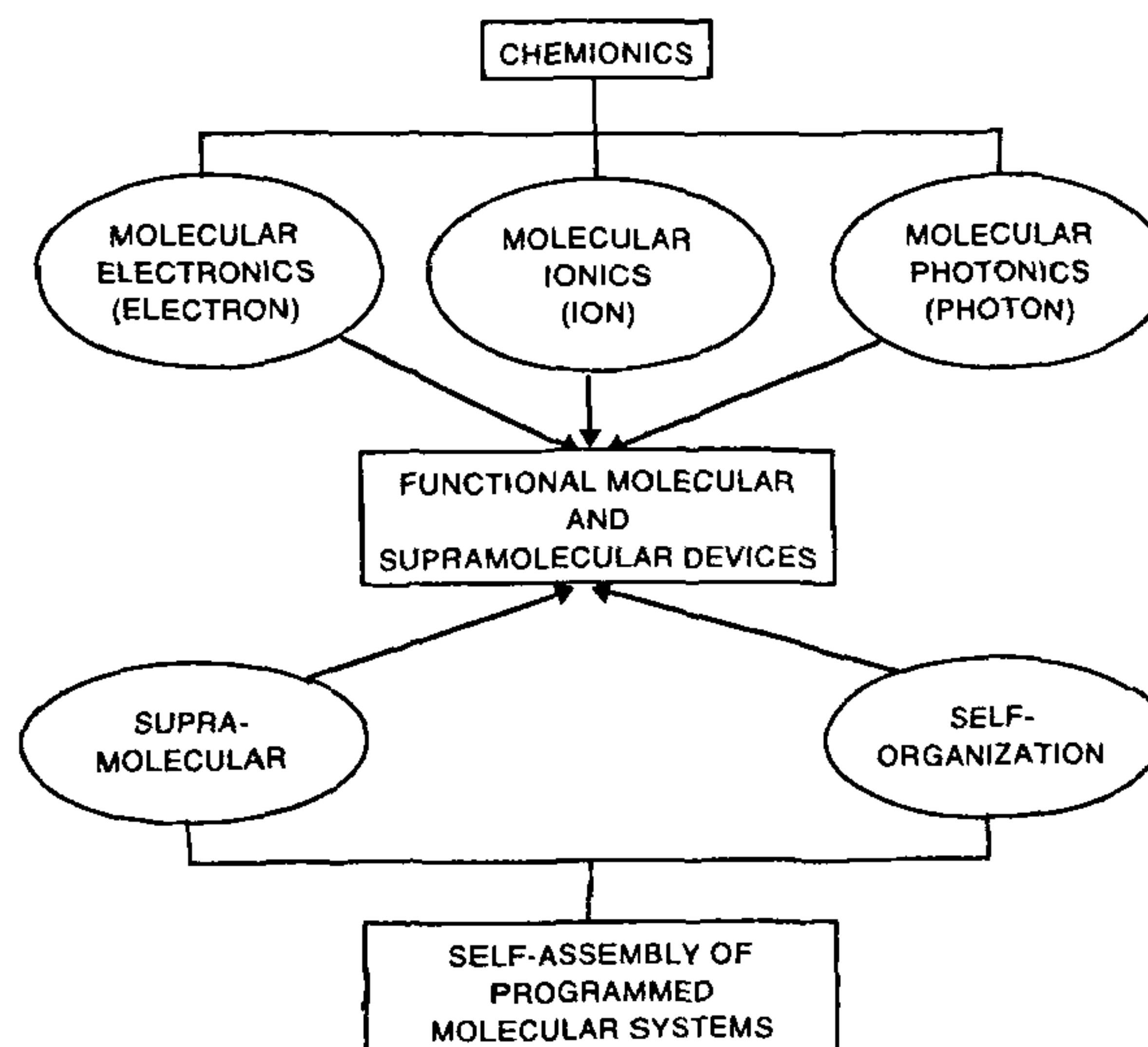


Figure 3. Chemionics as the chemistry of recognition-directed and self-organized photonic, electronic and ionic molecular and supramolecular devices.

But how do we enter this exciting field? The chemistry of molecular signal generation, processing, transfer, conversion and detection is already being hotly pursued by innovative chemists. The job of a molecular information engineer, if I may use that term, will be simply to design, build and operate molecular devices, which will be structurally organized and functionally integrated chemical systems built into supramolecular architectures. The function performed by such molecular devices will be the result of the integration of the elementary acts performed by the components, which may be photoactive, electroactive or ionoactive, depending upon whether they operate with photons, electrons or ions (See Figure 3). Strategies towards properties and

functions rather than towards structures will be the goal of a molecular information engineer. He will continuously seek to express a desired property in a molecule or a material, whatever be the composition and the structure.

What I have said so far sets out the general background. But now let me give a specific example of how CE scientists can use molecular information engineering in polymers to solve some challenging unsolved problems. I focus on the exciting idea of creating molecularly imprinted polymers. Molecular imprinting in polymers involves the idea of using a specific imprinting molecule to coordinate the assembly of synthetic monomers around a molecule of interest. The functional monomers are polymerized in the presence of a print molecule. The functionality in the print molecule interacting with the complementary functionality is found in the monomer units. A cocktail of functionalized monomers is 'prearranged' around the imprint molecule by noncovalent interactions, which could be ionic, hydrophobic, hydrogen bonding, etc. After polymerization, the imprint molecule is removed from the polymer. This leaves a polymer with recognition sites that are complementary to the imprint species with regard to both shape and functionality. This site will constitute an 'induced molecular memory' which will be capable of

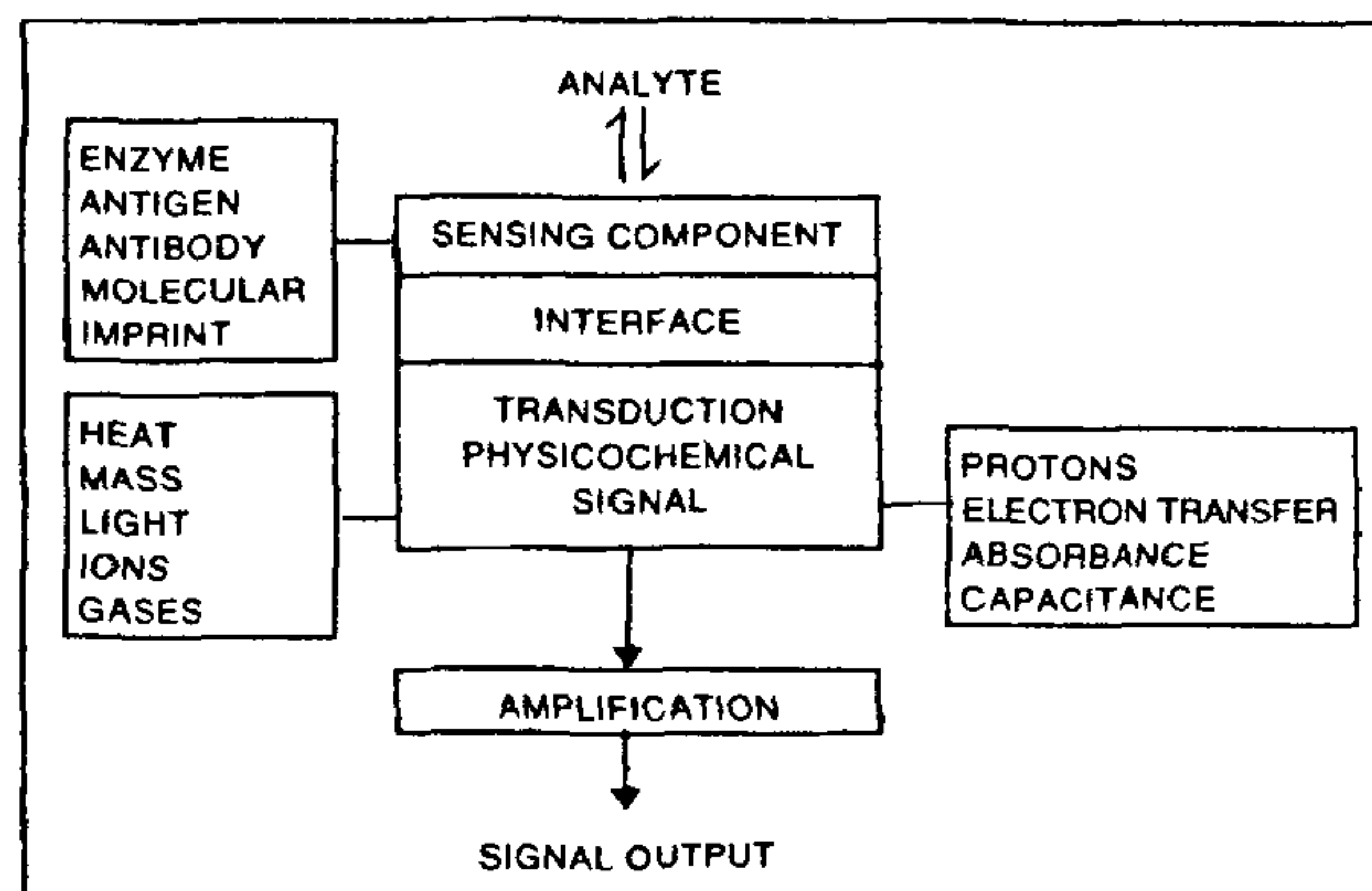


Figure 5. The principles underlying conventional biosensor operations and the possible role of MIPs in their function

selectively recognizing the imprint species. The polymer will have a macroporous structure which will allow an imprint molecule diffusion into and out of the polymer matrix.

Molecularly imprinted polymers (MIPs) are exciting, since they have a fascinating range of applications. Figure 4 shows a schematic representation of molecular imprinting through a noncovalent approach using an amino acid derivative demonstrated by Mosbach²⁷. Here, after mixing the imprint species with functional monomer and crosslinker, polymerization is initiated and the print molecule extracted from the resultant polymer under acidic conditions. Such MIPs find immediate applications in the challenging task of separation of racemic mixtures. Separation factors of between 2 and 8 have been achieved. What is impressive is that the molecular memory of the MIPs is not lost despite their manifold use in racemic resolutions over a period of several months.

This opens up an exciting new field of separation science for us in a challenging area such as chiral separations, where so far traditional chiral stationary phases (CSPs) have been used. Tailor-making binding polymers for a given separation process without involving the 'trial and error approach' inherent with different CSPs will be a big gain if we followed this strategy. The science-business connection is obvious here too. Please remember that of 500 or more optically active drugs presently in the market, about 90% are administered as racemic mixtures. Food and Drugs Administration regulations now require that for any new optically active drug, both enantiomers must be treated as separate substances in pharmacokinetic and toxicological profiling. Molecular imprinting might be the way to permit enantiopurification, i.e. the removal of small amounts of contaminating optical isomers on a commercial scale. Separation and purification of wide ranges of molecules by exploiting the stereospecificity and regiospecificity

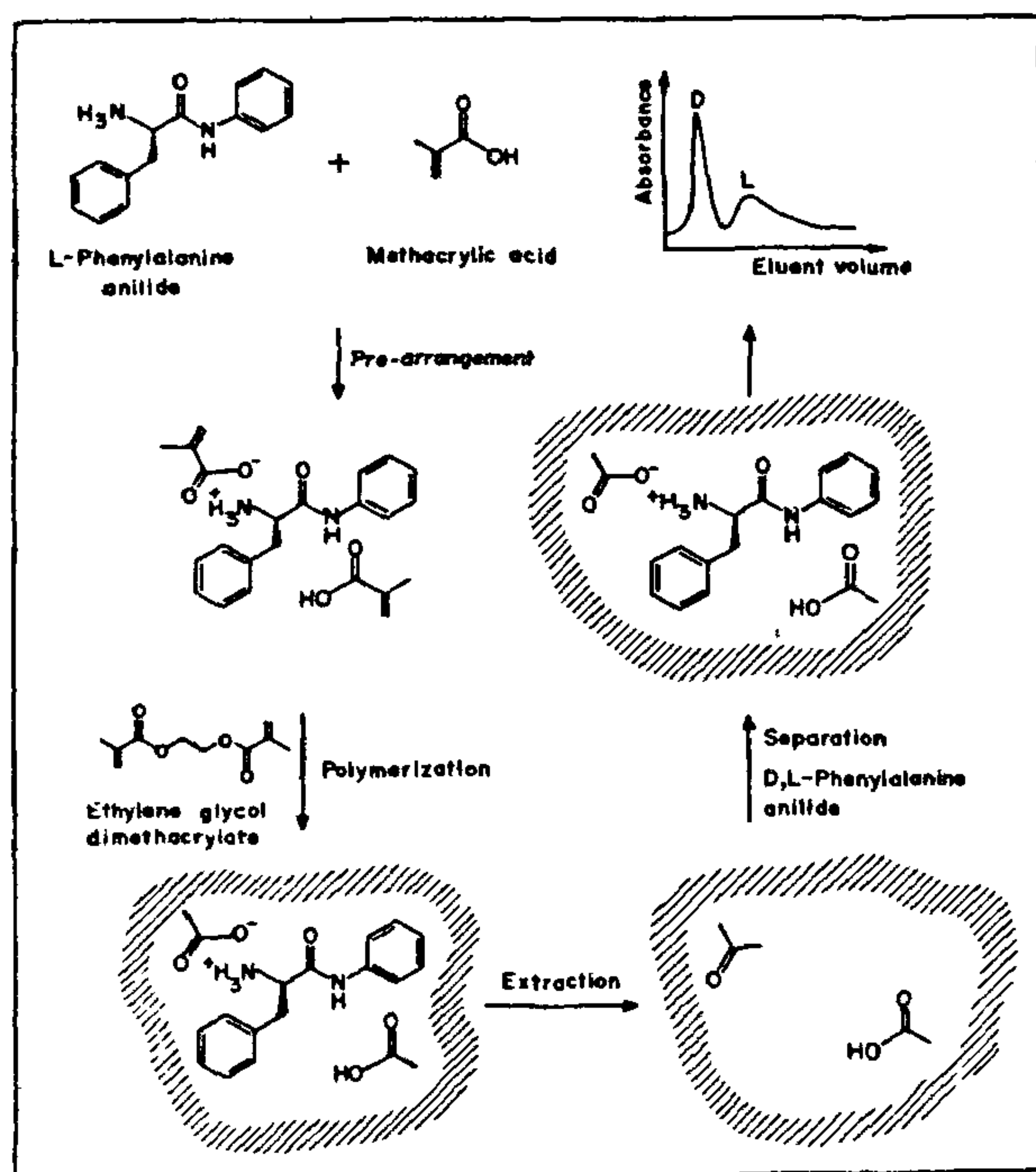


Figure 4. Schematic representation of molecular imprinting by a noncovalent approach of Mosbach²⁷. An amino acid derivative is used. Different stages in imprinting technique leading to a molecularly imprinted polymer (MIP) capable of baseline separation of racemic mixtures are shown

promises enormous potential with applications in differentiation of isoenzymes, conformers or epitopes and so on.

One can extend this molecular information engineering further, since MIPs can also move into substrate-selective polymers as sensory components. The idea will be to substitute the bio part in an enzyme- or antibody-based sensor with catalytically active or ligand-specific polymers prepared from specific polymers imprints. These can then move towards more robust sensing element systems (Figure 5).

In many cases no suitable biomolecule will be available. It is here that molecular imprinting will have the greatest potential. It will be able to create the custom-tailored synthetic binding site for a given molecule. The possibility of 'direct contact' systems, where 'molecular wires' could be created linking the binding cavity directly to a transducer, such as an electrode, to give rise to an instant signal upon binding follow naturally. A whole range of exciting possibilities will open up as soon as the real prowess of molecular information engineering is seen by CE scientists.

CE scientists and living systems

The fascination of chemical engineers for living systems dates back to several years. Whether it is transport phenomena²⁸ or reaction engineering²⁹ in living systems, CE scientists have brought elegant tools of sophisticated analysis to this field. Modern biotechnology, be it industrial, medical, environmental or some other, has always put a great demand on truly borderless behaviour between diverse disciplines. For instance, medical biotechnology thrived only because of a close cooperation between biologists, biochemists, geneticists, immunologists, medical specialists, chemical engineers and so on. Challenges of implantable and extracorporeal devices that duplicate the function of mammalian organs or facilitate the prevention or treatment of diseases are being met only through borderless laboratories combining several disciplines. Metabolic engineering and tissue engineering, in which CE scientists have got involved, require strong interdisciplinary teams. Search of novel biocompatible materials for prosthetic replacement and repair of both hard and soft mammalian tissue is also showing promising results only due to such synergy of action. Unresolved problems in industrial biotechnology of development of highly accurate, sensitive, and selective sensing devices capable of measuring concentrations of bioactive substances and metabolic components in bioprocess streams and monitoring these parameters for computer control also require strong interdisciplinary teams.

What chemical engineers have already achieved is something to be proud of. Significant contributions have

been made in industrial biotransformation processes³⁰, the subject of last year's Danckwerts memorial lecture. Chemical engineers had the lion's share in the development of artificial kidney, pursued initially as a natural extension of their work on membranes. They were at the centre stage when insulin was produced on a large scale using recombinant DNA technique. Now they have moved a step further by developing hybrid pancreas. The idea is to take live pancreas cells and immobilize them in an inert matrix to be used as hybrid pancreas. In drug delivery systems, we are now talking of low flow pumps and smart membranes. In low flow pumps, microcapsules are so produced that each releases its contents at a specified time. Smart membranes will sense the glucose level of the blood and release the required amount of insulin. Attempts are even being made to generate artificial red blood cells, which will not contain any living matter and yet perform the functions of the cells in great detail.

In this context it is worth quoting from an editorial that was written by Frauenfelder and Berg³¹ in connection with a special issue of *Physics Today* that dealt exclusively with the emerging new relations between physics and biology. They said 'interface between physics and biology ... is a cross-field endeavour to which physicists can make major contributions. But to do so, they need to learn enough biology to be able to talk with biologists and to distinguish problems that are central from those that are peripheral. Since much of biology is descriptive, the physicist has a strong advantage: It is much easier for a physicist to learn biology than for a biologist to learn physics'.

Just replace the word 'physicist' with 'CE scientist' and read the above paragraph again. The idea is clear. CE scientists have already played a crucial role in bringing quantitation to biology³². The tools and skills that we will use in future will also come from diverse disciplines again. My chemical engineering colleague in NCL, Bhaskar Kulkarni, recently wrote a paper³³ on the application of artificial neural networks for procaryotic transcription terminator predictor and it featured on the front cover of the journal *FEBS Letters*. The interesting point here is that a chemical engineer has picked up a tool developed by electrical engineers and mathematicians and contributed to quantitation of a biological problem!

CE scientists are making headway in developing more advanced methods. The growth of procaryotic cells has been predicted in a rigorous quantitative way – a far cry from our gross Monod and Michaelis-Menten equations. Such new models consider the formation of proteins from amino acids, RNA as well as DNA from nucleotides and cell wall membranes from lipids, not only for the parent cell but also for the plasmids contained in it. The distribution of plasmids as the cells multiply has also been predicted.

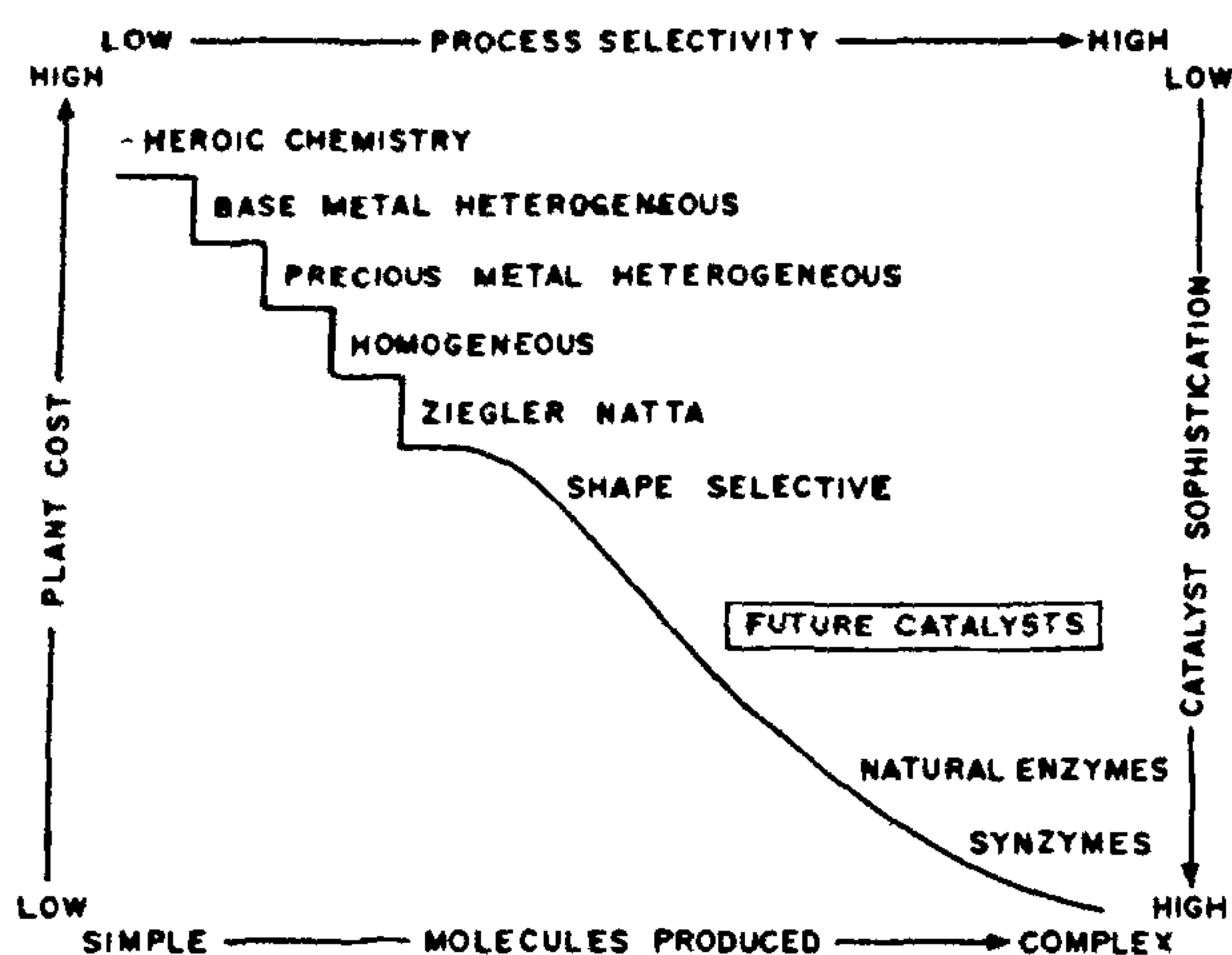


Figure 6. Historical trends in the development of catalysts

Let us, for a moment, look at enzymes, which the CE community is looking at as catalysts of the future. Figure 6 shows the way in which catalyst development has moved over the years. The chemical engineers have so far contributed to the development of production processes of commercial enzymes. They have tried to immobilize them and so on. However, once again if they become borderless then they can get involved in an even more exciting game, namely displacing the enzymes themselves. Indeed, designing catalysts functioning in a manner similar to natural enzymes, i.e. creating synzymes, is emerging as an exciting challenge, as we can see from Figure 6.

Enzyme catalysis involves binding of the reacting substrate in a perfectly fitting cavity or cleft of the enzyme that contains functional groups in the correct stereochemistry for binding, catalysis, and group transfer. The idea of using zeolites as hosts has opened up the field of zeozymes. Use of molecularly imprinted polymers now offers interesting possibility for creating enzyme-like catalysts too. But as we become more and more borderless, we can start bringing in diverse ideas from different disciplines. A recent breakthrough³⁴ is worth describing.

Many attempts have so far been made to create a synzyme for the purpose of catalytic oxidation on lines of the enzyme cytochrome P-450. Heterogeneous mimics have been designed that use organometallic complexes encapsulated in the supercages of zeolites, which are the so-called zeozymes. However, these systems have no real mechanistic analogy with the enzymatic process, and the oxidation rates tend to be low. Parton *et al.*³⁴ tackled this problem by developing a composite

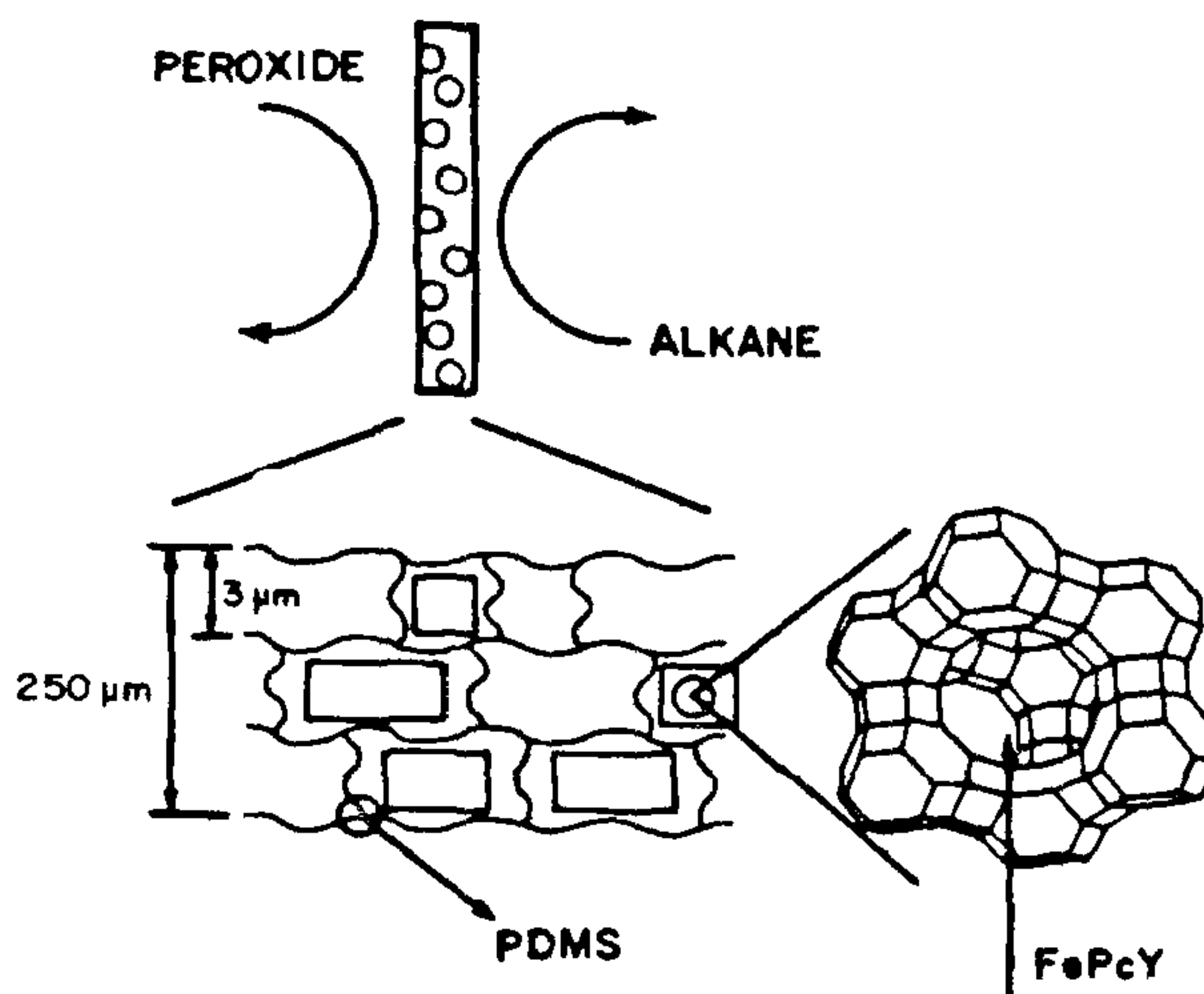


Figure 7. Zeozyme in a polymer membrane providing a mimic of cytochrome P-450.

catalytic system by incorporating iron phthalocyanine complexes encapsulated in crystals of zeolite Y, which were in turn embedded in a polydimethylsiloxane membrane (Figure 7). The polymer served three purposes. It acted as a mimic of the phospholipid membrane in which cytochrome P-450 resides. It acted as an interface between the two immiscible phases. It avoided the need for solvents or phase transfer agents. The system oxidized alkanes at room temperature and showed amazing turnover. The premium here again was on creativity, daring and combining concepts from diverse disciplines in an uninhibited fashion!

The way the field will move will be hard to predict by any logical and structural analysis. We already have examples of animals as bioreactors—take the case of transgenic cows producing human lactoferrin or transgenic sheep producing α -1 antitrypsin. Modern biotechnology is thus helping us to replace bioreactors by animals. On the other hand, modern polymer science is helping us replace animals by plastics! Let me explain this.

Immunoassay techniques require antibodies produced from laboratory animals. How about making plastic antibodies? This is not a dream anymore. All that we need is an exploitation of molecular information engineering done on chosen polymers so that they will become antibody mimics which will be comparable to biological

antibodies. It has been shown³⁵ that molecularly imprinted polymers could be made which show strong binding and cross-reactivity profiles very similar to antibodies. Now this opens up an enormous opportunity, since MIPs can be made against a great number of organic molecules, for example, drugs, metabolites, hormones and toxins, provided they have suitable interaction points. It is easy to see then the amazing synergistic effect of diverse disciplines merging together.

CES and nanotechnology

Great expectations on nanosystems (1–100 nm) have been raised recently. Exciting pictures of nanoscopic machines that replicate, build crystalline rocket engines, repair cells and extend life spans have been painted^{36,37} and even new strategies of doing all this by micromachining have been suggested. However, there is a problem here, since such nanomachines must themselves be put together by other nanomachines! Ideas of building molecules by pushing together atoms by the tip of the scanning tunnelling microscope have also been suggested. We can only imagine how slow and cumbersome these processes will be. Solid-state physicists, materials scientists, and electrical engineers build nanostructures through techniques such as chemical vapour deposition, etc. However, fabrication of microstructures and devices requires increasingly substantial effort as they are extended to the range below 100 nm. Then how can we proceed?

While we are all struggling, biology abounds in nanostructures with dimensions of about 1–100 nm (ref. 38). Just consider the range of biological structures – from proteins to viruses to cellular organelles. The challenge is to make structures of the size and complexity of biological structures, but without using biological catalysts or the information coded in genes. Nanotechnology, therefore, requires new strategies and technologies.

Self-assembly is emerging as a new strategy in chemical synthesis, with the potential of generating nonbiological structures with dimensions of 1–100 nm. Structures in the upper part of this range of sizes are presently inaccessible through the chemical synthesis route and the ability to prepare them would open a route to structures comparable in size (and perhaps complementary in function) to those that can be prepared by microlithography and other techniques of microfabrication.

What can CE scientists do here? One option is to look at the nature and see how we can exploit the self-organized structures that it has already created. The second is to understand the process of self-organization and simulate it synthetically to create new structures. Both

approaches require ingenuity but both are possible, as I will show.

Surface layers (S-layers) represent the outermost cell wall component of many eubacteria and archaebacteria. These S-layers are arrays of protein or glycoprotein subunits that are linked by noncovalent interactions. Channels of 2–6 nm diameter exist in S-layer lattices. This beautiful S-layer material was isolated from highly thermophilic eubacteria, crosslinked with glutaraldehyde and then it was deposited on commercially available microfiltration membranes³⁹. The only function of the microfiltration membrane was to provide mechanical support. These membranes displayed unusually steep rejection curves. Such new types of UF membranes will have considerable potential in opening up new doors to ultrafiltration technology.

Let us now turn to synthetic methodologies. Block copolymers have particularly interesting features with respect to equilibrium statistical mechanics, forming various phase-separated domain structures with nanometer periodicities, the so-called nanopatterns. Recently, a breakthrough was achieved⁴⁰ in using the process of self-organization in block copolymers of polystyrene–polyparaphenylene. The films, of 10–30 μm thickness, were produced by evaporating solutions in carbon disulphide under the flow of a moist gas. Empty spherical cells about 0.2–10 μm in diameter appeared spontaneously in a beautiful hexagonal array. Such membranes might find application in controlled release of drugs or other bioactive species, or as materials with useful optical properties, moulds or scaffolding for forming ordered microstructures, and model substrates for surface science. What is remarkable is that the polymer architecture is able to induce a complex regular morphology at a scale two or three orders larger than the molecular scale. The mechanism of formation of this new regular morphology involves a combination of complicated thermodynamics and transport phenomena and provides an interesting challenge to CE scientists.

Nanobiotechnology is emerging as an exciting field. Fabricating organized biomolecular structures is a new challenge that is being met by bringing in diverse disciplines. Genetic engineering will tailor protein's makeup and also its function. Organic chemistry will provide new materials for anchoring and preserving the altered proteins. Electrical engineering will offer ways to detect signals from internal working of proteins. We can finally turn a small assembly of biomolecules into a custom-designed molecular machine.

Another exciting area is where proteins are being turned into nanoscale chemical processing plants. Proteins can be used as reaction vessels for controlling the particle size of other materials. They can cage several compounds. If the chemical affinity of the protein can be changed, then the protein can be engineered to fit the mineralization product that one wants inside it. Such

caged particles will pass through the human body in an unrestricted way. They will be useful in diagnosing and treating diseases. It is clear that CE scientists can share the grand challenges of nanotechnology by joining hands with others working in protein engineering, organometallic chemistry, semiconductor technology, etc.

Entering new territories

Venturing into new fields will be both exciting and rewarding for CE scientists. Nontraditional thinking, whether it is in terms of creative use of ultrasound, photoenergy, microwaves or some other means, will continuously give the CE scientists new challenges and new opportunities. Laboratory curiosities or chance observations in other disciplines can be turned into major opportunities with winning technologies if we are both vigilant in watching other fields and daring. Let me take one specific example in detail, namely sonochemical reaction engineering.

Chemists have shown over the years that application of ultrasound yields entirely different products from the same reactants, enhances the rates of the reactions phenomenally and even permits at very mild reaction conditions synthesis of products that can normally be done only under very high temperatures. Although catalogues of the use of ultrasound by chemists are available⁴¹, little or no work aimed at quantitative prediction of the effects of ultrasound on the course of chemical reactions has been carried out. Now sonochemical reaction engineering is beginning to emerge as an exciting area of research for CE scientists, since it combines so many novel elements of cavitation dynamics, transport phenomena and reaction engineering.

The influence of ultrasound on chemical reactions is known to come from the cavitation phenomena. Very small bubbles of dissolved gases that are omnipresent in the liquid can grow in the rarefaction cycle of the sound wave and collapse rapidly and adiabatically during the compression cycle. The adiabatic compression generates very high temperatures and pressures in the bubble. Reactive intermediates are then born, which can diffuse out and react with other reactants present in the surrounding liquid phase. Further, when a cavitating bubble collapses near a solid surface, it does so asymmetrically and generates microjets of high velocity. The resulting microjets can clean the solid surfaces. Such a cleaning action leads to reactivation of passivated catalytic surfaces and also local heating of catalytic surfaces. This results in impressive enhancement of the rates of reaction. The high velocities generated can also decrease any diffusional resistance present and, once again, enhance the rates of the reactions.

The big question is how can sonochemistry be taken through the path of sonochemical reaction engineering

to sonochemical technology? A body of engineering knowledge has still to be acquired before design of reactors or even scale-up can be achieved. The first paper on sonochemical reaction engineering, which provides a high level of predictive ability, appeared a few months ago⁴². It is interesting to see that a multidisciplinary team of chemical engineers, mechanical engineers and chemists worked together to provide insights into the fluid-dynamical phenomena as well as the reaction events.

A lot more needs to be done in sonochemical reaction engineering. Capturing the dynamics of a cavitating bubble, postulating the rates of reactions occurring in the bubble that produce reactive intermediates, modelling of convection created by microjets and acoustic streaming, investigation of pitting and its effects on creation of new surfaces, understanding the physics of the fusion of particles and the new catalytic chemistry are some of the interesting challenges in modelling. But an even bigger challenge is to make a sonochemical reactor work in practice. New ideas on loop reactors are emerging⁴³. Normal sonicators have the problem of erosion of the power-transmitting surfaces due to cavitation. How do we concentrate the power away from the transducer surfaces? The use of spherical vessels for batch reactors or hollow cylindrical-type transducers to position the power around the centre of the axis seems to be a possibility. However, only a close interaction with acoustic engineers, mechanical engineers, chemists, etc., can move this field further.

The use of ultrasound is just one possibility. Interesting opportunities exist for the development of applications of both electrochemistry and photochemistry. Unusual cross-disciplinary thinking is needed though. The concept of using electrical potentials impressed upon metallic or semiconductor catalysts to bias either the rate or pathway of a heterogeneous catalytic reaction to affect the reaction kinetics or product distribution is an unexplored area. Can we carry out electrochemical (i.e. electron insertion/withdrawal) processes at electrode surfaces in the proximity of immobilized enzyme systems as a means of conducting oxidative or reductive enzymatic transformations? This will do away with the necessity of cofactor reactants. Another interesting challenge is the simultaneous generation of electric power with production of useful organic intermediates by controlled catalytic oxidation or reduction at an electrochemical cell electrode. Such 'bootstrap' chemical processes, which are energy- and raw-materials-conserving, will make the profession leap-frog.

If we go really borderless, then we can think in terms of the combined-fields approach⁴⁴. We can generate additional driving forces in a process that works simultaneously with the conventional driving force of the process. The additional forces may evolve from the application of external fields or body forces. Electric

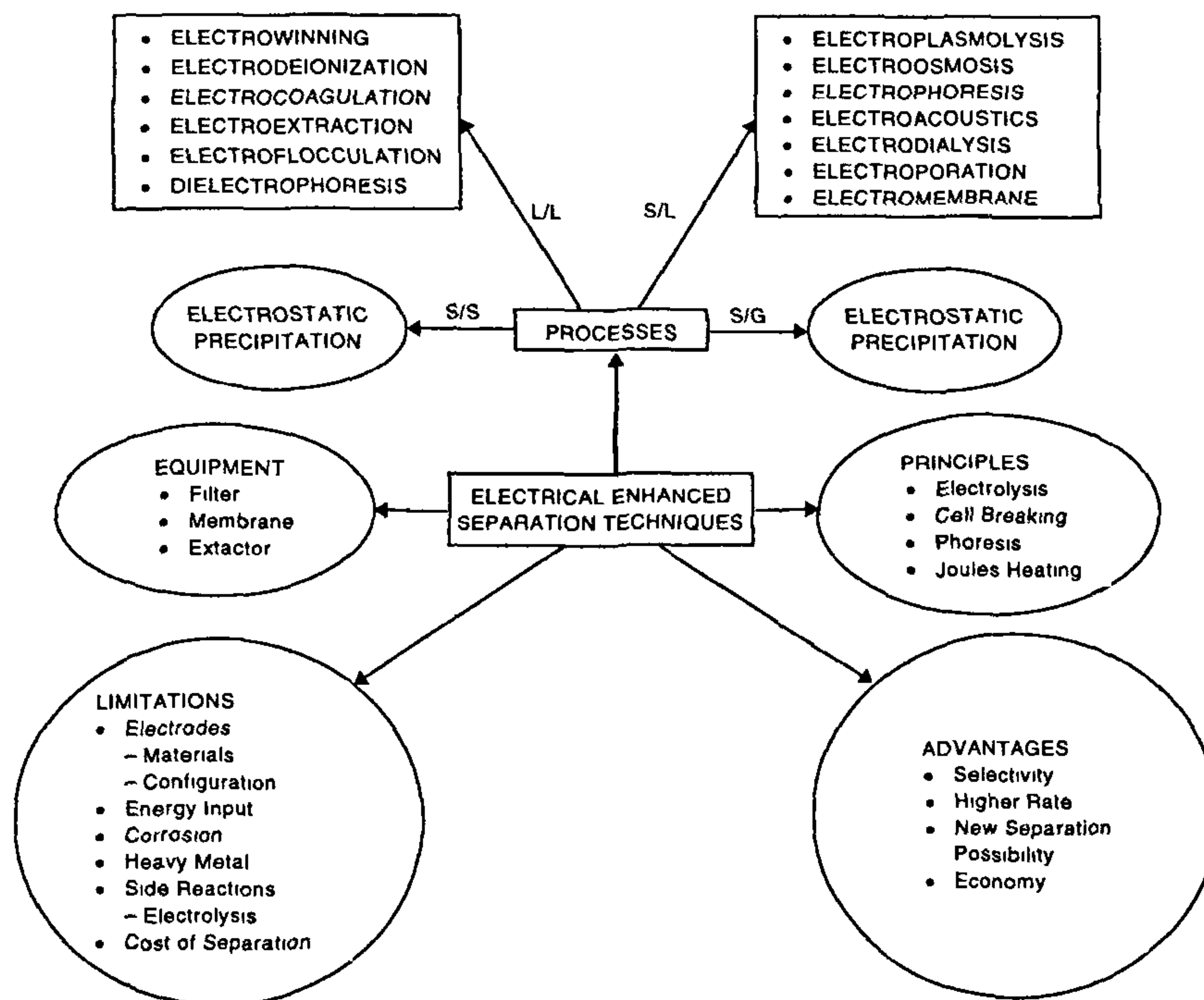


Figure 8. Range of electrical enhanced-separation techniques

field, which is one possibility, has already been explored for enhanced-separation techniques (Figure 8), but my feeling is that we have only been scraping the surface so far and a lot of unconventional thinking has to go on here.

Take, for instance, an imaginative use of the electrical field in the pulsing mode. We know⁴⁵ that an electric pulse of intensity in kilovolts per centimeter and of duration in microseconds to milliseconds can cause a temporary loss of the semipermeability of cell membranes, thus leading to ion leakage, escape of metabolites, and increased uptake of drugs, molecular probes and DNA by cells. This phenomenon is referred to as 'electroporation'. Electroporation can find applications in insertion of proteins into cell membranes, improving drug delivery and hence effectiveness in chemotherapy of cancerous cells, activation of membrane transporters and enzymes, etc. Why not design very cheap disinfection or water purification processes based on electroporation?

Let us pursue the idea of pulsing and look at other possibilities. Consider membrane fouling during cross-flow microfiltration. We can imaginatively use electrolytic membrane cleaning. Here again, intermittent electric field pulses can be used to clean membranes without the interruption of the separation process. It has already been shown⁴⁶ that this technique can improve the overall membrane permeation rates by a factor of up to 10 with

only a modest electrical energy requirement. Another technique, namely the *in situ* electrolytic membrane restoration, is very effective in restoring membrane water permeation rates under mild chemical conditions. Used in combination, these techniques have the potential of obviating the requirement of membrane backflushing and conventional chemical cleaning.

Let me emphasize again that these examples are by no means exhaustive but are only typical of the opportunities that exist. Photochemical and electrochemical reaction engineering have already matured. Sonochemical and microwave reaction engineering are emerging as new disciplines. Asimov's orbital reaction engineering⁴⁷ may be a long way away – but emergence of other fields will depend on our creativity and daring again.

New look at old materials through seamless science

With rapid advances in science, a CE scientist will have an opportunity to look at old materials and make them perform new functions. He may even convert them into smart materials with attributes of selectivity, sensitivity, shapability, self-recovery, self-repair, self-diagnosis, self-tuning and switchability. Use of some severe interdisciplinary science is required here to make this happen. For instance, 'dumb' water-swollen gels, which are

just used as passive supports, can be so transformed that they bend, walk and even mimic enzymes! To show such an exciting range of possibilities, I will just choose three familiar materials, namely gels, zeolites and clays.

Let me focus on gels first. Biological materials in the body are usually composed of soft and wet materials. This is in contrast with most industrial materials that we chemical engineers use. Take, for instance, metals, ceramics and plastics. These are dry and hard. Seldom do we use soft materials. But it is beginning to emerge now that 'soft and wet' materials can be important not only as biological materials that construct the body but also for displaying their functions. Designing mobile machines using soft and wet materials, furnishing soft materials so that they are able to make shape changes, or to generate tensile stresses that can lead to motility without the requirement of a rigid structure are challenges that will be met in the new world of seamless science.

Let me discuss more specifically polymeric gels, which are swollen polymeric networks. They possess the cohesive properties of solids and the diffusive transport properties of liquids. The combination of elastic properties and osmotic reactivity makes them very special. Gels are held in place by a hydrophilic lattice of long-chain molecules. The fragile balance between the electrostatic repulsion of the adjacent polymer strands and the osmotic pressure exerted by the ions in the solvent holds the key to the behaviour of gels. Disrupting a gel's charge distribution by altering its environment can trigger it to swell or shrink suddenly^{48,49}. Such phase transitions can be exploited imaginatively.

The thermodynamics of phase transitions, aspects of transport phenomena as well as the energy conversion phenomena in these gels will be best understood by CE scientists. Indeed, the entry of CE scientists in this area is giving rise to the development of several systems of interest, including separation technology^{50,51}, sustained release systems⁵² and so on.

It is rather interesting to notice the simultaneous generation of ideas in such fields that take place between different disciplines driving different applications using similar principles. Our research group recently used the pH sensitivity of the hydrogels for attaining time-invariant diffusional flux through bilayered membranes with collapsible barriers⁵². The novelty of the approach was that the bilayers were formed *in situ* and the diffusional behaviour was manipulated at will depending on the external stimuli. The idea rested, however, on making both surfaces of a gel slab collapsible. Our Japanese friends⁵³ decided that they would collapse only one of the surfaces of the gel. Their idea was to create a bending motion (Figure 9). By exploiting this asymmetric collapse with the help of a ratchet-type 'gel looper', they showed that a gel could 'walk' along a bar! As chemical engineers, it is easy to see that we were interested in controlling diffusion and the Japanese were interested in

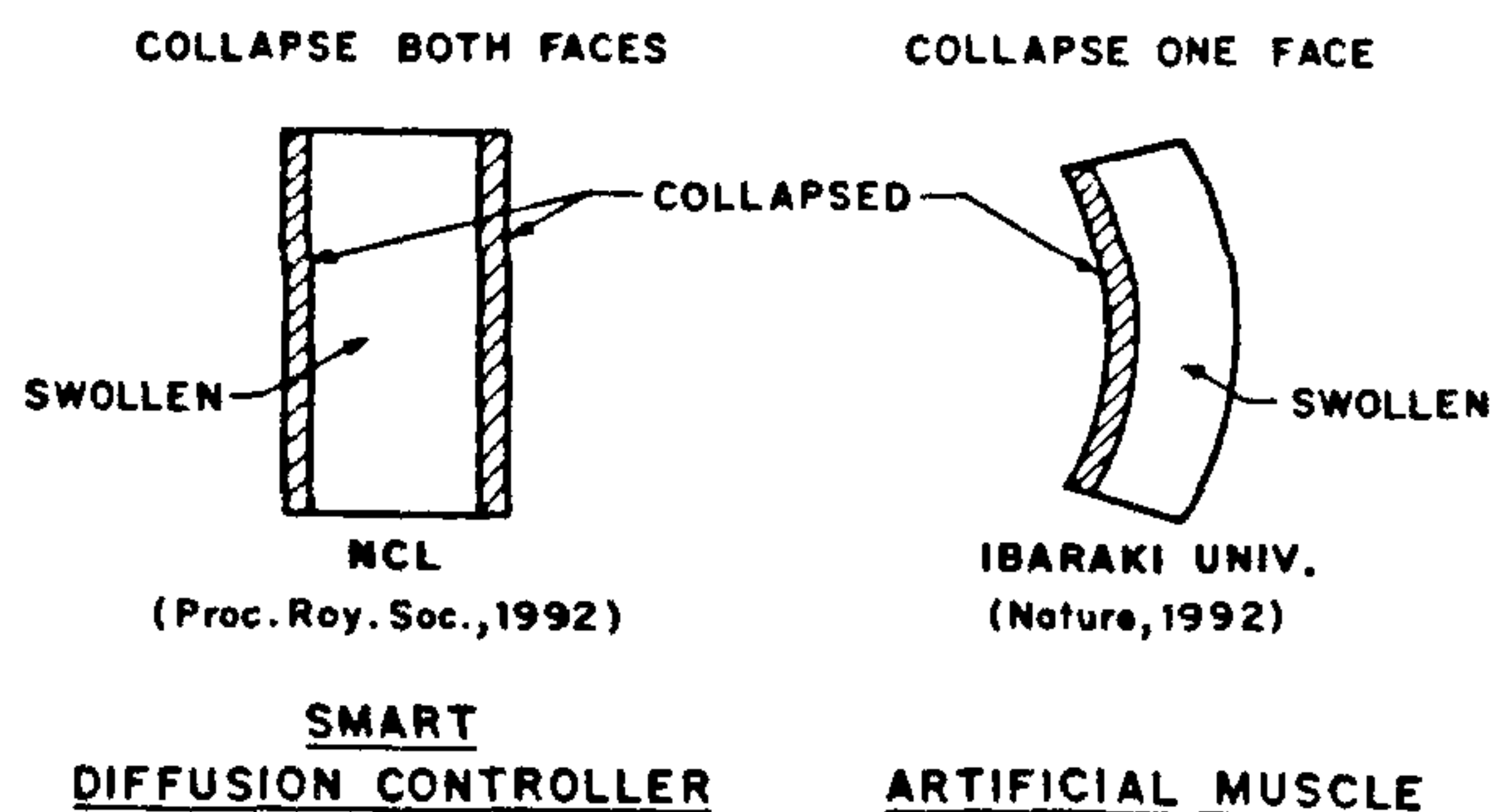


Figure 9. Schematic presentation of two applications of a reversible collapse of a gel bar surface used for designing a smart diffusion controller⁵² and a mimic of artificial muscle⁵³.

soft robots – but the phenomena exploited by us were exactly the same.

In contrast to motors and hydrodynamic pumps, the motion of a polymeric gel demonstrated by Osada *et al.*⁵³ is produced by the chemical free energy of the polymer network. Thereafter, electrical or thermal energy is used to drive the direction and control the state of the equilibrium. Thus, the chemomechanical gel driven by outside stimulus is able to exhibit 'gentle' and 'flexible' action, and its movement is more akin to that observed in a muscle than in the metallic machine systems. The application of chemomechanical gel as an 'actuator' for robots and other systems has special interest. The molecular machine that is capable of biomimetic motility by using gel will allow entry into a new world of movement where the system works smoothly and gently without noise, heat evolution and exhaustion^{48,54}. Applications might eventually include the construction of devices that can be inserted into muscle and even emulate the nervous system. This field opens up so many new exciting vistas for CE scientists.

Let us now move to zeolites, which were initially discovered as naturally occurring materials. Much zeolite research and development with which chemical engineering scientists are associated is still aimed at the traditional uses such as catalysts and adsorbents. However, over the past few years we have seen zeolites emerge as advanced materials⁵⁵. Indeed, zeolites as microporous materials with nanometer dimension window, channel and cavity architecture present new opportunities. The key in assembling and maintaining controlled microstructure is to use solid host lattices that serve as templates within which a guest structure of nanometer architecture can be assembled. This opens up new possibilities.

Take the field of solar energy conversion. Here a spatially well-organized molecular system is required that models photosynthetic mechanisms. This will enable

redox reactions to proceed efficiently along the desired paths. Other potential applications include zeolite electrodes and electron relays, zeolite batteries, zeolite fast-ion conductors, intrazeolite semiconductors, zeolite chemical sensors, zeolite imaging and data storage materials, zeolite lasers and displays, as well as zeolite composites to form perm-selective membranes or thin films.

The stage is set for rapid developments of zeolite-based electronic, optical, magnetic and dielectric materials. Zeolite semiconductors may not be far away. The marked proton conductivity of certain acid zeolites may open up the ways to electrochromic zeolites. The emergence of acentric zeolites may lead to the design of zeolite piezoelectric devices. The molecule-sized pore and channel structure of zeolites could provide a novel medium in which to create ultrahigh resolution images and package and process information at high storage densities. The unidimensional channel architecture of certain zeolites may even permit the assembly of low-dimensional zeolite conductors and the control of energy transfer and energy migration in restricted dimensions. How do we overcome the present disadvantages of zeolites, namely pore plugging, poisoning, structural defects, the difficulties of growing large single crystals, and interfacing a zeolite device with the outside world? A CE scientist is well poised to take upon himself some of these challenges. But he must operate in the borderless way interacting with materials scientists, physicists, electronic engineers and so on.

Let us look at another old material that we are so familiar with – namely, clays. There have been suggestions that clays may have served as templates for the first self-replicating systems on this planet⁵⁶. Indeed, clays have been considered as possible chemical microreactors in the prebiotic synthesis. They may very well have served as 'low-tech' precursors to the self-replicating biomolecules. Oligomers of glycine have been formed in the presence of clays subjected to cycles of wetting and drying simulating natural cycles. It has been demonstrated that energy due to mechanical stress could be stored within the lattice as trapped holes, and released in the form of additional acidic catalytic sites. Luminescence can be induced by dehydration of a clay and mechanical stress can translate into triboluminescence. In short, clays can store energy from the environment and release it in various forms.

Is it not then possible to let our imagination run wild and aggressively move into this area? We can raise a number of questions. Can clays oligomerize simple molecules into biomolecules? Can the required dehydration reactions occur in an aqueous environment? Can clays protect their reaction products from photodecomposition under intense irradiation from sunlight? Can clays store energy and release it by transforming it into chemical energy to operate these condensation reac-

tions? Can clays distinguish stereoisomers to form certain products selectively? The answers to most of these questions are positive. Can the CE scientist not move aggressively to exploit these materials?

What I have tried to emphasize here is that innovation is the key to making mundane materials smart or adding enormous value to them. However, the innovation will emerge only if we intermesh intimately with other adjacent sciences.

Acquiring new tools from other disciplines

We must empower a CE scientist with sophisticated tools, both experimental and computational, for him to march ahead. The quest of a CE scientist to probe molecular-level events and structure on the one hand and to gain access to the spatially resolved macroscopic processes on the other will mean that he will be in constant search of new tools. Especially valuable are those tools which allow the measurement of the dynamics of the events (say during mixing) or allow *in situ* measurements during say a reaction-diffusion event on a working catalyst. Once again these tools will be available elsewhere and the real ingenuity will lie in locating them and using them. Thus, tomography technologies are extensively used in medical diagnostics. A thermal neutron-based Computerized Tomography (CT) system may be used conventionally for industrial diagnostics. It is up to the CE scientist to know the relevance and the worth of these tools and bring them into the profession.

If we look around, we see that NMR spectroscopy and imaging, tomography, trajectography, image processing capability, etc., are serving as powerful aids for CE scientists, who are searching for more and more detailed information. Let us see how this is being achieved by taking a few specific examples.

Tomography techniques used in the medical field cover a wide range of tomographic sensing techniques. These include nucleonic (X-ray, γ -rays), optical, ultrasonic and electrical methods. Some of these methods would have limitations for CE problems at hand. For instance, optical sensors are not useful in opaque systems. Radiation-based sensors are slow, expensive and have safety constraints. However, the scope for the use of these techniques is enormous. Electrical capacitance tomography can be used for nonconducting systems. Electrical resistance tomography can be used for conducting systems. Optical tomography has already been used for imaging mixing process within agitated vessels.

An eye for application of new tools will take us a long way. For instance, consider positron emission tomography (PET), an imaging technique widely developed for diagnostic medicine. It was imaginatively applied by chemical engineers to examine the problems of mixing of powders and gain some valuable new insights^{57,58}.

Similarly consider a commonly used technique in industrial diagnostics, namely thermal-neutron-based CT system. It can be operated in a radiograph mode to obtain 2-D transmission images or in the real-time mode to image dynamic events. Both systems can be used in conjunction with computerized tomography for 3-D imaging. Jasti and Fogler⁵⁹ used this technique imaginatively recently in getting some important insights into porous media flow.

Let us cite a specific example to illustrate the power of these techniques. Williams *et al.*⁶⁰ exploited electrical impedance tomography to study mixing in stirred vessels. The batch mixing of a slug of brine tracer was mapped out. Simultaneous capture of video images of the tracer mixing provided a visual confirmation of the tomography reconstruction. The experimental acquisition of fully 3-D concentration field information was particularly satisfying. Such work provides a powerful incentive to develop and implement fully 3-D models of the flow and mixing, since the details available now are precisely commensurate with the details that are capable of being provided by computational fluid dynamic (CFD) models.

CE scientists getting involved in such endeavours must not be just at the periphery but must also get involved in obtaining deeper insights into image reconstruction problems connected with spatial nonlinearities and also the utilization of 3-D data. Furthermore, after a while, it is also important that they move from the 'comfort zone' of studying 'clean model systems' to 'real-life systems' with these powerful tools. The idea is to solve the 'problems that need to be solved' rather than those that 'can be solved'.

Let us move on to NMR techniques now. Excellent reviews by Gladden^{61,62} show the great power of this tool in chemical engineering. NMR probes physical and chemical phenomena occurring over a vast range of both length and time scales. While NMR spectroscopy yields information on structure and dynamics at the molecular level, NMR imaging probes macroscopic phenomena such as structural heterogeneities within materials, filtration processes, concentration and velocity profiles, etc. Such studies enable additional insights into the physics of the problems and may even suggest new strategies.

We ourselves have used NMR extensively over the past few years and found it to be a very versatile tool – for probing both microscopic as well as macroscopic events that take place during the swelling and dissolution of polymers^{63–65} as well as during the hydration of superabsorbing polymers^{66–68}. Let me just illustrate the point by giving an example. We looked at the molecular-level events while studying the dynamics of mobilization in swelling-dissolving polymers. We saw strange plateau appears in the averaged molecular mobility vs. time curves (Figure 10a) as well as in fraction of

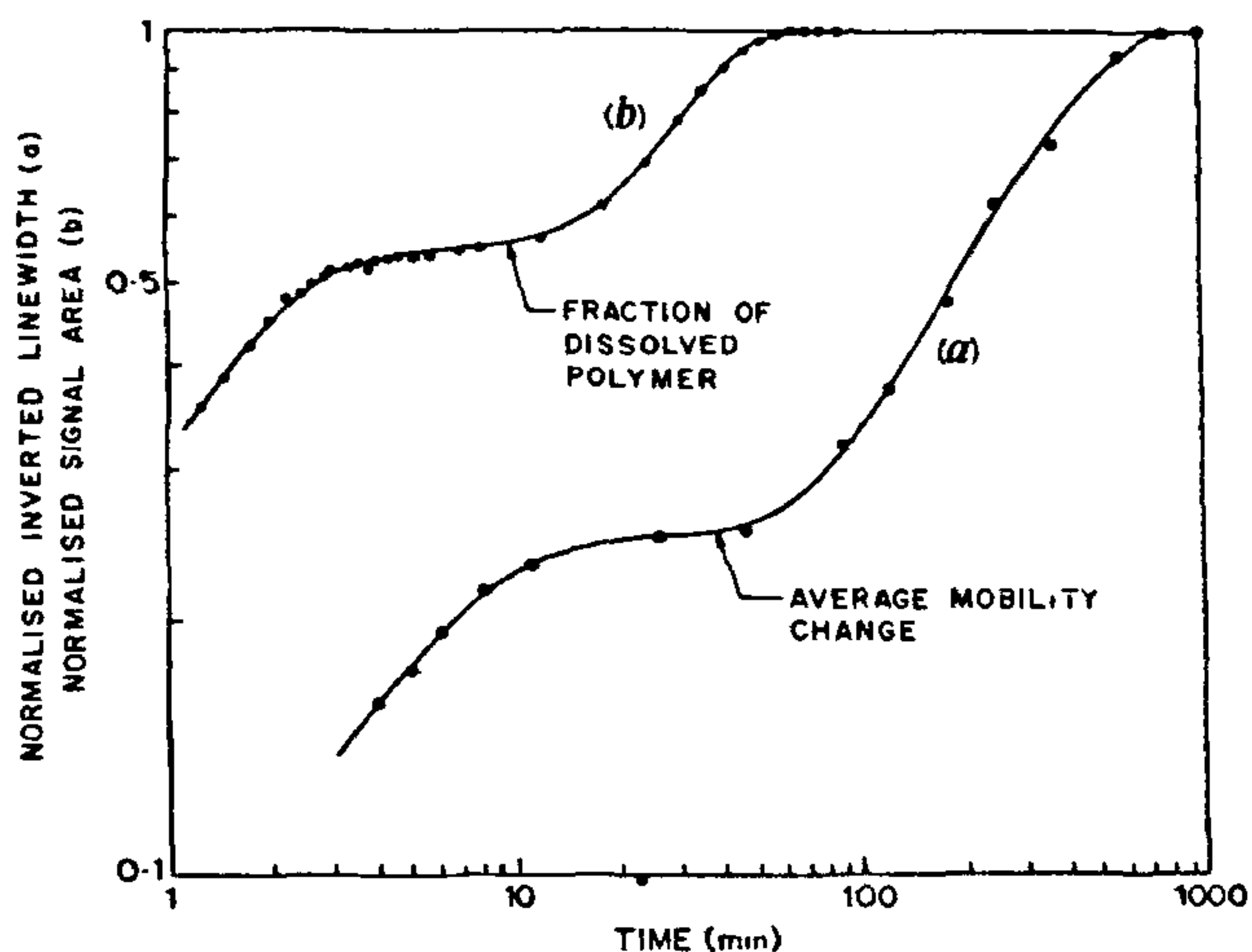


Figure 10. *a*, Reciprocal olefinic proton line width reflects on the average mobility in a swelling-dissolving polyisoprene polymer. The non-monotonous increase of mobility with time is striking⁶⁵. *b*, Normalized signal area measured during dissolution of high molecular weight polystyrene reflects on the dissolved fraction of polystyrene in CDCl_3 solvent. The plateau is striking and is influenced by disengagement dynamics⁶⁴.

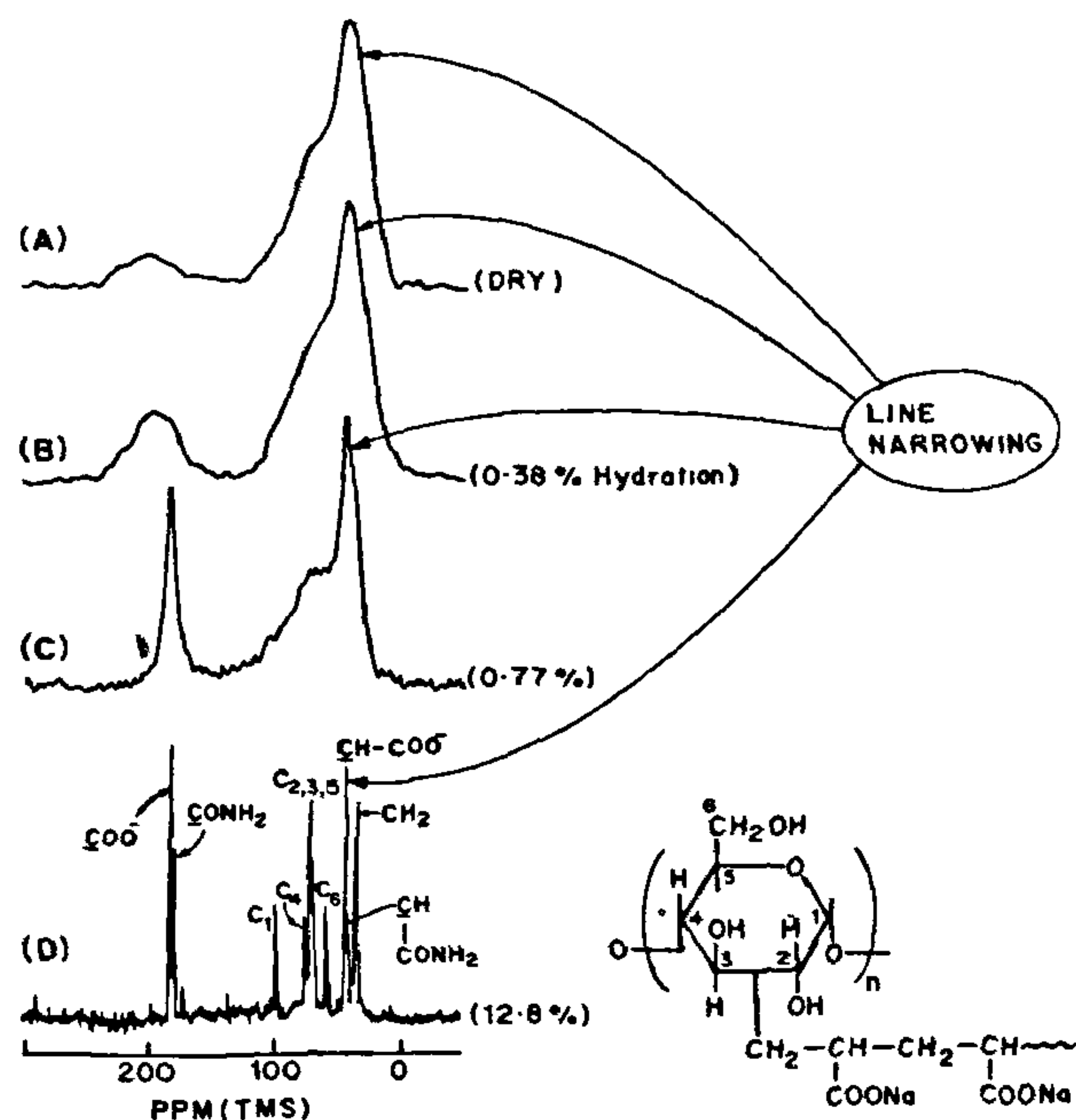


Figure 11. Specific hydration of a superabsorbing polymer (with the structure shown) studied by high-resolution solid-state NMR by Rajamohan *et al.*⁶⁸. Line narrowing at the carboxyl shows preferential hydration at that site despite other hydrophilic groups present in the polymer.

polymer dissolved vs. time curves (Figure 10 b). These unexpected observations helped us understand the role of disengagement dynamics at the gel-fluid interface for the first time. We have even been able to examine specific hydration sites in superabsorbing polymers (Figure 11), showing how water mobilizes the carboxyls preferentially, first in preference to other hydrophilic groups. Thus, NMR is a powerful tool that gives important insights into both macroscopic and microscopic phenomena.

In the above example, although we studied molecular mobility of macromolecules, it was still averaged over the sample dimension. However, some recent spectacular advances enable us to observe the dynamic events of reptation of a macromolecule even at a single-molecule level.

Perkins *et al.*⁶⁹ observed the tube-like motion of a single flexible DNA molecule by using fluorescence microscopy. Kas *et al.*⁷⁰ reported direct observation of reptation obtained by video microscopy of fluorescent labelled filaments of actin in a solution. How such improved understanding of molecular processes of migration and reorientation of DNA molecules undergoing conventional and pulsed field gel electrophoresis, as obtained by direct observations from a microscope and computer modelling studies, has helped in improving these sophisticated separation processes has been shown by Bustamante *et al.*⁷¹. Advent of such studies at molecular level will empower CE scientists to examine problems of interest to them with even greater rigour.

Let us move from experimental tools to computing tools. CE scientists have not been found wanting in moving quickly and exploiting new advances, be they in artificial intelligence (AI) techniques or in parallel processing, or in some other areas. They have not caught on to virtual reality as yet, but I am sure they ought to – and they will indeed do it soon.

A recent AI application in chemical engineering is the use of artificial neural network (ANN). ANN is a numerical (not symbolic), empirical modelling tool that has received much attention recently⁷². The ANN developments began with computer modelling of the human brain with a view to emulate neuron interactions. The universal approximation characteristic of ANN makes them extremely useful for applications such as on-line fault diagnosis, process control, process modelling, process and product design, trend analysis, etc. The ground is now ripe for wide-ranging applications. The ability to adapt, learn from noisy, incomplete or inconsistent data, better filtering capacity and true multiple-input-multiple-output nature make them indispensable in modern times. In most situations in real-world applications, a chemical engineer would neither have a formal model nor complete experimental data and ANN can help him greatly. Besides serving as a numerical modelling tool in intelligent process manipulations,

when combined with symbolic information processing, ANN supports the expert systems and the combination holds very significant technological promise.

Uncertainties abound human endeavours and associated information and data are often vague. Conventional techniques are, therefore, less useful when it comes to modelling and newer tools such as ANN provide some hope. The theory of chaos has already pointed out that apparently random behaviour may, in fact, be deterministic. The notion of fuzziness that prevails has prompted the development of fuzzy models and tools based on fuzzy set theory and logic, and applications in engineering such as reliability modelling, critical-path optimization and fuzzy logic controls are gaining ground. Future developments will, therefore, be clearly dominated by these new emerging tools.

Seeking solutions through new seamless science

Chemical engineers are expected to solve problems. Sometimes one finds a tendency to skirt around these and try and model them. Consider the problem of fouling in polymer membrane devices. Endless number of papers have modelled this phenomenon. But just modelling fouling is being a 'part of a problem' and not a 'part of a solution'. We really need to think creatively of ways and means by which fouling can be prevented. The solutions may require again the use of most severe interdisciplinary science. For instance, now that we know how to use molecular information engineering, why not develop a membrane with a molecularly imprinted polymer? May be a smart self-cleaning surface using 2-D imprint with an attribute of an enzyme mimic might do the trick! Or why not use a piezoelectric polymer which enables generation of mild turbulence at the membrane surface for a continuous cleaning action? However, such solutions require CE scientists with borderless attitude, who will go beyond the traditional thinking and seek solutions from other fields, and this is the new generation of CE scientists we will have to create.

Let me speak from a personal experience on drag reduction. Over 2000 papers have appeared on drag reduction under turbulent-flow conditions in polymer solutions. But these papers have not helped us in resolving the issue of the basic limitation of these polymers, which arises due to their poor shear stability in turbulent fields. Many of us in the chemical engineering community have continued to model the degradation phenomenon. This modelling started in the seventies and continues even today in the nineties⁷³. But have we solved the basic problem of *generating* shear-stable drag-reducing polymers? The only way we can solve the problem is by moving from the quest of 'new analysis' to new 'synthesis'. This new synthesis has to be again

based on an understanding of the molecular behaviour of these polymers under turbulent conditions, appreciation of the mechanochemistry of degradation and then finally designing some new synthetic strategies by using good contemporary chemistry⁷.

We recently tried to make a modest effort towards this and achieved at least partial success. We used the knowledge of polymer chain breakage developed by polymer physicists⁷⁴. Then we performed the mechanistic analysis of a perfectly 'zipped' assembly of a fully extended bead rod chain model of macromolecules in an elongational flow⁷⁵. We showed that the enhanced stability of such zipped structures was a result of the distribution (near the chain centre) of the drag tension into the two parallel 'zipped' chains and reduction of the drag force due to the enhanced hydrodynamic shielding. This helped us in devising quantitative guidelines for the optimum design of shear-stable and effective drag reducers. But then we needed some ideas from chemistry to exploit this further. The final idea was to introduce some chemical moieties with interacting functionalities on the backbone of a polymer to bring in the association effect. We created a shear-stable drag reducer by using hydrogen bonding as a tool, which led to an interpolymer complex formed when dilute solutions of two polymers bearing complementary proton-accepting and proton-donating functional groups were mixed^{76,77}. Zipped chains of the kind shown in Figure 12 were formed, with the 'zips' occurring due to hydrogen bonding. Such zipped molecules were far more shear-

stable and also provided 2–6 times higher levels of drag reduction.

The key point is that as CE scientists we had to take the clues from developments in polymer physics, perform an analysis based on a molecular model and finally shift to chemical synthesis of hydrogen-bonding-mediated systems to arrive at more effective systems. Remaining borderless or not shifting from 'analysis' to 'synthesis' would not have helped us to make progress. Of course, it is not that we claim that the problem of having shear-stable polymeric drag reducers is solved – but at least a modest beginning has been made.

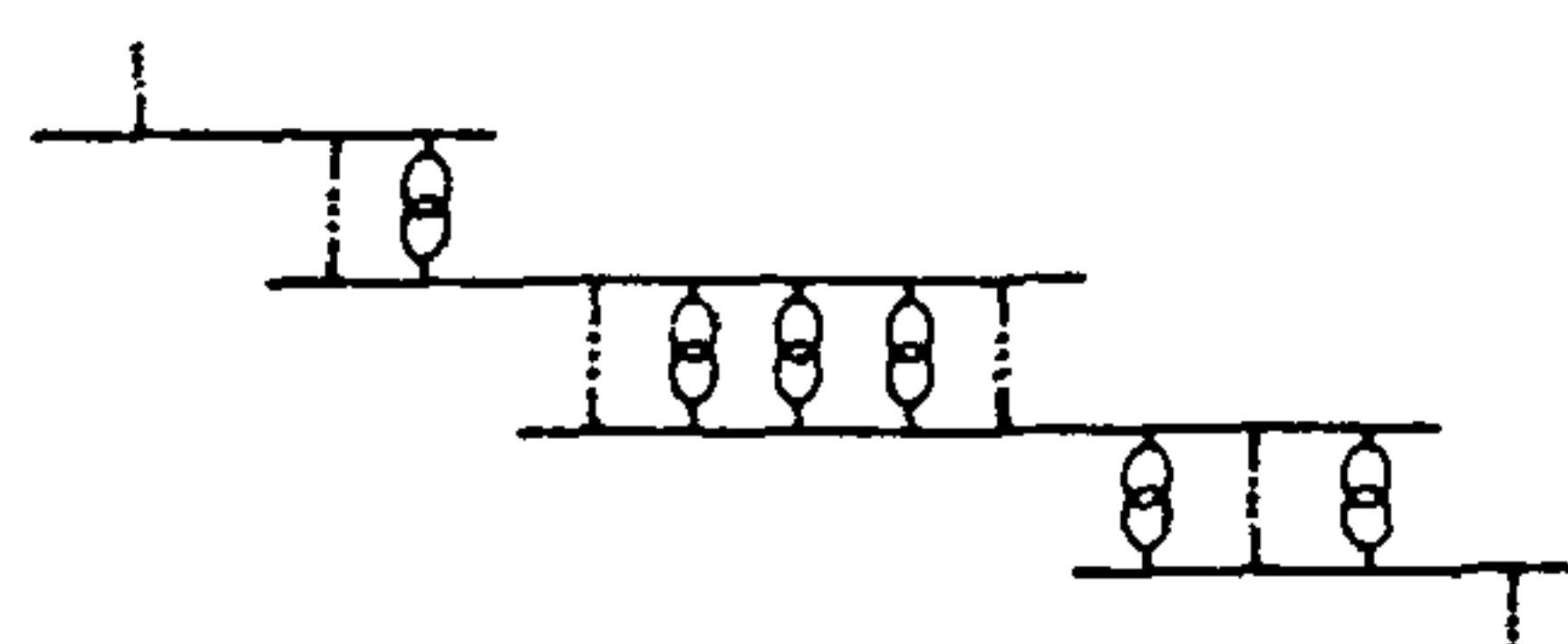
Creating the seamless chemical engineering science: Some concerns

I have spoken on seamless chemical engineering science. I have referred to how the boundaries between different disciplines of sciences as well as engineering science are vanishing today. How do we make this boundaryless world work though? Let me now discuss some of my concerns in this respect.

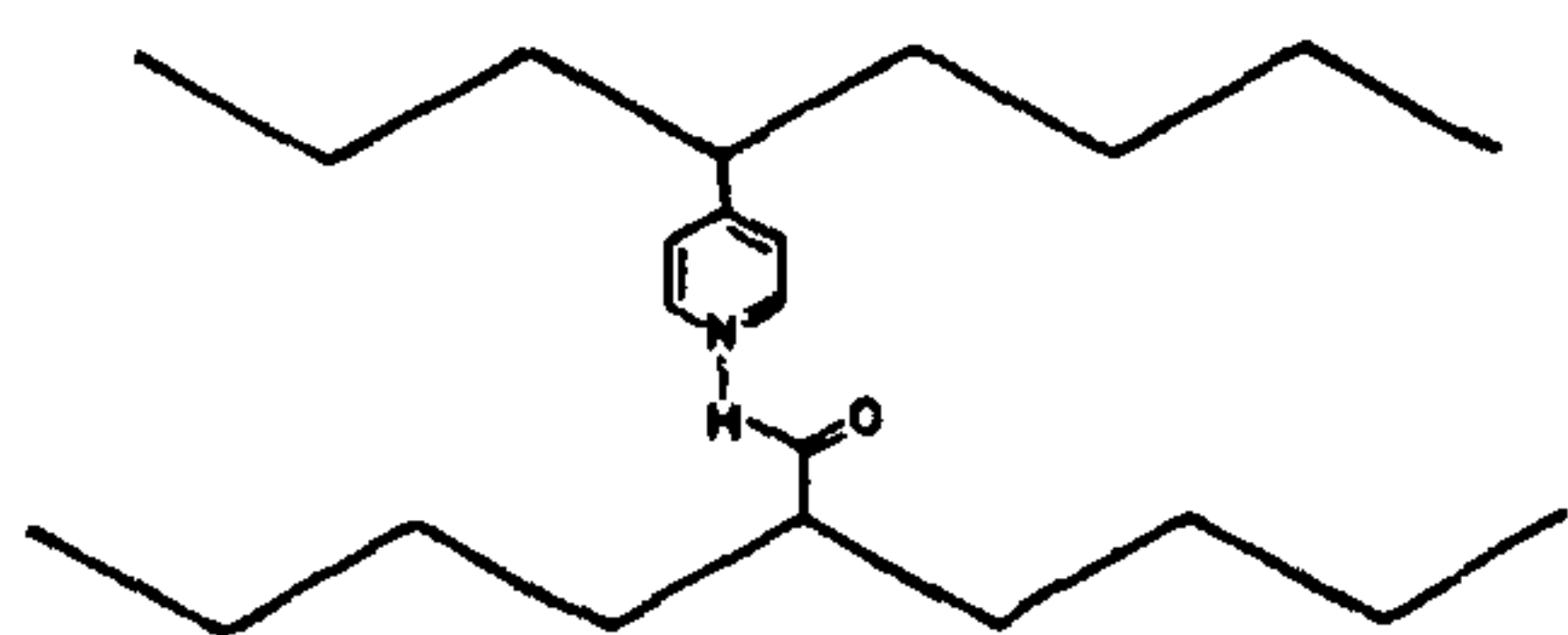
First of all we all live in a world of very high specialization. This automatically implies that we are continuously erecting our own new boundaries, creating our own small clubs and generating our own special language and jargon all the time. However, boundarylessness implies interconnectedness. There itself lies the contradiction! How do we take care of these contradictions?

Another problem is that of dealing with adjacent sciences, where new mergers are continuously taking place and new territories are being continuously built. How do we deal with a moving target? What happens, for instance, when chemistry itself starts merging its boundaries with other disciplines, such as biology, in a profound way? Let me explain my worries by giving a specific example of the way chemists are trying to meet the challenge of generating and identifying biologically active compounds for pharmaceutical developments. Here, ideally, one would like to have access to an infinite source of compounds, encompassing the entire realm of structural and conformational space, that could be screened rapidly for individual molecules with desired biological properties. Chemists have now moved to combinatorial methods in biology and chemistry, which are powerful methods for generating molecular diversity (Figure 13). One approach, light-directed chemical synthesis, combines semiconductor-based photolithography technologies with solid-phase organic chemistry to synthesize large arrays of molecules with potential biological activity. A CE scientist is then confounded with the prospect of dealing with a phenomenon of rapidly emerging area, where boundaries between several adjacent disciplines have vanished. How does he cope with this challenge?

18



STAGGERED STRUCTURES



HYDROGEN BONDING MEDIATED STRUCTURES

Figure 12. Design of shear-stable polymers by using hydrogen-bonding-mediated copolymeric structures, proton acceptor (containing 4-vinyl pyridine) and proton donor chains (containing methacrylic acid) create the staggered structures, which provide enhanced drag reduction⁷⁷.

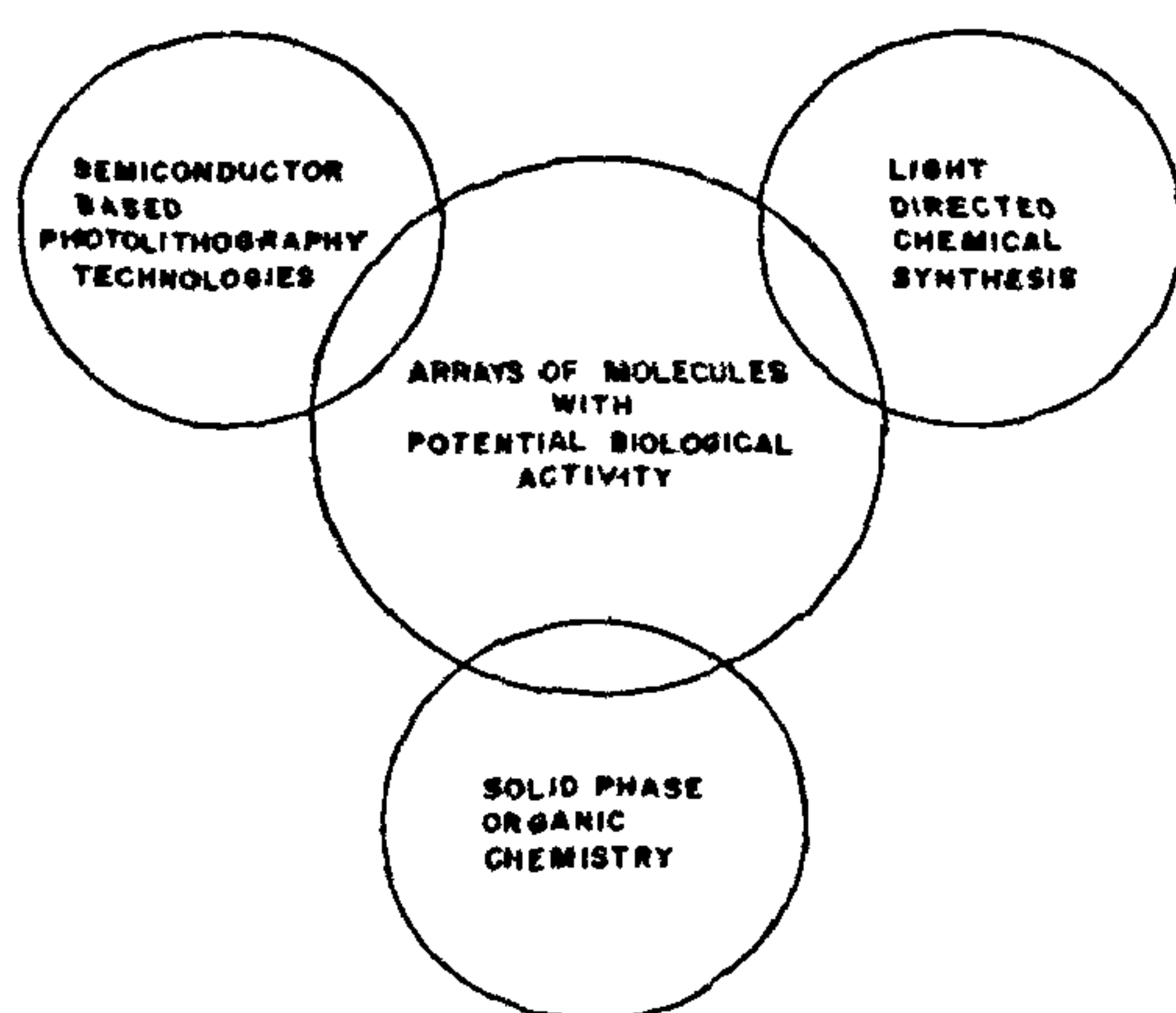


Figure 13. The principle of combinatorial chemistry, which combines diverse skills and technologies.

Then there is the problem of the language and the cultural barriers between different disciplines. Learning the language from another discipline and also teaching the language of CES to another discipline is not an easy job. Only those CE scientists who have dared to learn other skills and languages from adjacent disciplines will eventually make a mark. It also seems to me that interdisciplinary scientists will have to be great communicators too. They will have to constantly exchange information in a 'jargonless' way and also pass on their infectious enthusiasm by communicating well.

A CE scientist picks up tools and ideas generated in adjacent sciences and begins to publish papers in hardcore leading journals in chemical engineering. However, the elegance of the new tools or the sophistication of the new language may be mistaken for *novelty* and the problem solved may indeed be a trivial one. Many times a new tool from adjacent science, just because of its glamour value, may be applied to a trivial CE problem, which may not require that sophistication at all. This is misuse of tools and should be guarded against.

What are the forums for the presentation of results of research in interdisciplinary fields? Not many, I am afraid. More and more specialized clubs are mushrooming with little or no interaction between them. I saw someone make a suggestion that in a CES symposium dealing with an interface problem with other sciences, we should invite some scientists who may be able to give an alternative viewpoint. However, he was promptly turned down. Have we become too parochial? Will we be able to make progress if we continue this way?

We have another problem of peer recognition for those who work in interdisciplinary areas. As someone

involved with the election of the Fellows of the National Academy of Science and National Academy of Engineering, I have found that engineers and scientists who are working on borders or trying to fuse these borders end up in difficulty in seeking recognition. Invariably, they fall between stools. Thus, somebody working in biomedical electronics does not get considered in either medical sciences or engineering sciences committees. Where does he go then? This is truly demotivating. The academies will have to recognize this problem and evolve special ways of solving these problems.

Many chemical engineering departments have recognized today the importance of having basic scientists with training and research experience from non-CE areas, be they in natural sciences or other branches of engineering. Thus, a chemical engineering department might employ an NMR specialist or a solid-state chemist. Sometimes the cultural and language barriers posed before these new entrants create great difficulties. A long time passes before they are accepted as part of the family. While speaking to some of them, it became clear to me that they also face difficulties on acceptance in academies or professional bodies. For instance, a physicist specializing in NMR in a chemical engineering department and applying NMR for solving problems of interest to chemical engineers does not get accepted as a Fellow of the Institute of Physics. At the same time the concerned Institute of Chemical Engineers also turns him down because it looks at his basic qualifications and finds that he is a non-chemical engineer! What a penalty to pay for working on borderline areas! Should not our professional bodies reexamine this and take new and bold approaches?

Then there is the question of how far does an engineering scientist go. There are some shining examples in our profession. Mark Davis from Virginia Polytechnic was educated as a traditional chemical engineer. He did his PhD in kinetics and mathematical modelling. He wrote a book on numerical methods for chemical engineers. Then he contributed to the synthesis of zeolite A containing a transition metal. He exploited the use of ESR in the study of zeolites. Finally, he succeeded in synthesizing zeolite VPI-5, the first 18-ring opening crystal, which sparked off a renaissance in zeolite synthesis! A CE scientist is so well endowed due to his training that, if he dares to learn, he can conquer many territories. Extending this theme, I have reconsidered (Figure 14) the molecular heterogeneous hexagon conceptualized by van Santen⁷⁸. It is clear that CE scientists will invade this hexagon in years to come with telling results!

With the boundaries between engineering science and science themselves merging, some basic conflicts are likely to arise. What is the role of an engineer and what is the role of a scientist? To my mind, a scientist 'explores', whereas an engineer 'exploits'. I looked for a

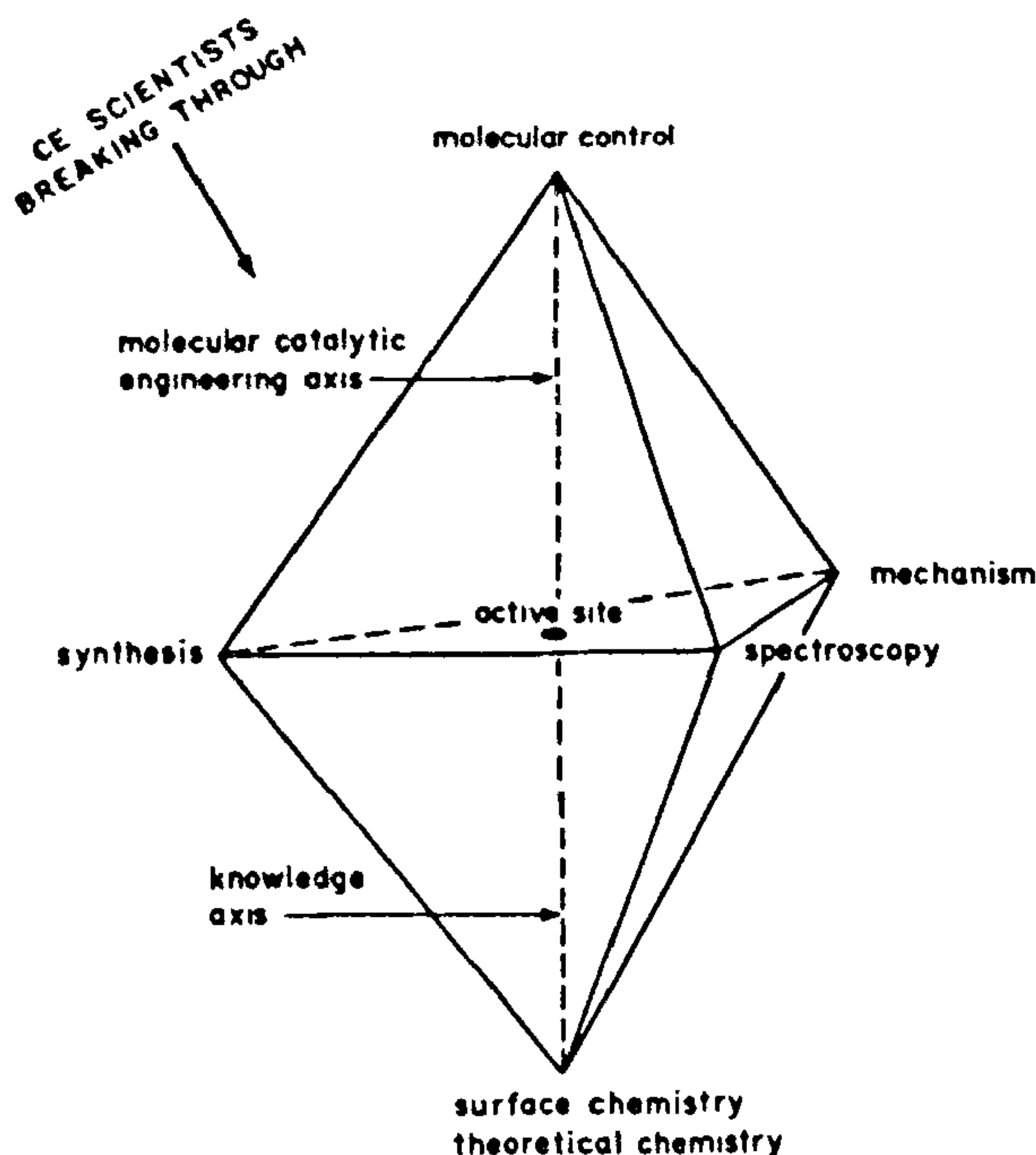


Figure 14. Molecular heterogeneous hexagon model due to van Santen⁷⁸. Note the entry of CE scientists into this hexagon.

good definition of a scientist. I found one provided by Sir Peter Medawar. He says: 'A scientist is one, who weighs the earth and ascertains the temperature of the sun. He destroys matter and invents new forms of matter and one day he will invent new forms of life.' Then I looked for a definition of an engineer and found one given by Eric Laithwaite. He built on Sir Peter Medawar's definition and said: 'An engineer is one who uses the earth and tries to capture the sun's energy more effectively. He controls the rate of destruction of matter and tries to find alternative sources of energy and new materials. He invents new shapes of matter and strives to improve the quality of life in whatever form he finds it.' The basic goals of exploration and exploitation could not have been spelt out more clearly.

And that is precisely the problem that I am more concerned with. How does a CE scientist ensure that rather than getting possessed by the new tool that he has picked up and rather than spending all his research career on sharpening and refining this tool, does he bring benefit to the profession by using this tool in problem solving? Let me illustrate this point by going back to my early remarks about nonlinear dynamics and CES-physics interface.

Coupling between different nonlinear systems to bring about synchronization of states holds significant promise for future technology developments. Already, a few examples of the use of these concepts have emerged. Con-

sider the spectacular success in enhancing the power of lasers by coupling them under chaotic conditions. In spite of the scores of papers on deterministic chaos, why is it that the CE scientists have not directed their attention to using this powerful technique to bring in similar spectacular results by, say, coupling chemical reactors? Here one is almost reminded of an inventor who endlessly refines his models but shies away from making a start for the fear that the real thing will not fly!

The challenges of the future will have to be met through both continuity and change. CES will extend itself, on the one hand, to the molecular focus of microscale processing and, on the other, to macroscale integration of processes and systems. Enormous flexibility and bewildering breadth have been the cornerstones of CES. However, the demand for enhanced flexibility in our approaches will be even higher in the coming years. The role of a CE scientist in this regard will be most crucial. He will have to be both very daring and innovative. In order to search for new tools and ideas, he may have to travel to the depths of the seas, climb new heights of the mountains, or he may have to go deep into the forests. If he does not dare to learn from other disciplines, then he will not be able to bring these jewels – these new ideas. The experience is that whenever this has happened, the results have been rewarding. Beckett *et al.*⁷⁹ borrowed the 'cold extrusion' idea from plastics and successfully applied it for the first time to milk chocolate, which is always melt-processed. This has opened up now endless possibilities of using plastics-processing techniques in chocolate processing. A CE scientist must not only dare to learn but he must also learn to dare.

Continuous improvements are fine – but discontinuities in knowledge create new technologies and that would not happen unless he dares. And most crucially, unless a CE scientist is himself 'boundaryless' and believes in seamless CES, all this will not happen.

Let us again remind ourselves that the word 'engineer' comes from the French word 'ingenieur', which literally means 'an ingenious one'. To my mind, our ingenuity of exploring the new tools of knowledge from adjacent disciplines is going to be the key to our success. Finally, I would like to repeat the inspiring inscription on the Lamme Medal of The Institute of Electrical and Electronics Engineers, USA, which simply says: 'The engineer views hopefully the hitherto unattainable.' I firmly believe that it is in this new seamless world of chemical engineering science that the CE scientists will not only 'view' the unattainable but also 'attain' the unattainable.

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