

New directions in chemical engineering *

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Abstract

Chemical engineering has a liberal base and is multicultural. The contents of chemical engineering science keep on changing in response to needs. The new chemical industry will demand safer and cleaner processes and 'selectivity engineering' will occupy a pivotal position demanding new homogeneous and heterogeneous catalysts and newer strategies in operating reactors. Separation processes have to be fine tuned for super-purity materials and hybrid systems, and reactor-separator configurations will become more important. Interfacial engineering will demand more attention. Biotechnology will become increasingly important and chemical engineers have to develop new strategies for recovering valuable chemicals from dilute streams.

Key words: Selectivity engineering, combo-reactor-separator, separation technology, membrane processes, interfacial engineering, biotechnology.

1. Introduction

The chemical industry occupies the centre stage in meeting the basic needs and desires of the society. The role of chemical engineering is crucial in our society. We hardly had any chemical industry before independence and our growth was very impressive in the 1970s and 1980s. However, at the present stage, we are very much behind developing countries like China and Brazil, as is evident from the per capita consumption of important chemicals, plastics, rubbers, synthetic fibres, etc. Even in the case of drugs, our per capita consumption is dismally low. Further, China has done very well in the development of indigenous technology and in the absorption of technology.

Most of the growth of the chemical industry has been based on imported technology, sometimes of repetitive nature, and there has been feeble in-house R&D and process design support. However, in recent years technocrat-based companies,

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particularly for speciality chemicals in pharmaceutical, agrochemicals, etc., have done a commendable job through in-house R&D and in some cases we can claim to have pioneered unique processes which are globally cost effective. Although the inputs into R&D in industry have improved, these are far behind contemporary figures globally for this highly science-based industry. The research in academia, as measured, for instance, by the number of doctoral theses in chemical engineering, has also been limited and there are only four or five schools of international standing.

The stimulus for research in applied sciences like chemical engineering comes from real problems and yet we need the cutting edge of science to solve problems. We cannot get too close to the art of practice as without the application of sound theoretical principles it would be sterile. Our research has to be justified on the basis of possible, and not fortuitous, linkages with industry. It would be appropriate to say that chemical engineering science (CES) is linked to the aspects of science developed by chemical engineers for their own purposes in fields not covered by other branches of technology.

The contents of CES keep on changing in response to changing scenarios in industry and to new scientific discovery. Thus, for instance, the enactment of environmental regulations alone has brought out a sea change in our work.

Since inception, chemical engineering has been characterised by a liberal base and is multicultural just as the chemical industry is polygamous and also an enabling industry. Chemical engineering continues to be an evolving discipline and it has the versatility to be tuned to micro or molecular level, meso or equipment scale, as well as to the macro-scale integrated plants. The orchestration of disparate subjects into a coherent theme is a special trait of chemical engineers. Chemical engineering continues to occupy the vital position to fill the gap that exists between natural sciences and the primary, physics-based discipline of mechanical, electrical and civil engineering. Chemical engineering is also uniquely placed in interfacing with biology and chemistry to convert inventions in biological sciences into innovations.

It would be desirable to note some important characteristics in the chemical industry (CI). We should recognise that no process is literally ever mature. The 75-year old ammonia technology continues to witness new developments which are largely engineering oriented and this is evident from the drastic reduction in energy consumption per tonne of ammonia and this is now approaching the theoretical figure. We should also declare that no process stream is a waste and we should treat this as a feedstock with a negative price and convert the liability into an asset. We would need cleaner and safer processes, independent of the incessant pressures of well-motivated environmental groups. We would have a strong driving force to convert very high pressure processes to low pressure ones and some spectacular successes, like in making linear low-density polyethylene, have been witnessed. We will need more friendly and 'robust' processes while approaching the concept of zero effluents. We will need intrinsically safe processes. The demands on separation processes will be very different in view of the requirements of ultra-high purity products and the need

to process dilute streams coming from biotransformation units. Since more than 70% of organic chemicals get linked to high polymers, getting more from known polymers through blends and alloys will demand more expertise in polymer physics. Our climatic conditions demand more friendly synthetic fibres, particularly polyester fibres and blends.

2. Selectivity engineering

A new area of 'selectivity engineering' is emerging which, through better catalysts and more rational operating strategies, allows highly selective synthesis¹. This is becoming all the more important in pharmaceuticals and agrochemicals due to the clear needs of having optically active material and avoiding the ballast of the unwanted isomer. This would demand newer processes, involving very innovative catalyst, and new methodologies in separations. We would need to evolve designs of small reactors, such as nozzle reactors, and get used to micro-engineering of small volume, high-value products. Along with the desire to have highly selective processes, it is becoming increasingly attractive to 'telescope' the number of steps in synthesising speciality chemicals.

The role of micromixing, even in single liquid-phase reactions, where the mixing and reaction times are comparable, needs to be more intensively studied as this affects the yield of unwanted products².

3. Process intensification

Process intensification will be yet another area which will receive increasing attention as this would allow smaller reactor/separator to be used. Consider the unusual demands that are placed on designers in offshore platforms where membrane separators or adsorbers may score over absorption-based separations. Intensification of heat transfer coefficients can lead to a substantial reduction in the area required for a specified duty.

4. Energy consumption: Combo-reactor-separator

The net energy consumption per tonne of the product will have to be reduced and in this context the strategy of combo-systems³, *i.e.*, reactor and separator as one unit, will gain momentum and demand new engineering practices. Thus, anionic polymerisation, which requires scrupulously dry conditions, allows the mixture of styrene and ethyl benzene, obtained from the dehydrogenation reactor, to be used and ethyl benzene can be recycled. Furthermore, in this type of polymerisation no unpolymerised monomer can exist thereby removing one of the specific points against the use of polystyrene in foods and pharmaceutical areas. For ethyl benzene itself, zeolite catalysts allow the use of lean ethylene from a variety of sources and ethane can be recycled. In areas where the per pass conversion is low due to reasons of selectivity associated with easier degradation of the wanted product the deployment of a membrane, which allows selective permeation of the desired product, can bring about an important change.

The recent success in making methyl *tert*-butyl ether in a distillation column reactor, where the heat of the etherification is gainfully employed for distillation, and where the ion-exchange resin beads provide the material for packings, has opened a new chapter in combo-reactor-separator. This will be extended to methyl *tert*-amyl ether and *tert*-butyl alcohol. Pilot-plant experiments have been reported for ethyl benzene and cumene, using zeolite-based catalysts, and here the heat of alkylation is utilised for the distillation of benzene. We need elaborate studies in such systems; we should recognise that the products have to be very pure and the content of close boiling components is often specified at ppm level.

In the case of dehydrogenation reactors, selectively permeable membranes (inorganic for higher temperature application) can lead to getting over equilibrium limitations and will lead to a substantial reduction in the energy consumption and possibly an improvement in the yield of the desired product. Ceramic and metallic membranes are expected to be robust and should be capable of performing at high temperatures over prolonged periods. We can also control the porosity. Thus, dehydrogenation reactions could possibly employ a Pd-based membrane which is highly permeable to hydrogen and on the other side, if required, air or O₂ can be used to oxidise H₂ to water. This will facilitate hydrogen permeation and provide heat of dehydrogenation as the membranes can be made conductive. We need to engineer such systems on a sound basis.

5. Role of chemical reactions⁴

Chemical reactions have been an important forte of chemical engineering as other branches of engineering have limited dealings with this subject. This is a niche area of great value and would demand greater attention in the area of science and engineering of homogeneous and heterogeneous catalysis. How to tailor-make a catalyst? The examples of the three-way catalyst for automobile exhaust, an altogether different area, can be cited as an outstanding contribution.

The example of ultra-active Ziegler-Natta catalysts for bulk polymers, high-density polyethylene and polypropylene, produced on a grand scale exceeding 35 mtpa, stands out as a remarkable example as the amount of the catalyst is so small that washing of the catalyst can be obviated⁵. These developments have brought in their wake new design features of large-size polymerisation reactors. Chiral synthesis is now demanding attention and the success in making L-DOPA, which has surpassed the performance of enzymes, can be referred to as a good example⁶.

The electronics industry, which is growing at a very rapid rate, demands extraordinarily pure materials and here new strategies in separations, which are benign on energy consumption have to be evolved.

6. Indigenous technology

We in India are short of capital in view of demands from many sectors. The availability of indigenous technology can itself act as a capital with a big 'C', apart

rom having know-how and know-why. Technology is really the most expensive equity capital. Indeed, we need to develop some 'exclusive' technologies to gain bargaining power. In recent years, there have been an increasing number of cases of denial of technology and this has forced us to adopt old and outdated technologies to our detriment or to depend on the import of the product. It may be noted that half of the scientists and engineers involved in research and development in industry in USA appear to be either chemists or chemical engineers.

7. New demands on CI

We need to recognise that, so far, much of the CI has been essentially product oriented but the future will surely see a transition towards a function oriented industry where integrated ranges of products and services will be required rather than merely supply of particular chemicals. Consider the simple case of water treatment where we need 'services' rather than just one chemical. Similarly, take the electroplating industry where we will need the entire gamut of chemicals including strategies for the treatment of waste liquors. Can we, for instance, recycle sodium cyanide or other cyanides? Some recent work involving membranes seems to show promising results. The wastewater treatment as a whole requires a 'function-oriented industry' approach. Many times the quality or the efficacy of the product is finally approved only on the basis of the function such as pour point depression in transportation of crude oils, particularly heavy waxy crude oils.

The future of the CI will also be guided by the new possibilities in molecular biology. Environmental concerns will dominate and there may well be insistence on safer processes. The breakthroughs in genetic engineering will also need a very different kind of scrutiny from safety point of view. Chemical engineers will have to adapt themselves to these new unfamiliar areas.

The emerging areas in material science of engineering ceramics, superconductors, supermagnets, etc., will place new demands on chemical engineers but they are well placed to utilise their multicultural attributes.

The penchant to get more from less will have to be intensified and the role of controlled release technology for drugs, agrochemicals, fertilisers, etc., will become prominent. The traditional expertise of chemical engineers in the role of diffusion in a host of processes/operations will be exploited in a meaningful way.

A more mundane guiding principle will be changing trends in raw material prices, notably methane *vs* ethane/propane/butane *vs* napath *vs* gas oil; large availability of C₅ and C₆s, due to changing specifications of motor gasoline, can be foreseen.

8. Replacement of processes/operations involving hazardous or toxic chemicals with 'safer' processes/operations^{1,4}

There will be incessant pressure to adopt safer processes. Thus, whenever phosgene can be replaced this may well be insisted upon. We in India have pioneered the

non-phosgene route for the well-known wheat weedicide, Isoproturon, where urea reacts with *p*-cumidine in the presence of dimethylamine (in the established process *p*-cumidine is reacted with phosgene to give the isocyanate which in turn is reacted with dimethylamine). Methylisocyanate (MIC) is already a taboo and no amount of scientific reasoning will convince local and national bodies to allow its use. There will be an intensive drive to make polycarbonates and urethanes without phosgene. In the existing phosgene-based plants, new strategies have been developed for safer operation through methods like 'on-demand' generation of phosgene (and hence no storage) followed by quick response disaster mitigation methods, including the use of ammonia curtain around the plant.

There will be demand to replace HCN-based processes and we already have the classic example, thirty years ago, of ammoxidation of propylene for acrylonitrile to supersede the HCN-based processes. It is ironic that HCN is obtained as a by-product in the ammoxidation process. Similarly, methyl methacrylate can be made from isobutylene and the HCN + acetone-based process can be supplanted.

The manufacture of adiponitrile from butadiene and HCN, which involves anti-Markownikoff addition, can be replaced by electrohydrodimerization of acrylonitrile or from adipic acid and ammonia. Even in the case of adipic acid, which is usually made by liquid-phase oxidation of cyclohexane, under somewhat hazardous conditions, attempts are being made to have selective dimerization of methyl acrylate to dimethyl ester of the adipic acid precursor hexenoic acid (acrylic acid itself is made by direct air oxidation of propylene in a two-stage reaction system). The carbonylation of butadiene, in the presence of methanol, to give dimethyl adipate is yet another candidate process.

It is good to remember that even after major developments in mercury cell-based caustic soda/chlorine plants, which leads to a design which meets the statutory regulations, its adoption is not favoured and there is insistence on membrane cells which brought in its wake many developments for the first time. Thus, saturated brine is required to be purified with respect to Ca and Mg ions down to ppb level and ion exchange resins with very specific chelating agents had to be developed.

In pharmaceutical and speciality chemical industry, wherever sodium metal in ammonia is used for reduction, attempts will be made to use electrochemical or other selective reduction processes. Similarly, whenever Grignard's reagent is used, attempts will be made to develop alternate processes. Small-volume high-price chemicals which are made *via* batch processes, involving hazards, will see transition to continuous processes where the reactor can be operated adiabatically with pre-cooling of reactants.

Wherever mercury salts are used as catalyst, *e.g.*, alpha sulphonation of anthraquinone for making alpha aminoanthraquinone, alternate processes will be developed.

The use of chlorine for bleaching in pulp and paper industry is under attack and we are looking for 'Mr Clean' and it seems hydrogen peroxide is in great demand (a reference will be made later about the recent breakthrough in making H₂O₂).

A number of alkylation reactions, notably the alkylation of isobutane with isobutylene/butenes/propylene to give alkylates for motor gasoline, benzene with lean C_{12} linear olefin for linear alkyl benzene (LAB), are conducted on a very large scale and hydrofluoric acid is used as a catalyst. There is pressure to change this and for alkylates required for motor gasoline, the use of sulfuric acid is once again in demand and there is an intense activity to develop zeolite-based catalysts. In the case of LAB, there is hope of using zeolites as catalyst and even cationic ion exchange resins could possibly be used advantageously. The use of oleum for sulphonation, particularly the purchased one, is being discouraged and on-site generation of lean SO_3 is recommended. This calls for new effective designs of small SO_3 plants where lean SO_3 is made available 'on demand'.

Chromium salts have been used as oxidants when other benign oxidants do not seem to work. Here, apart from building alternative oxidants, a total recycle, *via* electrochemical oxidation, has been successfully implemented. Similarly, in water treatment systems for cooling towers, the use of chromium salt has been supplanted with newer safer chemicals.

Arsenite-activated potash solutions for CO_2 removal in fertilizer plants were very popular in the 60s and the early 70s. Even though plant designs had been tightened and As in effluents was kept below the statutory limits, it became necessary to replace this with diethanolamine (or some other amine or amino acid) activated potash solutions. The key point to bear in mind is that the additives must be intrinsically safe.

The oxidation of cyclohexane to cyclohexanol/cyclohexanone involves potentially hazardous conditions and it is well known that after the Nypro accident in UK, the local authorities did not allow this process to be adopted and selective hydrogenation of phenol was recommended. Can we not have a much safer process apart from that based on phenol? The recent work on selective hydrogenation of benzene to cyclohexene/cyclohexane opens up a new safer process as direct hydration of cyclohexene to cyclohexanol is possible.

The replacement of the existing range of fluoro-chlorocarbons, used as refrigerants, blowing agents, etc., which were heralded as a major development in yesteryears, with ozone-friendly compounds has acquired worldwide attention of even politicians. This calls for skills in fluorine chemistry, thermodynamics, kinetics, etc., in uncharted areas. Indeed, it also provides an opportunity for chemical engineers to model the global reactor.

Whenever it is suspected that an intermediate compound is carcinogenic, there is a demand to look for alternatives. We need to plan this in advance and preempt many problems. Thus the conventional process of chloromethyl ether, which contains carcinogenic dichloro derivative, can be replaced by a process based on the reaction between HCl and methylal when the carcinogenic compound is not obtained.

The replacement of processes based on acetylene, which involve hazardous copper acetylide or related materials, has also drawn attention. Thus, 1,4-butanediol,

tetrahydrofuran, etc., can be made *via* low pressure hydrogenation of maleic anhydride. Even chloroprene can be made from butadiene supplanting the use of vinyl acetylene, which in turn is made from acetylene. There will be further demands on finding safer processes.

9. Replacement of high pressure processes with low pressure processes¹

The operation of plants at very high pressures poses many problems in design and safety. There is an ever-increasing demand to find alternatives and an early example was that for hydroformylation (oxo-reaction) reaction for converting olefins to primary alcohols. Here, the use of rhodium phosphine-based ligands allows pressures to be as low as 30 to 40 atm, compared to 200 to 300 atm in the case of the cobalt-based catalyst⁷. Even in the case of cobalt-based catalyst, modifications with phosphine ligand have allowed pressures to be as low as 30 to 40 atm. The carbonylation of methanol to acetic acid, which earlier required pressures approaching 1000 atm, can now be operated at 40 atm. This was preceded by the new low pressure (40 to 60 atm) process for methanol which supplanted the older process which operated at pressures 200 to 300 atm. Thus, the pressures in methanol and acetic acid plants are comparable and integration is possible.

The case of linear low-density polyethylene stands out as an outstanding example where the new process requires 40 to 50 atm compared to over 3000 atm in the older process.

The manufacture of ammonia is now receiving attention so that pressures could be around 75 atm, and with modifications in the reforming of methane/naphtha to make syn-gas utilising enriched O₂, pressure may be synchronised and the compressor may well be eliminated.

Thus, chemical engineers will be required to think afresh in process designs, integration of different parts of the plant, etc., and make processes work under friendlier conditions. The synthesis loop in the ammonia reactor was heralded as an engineering marvel in the 1910s.

The design of storage vessels for ammonia, ethylene, etc., has been changed and the current practice is to have atmospheric pressure, low temperature facility which is intrinsically safer. Such designs bring in new strategies and further penetration of this kind can be expected.

10. Catalysis, reactors and reaction engineering^{1,4}

It seems most likely that the science of catalysis will shape the technology. Thus chemical engineers should become, at least, bicultural and get into the innovation cycle and work and compete with 'purists'. It will be necessary to make quantum jumps through 'discontinuities' to have breakthroughs. Thus, for instance, would it be possible to convert methane directly to methanol, which is not only important by itself for conversion to MTBE, as a fuel, raw material for acetic acid, etc., but can

be very easily dissociated to CO and H₂ to provide syn-gas for ammonia and other purposes? Alternatively, would we succeed in making ethylene directly from methane? We already have zeolite-based catalysts to convert methanol to olefins and then to aromatics or middle distillates. Would it be possible for us to develop a catalyst which will allow low temperature dissociation of NO?

We can expect newer oxidation reactions with 'Mr Clean' H₂O₂ or *tert*-butyl hydroperoxide (TBHP), including activation of alkanes. The 'discontinuity' in the science and practice of catalysis is evident from the direct conversion, in liquid phase, with noble metal catalyst, of hydrogen and oxygen to make hydrogen peroxide⁸. Here, apart from the design of the ingenious catalysts, articulate design of reactors is called for. The use of TBHP is expected to expand vigorously as this is a cheap source of 'peroxide O' and *tert*-butanol can be blended with gasoline directly or *via* isobutylene and MTBE. The asymmetric epoxidation of allylic alcohols, with TBHP and Mo/Ti ligands containing optically active tartaric acid, has opened up new vistas and optically active glycidol is now commercially available. The epoxidation of propylene with TBHP with heterogeneous Ti-based catalyst was itself an important breakthrough. The use of sodium perborate, obtained from H₂O₂, as an oxidant will merit attention. Further use of aqueous sodium hypochlorite as an oxidant will be explored.

The use of butane/isobutane as a raw material will expand. We will have to develop expertise in selective dehydrogenation/oxidative dehydrogenation of ethane/propane. The dehydrogenation reactors will demand much greater expertise and reliability in continuous catalyst regeneration (CCR) units. Non-zeolite molecular sieves are expected to be developed. The possibilities of using zeolites to coax isobutylene to react with ammonia to give *tert*-butyl amine exist.

The use of zeolites in making speciality chemicals, *via* liquid phase processes, will gain momentum. The hydroxylation of phenol with H₂O₂ to give catechol with Ti-silicate stands out as a good case⁹. Selective chlorination, nitration, etc., stand to benefit and both analysis and design of such units will demand attention.

The breakthrough realised through metathesis reactions, which may well be described as an elegant example of chopping and stitching or scrambling of molecules, should be pushed further to make value-added products.

A reference was made to the new generation Ziegler-Natta catalysts. The design and operation of large-size fluidised bed polymerization reactors to make LLDPE, HDPE, and even flexomers (ethylene-propylene rubbers, including those containing dienes), requires much more systematic study.

In recent years, homogeneous catalysis, based on newly acquired skills in coordination chemistry, has made a major impact through oxidation, oxo-reaction, carbonylation, oligomerization, etc., reactions. We can expect further improvements. Thus, for instance, catalysts and reactor design will be modified to give the wanted C₄ to C₁₈ alpha olefins in oligomerization of ethylene. It is good to recollect that Mond gave wings to Ni *via* volatile carbonyl and we can now expect, through proper

ligands, novel uses of Ni catalysts and success is evident *via* 'ligand tailoring' to convert butadiene to 4-vinyl cyclohexene or 1,5-cyclooctadiene. Perhaps enantioselective dimerisation of olefins like styrene and ethylene to give (R)-(-)-3-phenyl-1-butene will gain momentum. In fact, the general area of enantioselective hydrogenation, oxidation, epoxidation, carbonylation, etc., will require much greater attention.

Homogeneous catalysis lends itself to molecular modelling and further work will be necessary. Can we arrive at a better catalyst *via* identifying possible catalytic mechanism?

Phase-transfer catalysis has made a great impact in speciality chemicals. Attention will be given to find catalysts which are stable at higher temperatures and can be recovered and recycled. Enantioselective synthesis will also be studied.

The role of modern spectroscopic and other methods has been crucial and this will gain momentum through the use of FT-IR, solid state NMR, ESCA, etc. The success achieved with the systematic study of functioning of Pt/Rh gauge catalyst for oxidation of ammonia to NO, ammoxidation of methane to HCN, etc., will give further impetus. The manner in which noble metals have been dispersed on catalyst supports has reduced the inventory to a much lower level and further improvements can be expected. The use of Raney nickel in pelleted form in fixed bed reactor may gain momentum. These call for a systematic study of engineering of catalysts as was the case with the major breakthrough in reforming of naphtha and low pressure synthesis of methanol.

Catalysis by enzymes, particularly exploiting two-liquid-phase systems, will need more intensive studies in view of mild operating conditions and high selectivity. It appears that the main field of application will be speciality chemicals. We will need to introduce 'switches' in enzymes and fine-tune their activity. We should tinker with their function and we can look for 'imprinting' common proteins to turn them into selective artificial receptors. Innovative approaches will be required for the design of bioreactors for plant and animal cells which would be shear free. Chemical engineers, including biochemical engineers, have not made an impact in this area comparable to the other areas of catalysis. The 'bicultural' character will have to be strengthened.

11. Separation technology³

The well-established separations based on distillation, absorption, extraction, crystallisation, etc., are now approaching the upper side of the 'S' curve and very intensive efforts are required to make improvements. Thus in distillation a more vigorous approach is required for the design of tray columns. A neglected area is the performance of columns with respect to removal of impurities which is vital to the process. A reference has been made to study combined distillation column reactors. The role of second liquid phase, particularly in packed columns, demands further studies.

The performance of liquid and gas distributors for packed column needs to be studied further. Can we come out with still cheaper structured packings? The performance of columns at conditions close to supercritical, like in demethaniser, needs to be studied.

It is interesting that many of the established operations are orchestrating together and the role of hybrid processes is being increasingly appreciated. Thus companies which had expertise in low-temperature fractionation of air moved into adsorptive and membrane separations. The optimisation of flowsheets, incorporating hybrid processes, will demand attention.

The marriage of different separation processes can be seen in having 'reactive' Cu exchanged zeolite adsorbents for the removal of CO from inert gases (*i.e.*, in the absence of oxygen)¹⁰. Reactive membranes are being considered even for resolution of optical isomers.

The use of hollow fibre membranes as dispersionless extractors¹¹ is gaining momentum, even in biotechnology, and we need very systematic studies including an unambiguous assessment of effective area of contact and values of mass-transfer coefficient that are realised. Hollow fibre membrane absorbers have also been considered.

The selection of solvents in liquid-liquid extraction¹², where temperature swing can be used to remove the major amount of solvent from the extract phase, needs to be studied. The use of aqueous solutions of hydrotropes for extraction merits attention. Further improvements in supercritical extraction, including the use of entrainers, can be foreseen.

Engineering of adsorbents, as seen through the success of zeolites and carbon molecular sieves, should be studied. Thus novel adsorbents have been recently developed which can remove malodorous compounds in a very elegant way.

Novel 'structured' absorbents, such as those based on the use of cyclodextrins, need to be developed.

The use of ion-exchange resins, which have long life in aqueous environment, with specific chelating agents will gain momentum and demands further study. The removal of Ca and Mg from saturated brine to ppb level has been an outstanding success, apart from demineralisation of water to remove dissolved solids to ppb level. The recovery of metal ions from lean solutions is an area of importance.

In the area of crystallisation, direct contact operation merits study. Reaction crystallisation is yet another area. The use of population balance method brought a whiff of fresh air in this area and modelling of crystallisers is now more systematic. However, the tailor making of crystal size distribution and avoiding inclusion of impurities merit further attention, in this area of 'molecular engineering'. The resolution of racemic mixtures in special fluidised conical bed crystallisers, without using external reagents, ought to be studied very intensively.

Membrane separations merit further attention, particularly with respect to inorganic membranes which can be used at higher temperatures and in biotechnology

area these can be sterilised. Can we tailor make membranes and manipulate operating conditions to avoid fouling? The recent success of pervaporation in dealing with azeotropes, like ethanol-water, isopropanol-water, to give anhydrous organic component has been impressive¹³ and this further lends support to 'hybrid' processes¹⁴. The role of pervaporation in dealing with systems like acetone-water, where water content has to be reduced below 1%, to a level like 0.1%, needs to be more intensively studied. Here no azeotrope is formed but capital and recurring costs are very high due to a large number of theoretical stages and need to have high reflux ratio. Membranes containing liquid crystals are being considered for separating butane/isobutane and this will be a remarkable feature.

The development of 'hot' membranes is still in a nebulous stage. The impact of such separations can be great as the operating conditions of the chemical process and the separation process can be synchronised. Consider the ammonia loop where per pass conversion, at about 450°C and pressure of 90–150 atm, is in the range of 10 to 16%, the removal of ammonia at 450°C will bring about a dramatic change in the technology.

The deployment of temperature-sensitive gels, particularly in biotechnology, has not yet been demonstrated in the market place. Affinity chromatography and aqueous-aqueous extraction have been found to be useful in biotechnology and further studies are necessary.

The strategy of combining reactions with separations has been outlined earlier. The exploitation of reactions, in a highly selective way, by the ingenious chemistry and manipulation of operating conditions, has been poor. The most well-known example is the separation of isobutylene from butene *via* methyl *tert*-butyl ether (MTBE)¹⁵ and this is practised on a scale of about 8 mtpa of MTBE. Isobutylene is separated only by chemical methods. Similarly, isoamylene is recovered from the C₅ fraction *via* reaction; cyclopentadiene is also recovered from the C₅ fraction *via* reaction. Other known examples of separation of close boiling substances like *m*- and *p*-xylene, *m*- and *p*-cresol, etc., still continue to attract attention. The availability of novel-structured zeolite catalysts, ion-exchange resins, pillared clays, etc., should be fully exploited. Consider the case of the separation of α - and β -naphthol. Here alkylation (*O*- and *C*-) with isobutylene has been exploited to separate the two isomers¹⁶.

Separation processes face their acid test when it comes to dealing with liquid effluents. This area is of vital importance as explained earlier.

12. Interfacial engineering

This area is pregnant with many challenges over a broad front. Even in the area of materials (*e.g.*, thin film coating in microelectronics, in advanced ceramics, etc.), we need to take greater interest. Recent studies, with advanced analysis based on a variety of spectroscopic data, have opened up new frontiers in emulsions,

microemulsions, etc., which have many important industrial applications. Thus the whole area of emulsion polymerisation, which now includes the use of microemulsions, can now be approached more rigorously and particle size (or latex size) distribution and molecular weight distribution can be tailored. Since water-based, rather than solvent-based, coatings are gaining importance due to restrictions on emission of volatile organic solvents, a study of emulsion polymerisation will become even more important.

Since micelles, microemulsions, solutions of hydrotropes, etc., are structured media they offer great scope in managing regioselectivity in organic reactions. Thus 1, 2 vs 1, 4 reductions of isophorone can be manipulated¹⁷. We need to develop predictive capabilities.

In transportation of heavy petroleum fractions and heavy crude oil the role of emulsions with a small amount of water has been recognised. How such mixtures can be tailor made is an area of relevance and more so when we link to their use as fuels. The enhanced oil recovery systems depend heavily on interfacial engineering.

Even in biotechnology, interfacial sciences are very important (immobilised animal cells, microencapsulation, etc.).

Surfactants can help us, in a cost-effective way, in cement/concrete. Our expertise in this area is poor.

In India, we have not witnessed a systematic study, in a concerted way, and there are hardly any schools of international standing. It is important for us to give impetus to this vital area and promote excellence.

13. Fertilisers, synthetic fibres; sugar and bagasse; cement/concrete; etc

These subjects have been covered at length in my Danckwerts Memorial Lecture¹⁸. There is an urgent need to develop novel processes for acidulation of phosphate rock, conversion of KCl to KNO₃, etc. We must improve polyester fibres and filaments to suit our climatic conditions; polypropylene fibres can be upgraded to meet many of our requirements. We are the largest sugar-producing country in the world and we do not have any technology of worldwide significance. The areas of purification of cane juice, crystallisation, etc., merit attention.

We have the largest bagasse resource in the world and simultaneously we are short of raw material for paper. It is important for us to develop novel technologies for delignification.

The role of polymer additives and superplasticisers for concrete should be studied systematically, particularly due to the corrosive atmosphere that is prevalent on account of our 7000-km long coastline.

14. Energy

14.1. Coal

The availability of energy in a sustained way and without interruptions will continue to be a source of concern for us. Coal will continue to occupy the pivotal position and we need to give more attention.

The fluidised bed combustion (FBC) of coals, with high ash content, middlings from washeries, etc., need to be studied more intensively and to be practised on a grand scale. This may provide an innovative approach to have an add-on, preceding unit, for low to medium temperature fluidised bed carbonisation with hot product coal transported directly into the FBC unit. The yield of liquids from carbonisation could be about 3% by wt and should also provide a valuable source of phenols. Thus, in a location where 2000 MW of power is generated we may have 60,000 tpa of liquids. Coal carbonisation needs to be studied further.

Integrated coal gasification power plants should be preferred and this also calls for a systematic study of pressurised fluid bed combustion. The engineering challenges in exploiting our huge reserves of unmineable coals in north Gujarat (estimated at more than 60 billion tonnes), at a depth of 1000 m and more, are enormous and we can be world leaders. The modelling of underground coal gasification is a real challenge.

The role of interface science in transporting coal as a slurry at high concentrations merits attention. We should consider high capacity, say 1 mtpa pit-head-coal-based 'fuel' methanol plants and transport coal as a slurry in methanol.

The liquefaction of coal will become important and we have to consider the design of large-size continuous reactors. The coal liquefaction, which is particularly attractive for coals containing higher amounts of volatile matter, can possibly be ingeniously combined with hydrocracking of heavy bottoms to maximise the yield of middle distillates which we need badly. Such combo-processes require engineering skills of high order. It is very likely that 65% of coal, on moisture and ash-free basis, can be converted to liquids and this clearly brings out the potential.

The recovery of chemicals from tar acids and tar bases continues to be an important subject, particularly with respect to getting purer fractions. Similarly, the recovery of naphthalene, anthracene, etc., from tars is very important. Our potential is great but our progress has been very unsatisfactory.

14.2. Nuclear power

This sector of industry perhaps has the highest content of science. We will unquestionably need nuclear power, particularly in parts of India where we do not have coal and natural gas.

New methods of enriching uranium will have to be explored, apart from exploring new sources of uranium including recovery from phosphoric acid obtained by acidulation of selected imported phosphate rocks.

We also need to improve our heavy water technology, apart from developing new processes. Here, we have an excellent opportunity to develop highly efficient column packings and even trays of new design. We need about 300 theoretical stages!

We are an important resource country globally for rare earths. We need to develop cost-effective technologies for Nd, Pd, Sm, Gd, etc. Technologies based on solvent extraction and/or ion exchange resins will be important.

15. Biotechnology

This area demands far greater attention than we have really devoted so far, particularly in downstream processing where we have to deal with dilute solutions. The role of membrane processes, affinity chromatography, solvent extraction in hollow fibre extractor, crystallisation and precipitation, etc., need to be emphasised. The vital role of biotechnology in producing human therapeutics and human diagnostics needs to be emphasised and in fact 'it's not science anymore' and needs to be converted into technology. The recent success in r-DNA-produced bovine and porcine somatropine in agriculture sector should act as a booster for us. The most promising direction appears to be in taking proteins to design small molecules that mimic or antagonise a protein, enzyme, or receptor. We are still not clear about the impact the first genetically engineered seeds will have and how soon they will reach the market place. The herbicide-resistant seeds are already in the market.

While the new areas of biotechnology are getting attention, it is a pity that our alcohol production, based on fermentation of molasses, is still based largely on outdated technology. We must correct this situation. We should also do innovative work on science and engineering of anaerobic digestion.

There is scope to develop the technique of bioremediation-used bacteria to break-down toxic elements and convert them into harmless products.

We should consider microorganisms to solubilise heavily weathered (oxidised) coals at ambient temperatures and fungi may be particularly effective.

The importance of having optically active molecules in pharmaceuticals and agrochemicals has already been emphasised and the role of enzymatic processes both in making the wanted molecules and in resolving racemic mixtures is crucial.

Chemical, including biochemical, engineers are particularly well suited in orchestrating different separation processes, conventional and new ones, for downstream processing. However, in the field of biotechnology as a whole our 'bicultural' feature has been weak and chemical engineers need to be more proficient in biology. We must recognise that the successful improvement of a process requires a high degree of the basic process knowledge and our ability to predict process response.

16. Concluding remarks

It is clear that in the future process design will have to be more accurate and an astute scale-up of processes will be required. It will become necessary for us to be

more innovative rather than imitative. However, the road to innovation requires a great deal of individual eclecticism; the multicultural character of chemical engineers should lead to uncanny skills in bringing disparate subjects together.

Chemical engineering has a tradition and culture of being an 'evolving discipline' with a unique blend and flavour of its own and this will remain our hallmark. The chemical engineer is a critical resource but we must greatly improve our propensity to take calculated risk in coming out with innovative processes.

The future of chemical engineering will be full of excitement and challenges and without fail will be stimulating, rewarding and edifying.

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