Om to Genome -
Chemical Engineering Transforming into Universal Molecular Engineering

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In our culture, OM has a great meaning- It is the beginning. The sound itself is spiritual. It is a trinity consisting of three sounds - A, U, M which in English has somehow been written as OM. Really it has to be pronounced as AUM- Brahma, Vishnu and Mahesh. Birth, Prosperity and Death- And Chemical Engineering can be linked to all these aspects very philosophically and technically.

The Beginning

Today's buzz word is Genome- Gene has come from the Sankrit word - Jan - i.e. to create and in genOMe, OM is already there as its part. All engineers are creators of the world that has never been and chemical engineers are at the heart and soul of all branches of engineering; the recently born "kid brother" called IT included. So is fascinating for me, at least, to present where we are heading during this century and whether "Chemical Engineering" represents what we have done since the word "Chemical Engineer" was born; creator of the profession is supposed to be George Davis, who tried to form a society of chemical engineers in England in 1880, but failed. In 1888, Professor Lewis Norton of the Massachusetts Institute of Technology introduced "Course X" (ten), thereby uniting chemical engineers through a formal degree. Davies started with industrial chemistry as a soul with input from the other three engineering branches, Norton did it for mechanical engineers with industrial chemistry as additional input. That was the time when there was a lot of excitement in chemistry; the hero Mandelee was making ripples and predicting existence of elements which were then unknown. Alfred Nobel had already made name for himself as "explosive" manufacture.

The Solvay process was well established and embraced the concepts of "Green Chemistry" which is now a buzz word, wherein the concepts of recycle, reuse, waste minimization, etc, were inherently practiced. No synthetic ammonia was born and it took another 25 years or so for the World War I to bring in synthetic ammonia of Haber (1913), which as been heralded as the greatest innovation of the twentieth century in chemistry and chemical engineering. Fritz Haber's process for synthesizing ammonia from hydrogen and nitrogen was turned into a viable commercial process by the German chemical company BASF. The crucial moment in their relationship was the demonstration by Haber to the company on 2 July 1909.Haber's British-born assistant Robert le Rossignol was present at the time and acquired a sample of the ammonia made on that historic occasion.

By my philosophy, ammonia symbolizes OM - birth, prosperity and death. A new chemical industry was born and taken to greater heights. Ammonia is not just a base, but basic to everything. The origin of life is linked to ammonia which in nature formed through a photochemical reaction. Llightning strikes at a rate of approximately 100 every second somewhere in the atmosphere and contributes to so many changes on molecular level which we have not yet properly understood.

Impact

The excitement of being chemical engineers would be short-lived if it was not to be practiced by industry. The societal impacts of chemicals is so enormous, but very poorly understood by the public or media. The United States is the largest chemical producer in the world, accounting for 27% of world production. With chemical shipments reaching nearly $460 billion in 2000, the chemical industry provides about 1.2% of the total U.S. GDP and nearly 12% of the manufacturing GDP. The industry exported a record $80 billion in chemicals in 2000 and registered a trade balance of $6.3 billion. On a value-added basis, chemicals is the largest U.S. manufacturing sector. The industry continues to grow, with profits in 2000 reaching $44 billion, an all-time high.

Historical Perspective

The history of evolution of chemical engineering profession is equally fascinating. The American Chemical Society (ACS) did not think much of chemical engineers when AIChE was born in 1908. The ACS had a division of Industrial and Engineering Chemistry established then just to undermine the existence of AIChE. Luckily they sorted out their differences and started working in tandem. In India, Dr. H. L. Roy had the honour of starting a chemical engineering course in 1923, while the chemical industry was in utter infancy..A cursory look at the evolution of syllabi and the persons associated with it will reveal that chemical engineering has indeed marched on as science. (Table 1 and Table 2). And some of the milestones are reflected in the Kirkpatrick awards (Table 3).

The New Generarion

Chemical engineers have been dealing with systems on - Megascopic, Mesoscopic, Macroscopic, Nanoscopic/Microscopic and Atomic scale. The reason is simple - Chemical Engineering is a highly science based and universal discipline now playing at molecular level. They talk of today- Structure activity relation , Electrophoresis, tissue engineering, controlled drug delivery, targeted medicine, recombinant DNA, molecular models, life cycle analysis, etc. Chemical Engineering, Universalism and Molecules

"All intelligence is collective," technology historian George Dyson writes in "Darwin Among the Machines," "... whether that of a billion neurons, a billion microprocessors, or a billion molecules forming a single cell." At the scale of human society, intelligence is evolving from centres and tops and spreading over the widest possible expanse. Technologies that facilitate this migration of intelligence to the edge already rank among the most important of our time. If you look at the research interests of the faculty hired in last decade in chemical engineering departments in the USA, the old times would start pinching themselves if they have been chemical engineers, in the first place.

Whosoever named that journal Chemical Engineering Science, which is incidentally celebrating its Golden Jubilee, must be a visionary since there is so much science in chemical engineering and in particular without chemistry it would be no engineering. So the joke that a chemical engineer is an engineer among chemists and chemists among engineers can boomerang. Chemistry is usually referred to as the central science. It is absolutely at the centre of improving conditions of human and animal life. One of the hallmarks of chemists is that they can create new molecules. In doing so they often outperform nature.

As chemical engineers we have been dealing with systems of scale from atom to atmosphere - we are building models- physical, chemical and physico-chemical, using complicated mathematics, minimizing the number of parameters to describe systems, events, and creating new molecules. Some of us are happy to be only in the physical world and some in mathematical world, whereas some do not see a link of their work with somebody else.

Chemistry as a science has broadened so much that we only talk of living and non-living systems. Chemical engineers are the biggest beneficiaries and have started taking control of creating new molecules on a grander scale. We may add a word "bio" to appear distinct, but it is rather elusive.

Chemistry Is Our Soul

Synthetic chemistry - organic, inorganic and organo-metallic, has been a virtual watershed of knowledge that has propelled the development of a wide spectrum of new industrial, commercial and health products and intermediates by the chemical and allied industry. With an avalanche of new techniques including new instruments over the years, chemists have continuously explored new structural designs and configurations in their attempts to develop better performing less expensive products or intermediates, pharmaceuticals and molecular understanding

Let us examine what has brought us to this level of molecular engineering. The desire to lead long comfortable life made spectacular advances in the pharmaceutical and drug industry. The distinct periods are as follows:

From 1800 till end of WWI - The era of predictable and safe drugs that we now enjoy did not begin until the end of the 19th century.

During 1920s - This was the era of vitamins and hormones and it witnessed the development of new drugs and vaccines.

During 1940s - It was an era of antibiotics and isotopes. Like the music of the Big Bands, Big Pharma zoomed the antibiotic era into full swing with a host of WWII-stimulated technological advances.

During 1950s : As America turned from world war to cold war, the economy and technology prospered, and a new vaccine brought victory over an old scourge, infantile paralysis

During 1960s- It was the pharmaceutical decade covering anodynes and estrogens. Against a backdrop of civil unrest, war, political assassinations, and men on the moon, drug use exploded for better and for worse

During 1970s- Chemistry, cancer, and ecology ,and environments of health occupied the centre stage and concerns over cancer and carcinogens grew against a backdrop of lingering warfare, political scandals, and the rising environmental movement. This period also started having a fresh look at chemicals and the functional groups which imparted them specific characteristics.

During 1980s- This period shattered the hopes of stray persons, like Rock Hudson. Aids, arteries, and engineering became new buzz words. An incurable retrovirus epidemic and rising biotechnology fever took centre stage in pharmaceutical development. Chemical engineers became more involved in this area of activity.

1990s- The closing of the Pharmaceutical Century witnessed harnessing genes, recasting flesh. Global genomic initiatives and marvels of miniaturization set the stage for a new century of "better living through biotechnology.

Beyond 2000s - The next pharmaceutical century and the future will get more attention,. Longevity will bring into focus new types of personalized diseases. Experts predict that genomics, gene therapy, and rejuvenative therapy will play major roles in medicine's future.

Human Genome

The 21st century is opening with the sequencing of the human genome. On June 26, 2001 Celera Genomics (Rockville, MD) and the international Human Genome Project jointly announced that they had completed 97-99% of the human genome. Using computer algorithms, the next step would be to reassemble the jumble of DNA fragments into a whole sequence.

Molecular Modeling

By the time many of today's students enter the workforce, career opportunities will have radically changed. Most if not all of the 100,000 genes in the Human Genome will have been sequenced. Using molecular modeling scientists will be better able to design new and more potent drugs against diseases such as Cancer, AIDS, and Arthritis. Molecular modeling not only has the potential to bring new drugs to the market, but a vast array of new materials. The discovery of fullerenes, and superconducting cuprates (as well as other complex inorganic compounds), are expected to produce new materials in the optics, ceramic, semiconductor and biomaterials markets. Chemical Engineers will be at the forefront of this activity.

What will be our future - Atomic Scale Engineering ?

The most important advance in the 21st century, according to some scientists, will be the introduction of atomic-scale prostheses to repair and restore human body function during 2050-2100 The most important revolution of the next century, which will be atomic-scale engineering.

Regenerative therapy will use naturally occurring biologic substances, whereas rejuvenative therapy will use human stem cells and synthetic engineered substances. Humans will be able to replace their body parts with a more durable substance and extend human performance in almost any area. The fusion of atomic-scale engineering technology with human body will enormously enhance human performance. So we need new monomers and better performing polymers and the understanding has to be on molecular level.

Tissue engineering-taking cells to restructure or rebuild damaged or congenitally defective tissues-is an important part of regenerative therapy. The first tissues are just now being reimplanted. That will grow over the next 5 to 15 years to be a major business. We will begin with blood vessels, cartilage, bone, bladder, trachea, and skin, moving on to more complicated organs like the liver and kidney. Twenty years from now, a number of major organs should be reimplanted, and by 30 years from now more complicated organs including the heart and lung can be transplanted.

Both regenerative and rejuvenative medicine will be important in the 21st century. Medicine will be moving toward the use of stem cells to rejuvenate the body. Fundamental breakthroughs will occur in our understanding of how stem cell arise during embryogenesis, what controls them, and how they can be used as medicine

In regenerative medicine, we would be able to take stem cells and train them to be cardiac muscle cells and replace the muscle tissue. Stem cells and anything related to them are going to be of extraordinary importance in the future.

We may even find ways to improve on our basic architecture. Nanorobots injected into the body may rebuild broken-down or worn-out body parts with materials more durable than our own native cells and proteins. Other nanorobots may be able to diagnose and eradicate now-fatal diseases such as heart disease and cancer. These visions may sound like the stuff of science fiction, but they aren't as far off as they seem.

Nano-science and technology

Ultimately, a fantastic challenge is to link *molecular sensing technologies with nanotechnology* for the idea of using such molecular machines to remotely sense molecular changes, know what they are, and know where they are. One can ultimately imagine the incorporation in a single molecular platform of sensing, signal generation, external decision-making, and local therapy. What we're talking about violates laws of physics as we understand them, but it is very far off in terms of what we're capable of doing.

Whether the future will bring true cures or simply more palliative therapies. The difference between palliation and cure relates to understanding the effect of intervening at a molecular target with a phenotype. It's going to require putting the system together, not just having the components. We need to understand the relationship between the components and the disease processes-*the processes that lead* to developing the disease, the symptoms of the disease, and the fundamental nature of the disease itself.

Ethics

The new areas of research will be protein therapeutics, personalized medicine and of course to find the fountain of youth. One of the stickier ethical issues for the future is the question of germ-line therapy-tinkering with the genes in sperm and eggs.

There are several other important milestones that have been achieved and I would rather give a cursory account of it.

Restoring sight with plastic implants

A polymer implant has been developed that can restore the ageing eye to the physiological condition of youth. This device is also expected to revolutionise treatments for ocular hypertension and glaucoma, the second most common cause of blindness.. Currently, almost 100% of older people are affected by an inability to focus, and this is the main reason why many people over the age of 42 require reading glasses. The implant restores the ability to focus by increasing the distance between the lens and the outer coating of the eye. The ability to focus is lost over time as the lens continues to grow. This cramps the muscles surrounding the lens, thereby reducing the amount of force the muscles can apply on the lens and hence the ability to focus. The implant consists of four separate segments made from injection-moulded polymethylmethacrylate that are implanted in four points in the eye. This increases the diameter of the eye, so that the effective working distance of the muscles surrounding the lens is increased. Renewing the eye's ability to focus also restores its ability to drain itself. This is because the tissues responsible for drainage are stretched and any fluid blockages that might have occurred, as in glaucoma, are relieved. Clinical trials conducted recently in Canada showed that the implants do effectively restore drainage to the ageing eye and are therefore suitable for treating ocular hypertension and glaucoma.

Schizophrenia Cure

Schizophrenia is caused by the brain's inability to produce enough proteins, the building blocks of nerve cells according to a new theory. If this theory proves correct, schizophrenia might be easily preventable and treatable, partly by immunisation against viruses that infect the brain and partly by new drugs that improve the rate at which the brain makes proteins. Insufficient protein synthesis could cause neurodegenerative defects due to incomplete regeneration and remodelling of neural networks,. The role of protein synthesis in the development of schizophrenia was applied to the analysis of data produced by the Human Genome Project by what is called a secondary Darwinian method to narrow the number of genes responsible for the susceptibility to schizophrenia. The large number of genes identified by the human genome project were treated as the population and their difference in function were the variations in the population. Several cycles of selection were then applied using criteria based on knowledge about schizophrenia. The results showed that many of the genes associated with a susceptibility for schizophrenia were associated with protein synthesis.

Chiral Engineering

A cactus found in the deserts of Arizona is a good example of chiral catalysis. The flowers first appear only when the plant is about 50 years old. An attractive parallel can be seen between this slowly maturing beauty and the development of asymmetric organocatalysis, the origin of which goes back to the emergence of the efficient homogeneous asymmetric catalysis. Since the importance of the spatial arrangement within molecules to the fundamental properties of the substances was recognized, chemists have become increasingly interested in enantioselective synthesis. In the course of time, the field of enantioselective synthesis has outgrown the academic environment. The chiral drug industry has become a rapidly growing segment of the drug market and represents close to one third of all drug sales worldwide.This has been driven by the increased regulatory control of enantiomeric composition of drug candidates, and the potential of isomerically pure drugs to provide improvements over the previously available racemates. Undoubtedly, the more elegant and economically most attractive way to introduce chirality into a molecule is by using a catalytic amount of chiral controller to induce the chiral transformation. Enantiocatalytic reactions have had the most significant impact on the development of synthetic organic chemistry in the last 30 years. Among them, methods based exclusively on metal-free chiral organic catalysts have become more significant. Helped by intuition, persistence, and good fortune, these new reactions are becoming powerful tools in the construction of complex molecular skeletons.

Chiral organic molecules have been used from the early days of chemistry to promote reactions. The emergence of homogeneous enantioselective organometallic catalysis has had a decisive effect on the development of enantioselective synthesis (P. I. Dalko, L. Moisan, Angew. Chem. Int. Ed. 2001, 40, 3726)

Carving on the Nanoscale

In biologically mineralized systems the constructive interaction of the inorganic crystal phase with the organic matrix material results in composite materials that are exceptional in their outward appearance and material properties. Of the 60 minerals known to be processed by living organisms, the most frequently used are calcium carbonate, calcium phosphate, and hydrous silica. They are used for the formation of scales, prickles, shells, or endoskeletons. The mineral is usually crystallized within a protein or polysaccharide matrix which has a number of functions: it shapes and aligns the singlecrystalline building blocks, and it serves as a ductile component for mechanical stress dissipation. The resulting nanoscale composite structures make biominerals such as bone or teeth superior to most artificial ceramics. (Anna Peytcheva and Markus Antonietti, Angew. Chem. Int. Ed. 2001, 40, No. 18, 3383)

Electrochemical Surface Science

The last 30 years have seen remarkable changes in interfacial electrochemistry, particularly in the kind of questions that were addressed in electrochemical studies. Ever since classical surface science, traditionally performed under ultrahigh vacuum conditions, has succeeded in describing surfaces and surface reactions on a molecular level, electrochemists longed for a microscopic understanding of the solid/electrolyte interface and, at the same time, searched widely for new experimental ways to reach that goal. Herein, studies are described concerning the structure and the dynamics of bare and adsorbate-covered electrode surfaces and of metal deposition as a simple, yet important, electrochemical process. In all these cases, the scanning tunneling microscope plays a pivotal role emphasizing the surface-science approach to the problems. (D. M. Kolb , Angew. Chem. Int. Ed. 2001, 40, 1163)

The application of l-proline as an enzyme mimic and further new asymmetric syntheses using small organic molecules as chiral catalysts has been demonstrated (Angew. Chem. Int. Ed. 2001, 40, No. 3, 529). It would represent a remarkable synthetic alternative to many established asymmetric transformations. In particular, such processes would allow the cost effective manufacture of chiral building blocks on an industrial scale. Furthermore, the application of enantiomerically pure, small organic molecules represents a promising alternative catalytic concept in addition to other frequently used syntheses based on metal-containing catalysts.

From Polymer Synthesis to Molecular -Engineered Surfactants

The highly versatile nature of CO_2 has been exploited in numerous industries and applications. CO_2 has been used for decades for food freezing and for pH control in the textile Although CO_2 is a good solvent for many small molecules, most polymeric materials have a very low solubility in CO_2. This presents major limitations for the applicability of CO_2 in many processes. These limitations lead researchers to the design and synthesis of molecules that would bring CO_2 into a new application areas. DeSimone et al. were the first to report a homogeneous free radical polymerization using a semifluorinated acrylate monomer in $scCO_2$. This milestone led to the homogeneous synthesis of many other fluorinated polymers including poly(2-(N ethylperfluorooctanesulfonamido) ethyl acrylate), poly(1,1-dihydroperfluorooctyl acrylate), and poly(perfluoroethyleneoxymethylstyrene). The polymerization of tetrafluoroethylene to PTFE in CO_2 is of particular importance because it emphasizes a safe new route to fluorolefin polymers. (Sharon L. Wells and Joseph DeSimone, Angew. Chem. Int. Ed. 2001, 40, 518)

Biotechnology and Material Science

The interesting aspects of nanoparticles, proteins, nucleic acids, biotechnology and material science have been a subject of great curiosity (C. M. Niemeyer, Angew. Chem. Int. Ed. 2001, 40, 4129). The essence of chemical science finds its full expression in the words of that epitome of the artist-scientist Leonardo da Vinci, "Where Nature finishes producing its own species, man begins, using natural things and with the help of this nature, to create an infinity of species". Supramolecular chemistry concerns the investigation of nature_s principles to produce fascinating complex and functional molecular assemblies, as well as the utilization of these principles to generate novel devices and materials, potentially useful for sensing, catalysis, transport, and other applications in medicinal or engineering science. Another example of modern technical achievements concerns the development of advanced, functional, and even ºsmartº materials for applications in highly integrated mechanical, optical, and electronic devices, sensors, or catalysts. The enormous advance attained in this area so far is illustrated impressively by comparing materials used in last centuries electrical devices such as millimeter-sized copper wires to today (sub)micrometer-sized optical and electronical parts, comprised of modern conducting and electroluminescent organic polymers. Similar advances have been made in the biological sciences. Natural evolution has led to highly functional assemblies of proteins, nucleic acids, and other (macro)molecules which perform complicated tasks that are still daunting for us to try to emulate. As an example, the 20 nm ribosome particle is an effective supramolecular machine which spontaneously selfassembles from more than 50 individual protein and nucleic acid building blocks, thereby impressively demonstrating the power of biologically programmed molecular recognition. Starting with the discovery of the double helix structure of DNA, biology has grown from a purely descriptive and phenomenological discipline to a molecular science. Recombinant DNA technology brought insights into the basic principles of many biochemical processes, and it has also opened the door to modern biotechnology. Today we are able to genetically engineer relatively simple bacterial cells, and we are on our way towards tailoring complex organisms. In view of such revolutionary developments, it seems particularly challenging to fuse biotechnology with materials science. Merging these disciplines will allow us to take advantage of the improved evolutionary biological components to generate new smart materials and, conversely, to apply today's advanced materials and physicochemical techniques to solve biological problems. Both biotechnology and materials science meet at the same length scale . On the one hand, biomolecular components have typical size dimensions in the range of about 5 to 200 nm. To exploit and to utilize the concepts administered in natural nanometer-scale systems, the development of nanochemistry is crucial. On the other hand, commercial requirements to produce increasingly miniaturize microelectronic devices strongly motivate the elaboration of nanoscale systems. The structural dimensions of computer microprocessors are currently in the range of about 200 nm. They are only just available by conventional topdown processes (miniaturization processes) such as photolithography, but for the foreseeable future, such technologies hardly allow the large-scale production of parts that are significantly smaller than 100 nanometers.

Architectural and Functional Molecular Engineering

Although selectivity, particularly in the control of absolute stereochemistry, is a major concern in modern organic synthesis, reactivity and productivity are also important in making reactions efficient and practical. Combinatorial approaches coupled with high-throughput screening techniques obviously facilitate the discovery process but their powers are still that not evident in the field of molecular catalysis. Most excellent new catalysts are optimized forms of existing catalysts rather than being truly novel. Nobel Laureate Noyori's work is a fine example of the functional molecular engineering

Table 1 : Evolution of Chemical Engineering Courses

Unit Operations and Unit Processes
Economics
Separation Processes
Material and Energy Balance
Mass Transfer
Heat Transfer and Fluid Flow
Transport Phenomena
Chemical Reaction Engineering
Biochemical Engineering
Environmental Engineering and Pollution Prevention
Molecular Engineering and Engineered Molecules
Green Chemistry and Technology
Genomics and Genetic Engineering

Table 2 : Some Important Persons Involved in Developing New Curricula and Texts until 1960

Arthur D. Little
McAdams,Walker,Lewis, Kern
Groggins, Shreve
Sherwood, Pigford
Hougen, Watson, Ragatz
Bird, Stewart , Lightfoot
Amundson, Aris
Levenspiel, Smith

Table 3 : Kirkpatrick Awards

2001 Awards

- Low temp adsorption of NOx (The BOC Group)
- New 7-ADCA chemistry (cephalosporins) (DSM Anti Infectives, Delft)
- Silver recovery from photographic waste (Itronics Inc.Reno,Nev.)
- Recovery of hazardous solvent THF Mistsubishi Chemical Co.)
- New approach to absorption of ammonia (TNO and Cirmac International, The Netherlands)

1999- Alkoxysilanes (CK Witco)
1997- Membrane recovery for unreacted monomer in polyolefin manufacture
1995- Oxygen based recycling of mixed office paper
1993- Catalytic manufacture of Ibuprofen (BHC)
1991- Anaerobic treatment of process wastewater (Amoco Chemical)
1985- Coal based acetic anhydride (Tennesse Eastmant)
1979- Low pressure process for LDPE
1971- Hollow fibre reverse osmosis (du Pont)
1969- Textured protein foods (General mills)
1961- Synthetic zeolite adsorbents
1955- Silicone products (Dow Corning)
1947- Large scale manufacture of streptomycin (Merck)
1943- Rapid commercialization of synthetic rubber during WWII (67 different companies jointly)
1941- Magensium from sea water (Dow)
1939- Aviation fuels (Standard Oil Development)
1933- Petrochemical Synthesis (Carbide & Car)

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His research interests are catalysis, enhanced oil recovery and green technologies. He has filed 19 patents including 8 foreign patents in USA, UK, Germany, and Japan on new catalysts UDCT-1 and UDCT-2 and new processes.

His research papers, over 100, are published in peer-reviewed international journals. He is a recipient of many prestigious national honours and awards. He is the recipient of Vasvik Award for excellence in chemical sciences and technology (1995). He is also elected as the Fellow of Maharashtra Academy of Sciences. He has served Indian Institute of Chemical Engineers as President of the Institute.