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Industrial Chemical Research : An International Outline*

Introduction

Good morning ladies and gentlemen. I am pleased to be with you at this impressive exposition whose theme is chemical research in the nineties. The title of my talk is "chemical research - an international outline" and Drs. Pregaglia and Sponzilli have asked me to analyze the state of the art and the prospects for the nineties in industrial chemical research at an international level.

One hour is a very short time to give any in-depth treatment to a subject with the breadth and depth of industrial chemical research. My colleagues and I have selected for an overview several areas of industrial chemical research that we believe will be important in the nineties - but time only permits us to cover a few areas. Therefore, we trust you will understand that if your area of interest is not included, it is because time and our knowledge base didn't permit us to include it in our talk.

As we start to discuss industrial chemical research, several of its key attributes stand out - and these justify special mention :

- International in nature.
- Pervasive throughout industry.
- Expanding in breadth and depth.
- Driven by needs.

First, industrial chemical research is truly international. Most of the major companies that do research are international or global and conduct research in many countries throughout the world - and in the process must coordinate their programs on a global basis.

Second, the application of chemical research is pervasive throughout industry. Few manufacturing industries can continually improve their products and processes without some level of chemical expertise and research and development.

Third, the importance of chemistry in industry continues to expand in both breadth of applications and the depth of understanding needed in them. Chemistry is truly the fundamental science.

Fourth, industrial chemical research is driven by the needs of industry and society in general. In the process of meeting those needs, it takes the «basics» of science from academic research and applies them to solve real world problems.

In my talk today, I would like to first present some information on international chemical research to characterize its size, location,

focus and growth trends. After that, I will briefly describe several segments of industrial chemical research that we believe will be important in the nineties. The following areas will be discussed :

- analytical chemistry,
- simulation,
- environmental chemistry,
- catalysis,
- thermoplastics polymers and composites,
- thermosetting polymers and composites,
- agricultural chemistry,
- advanced ceramics.

First, I'd like to give you some data on industrial chemical R & D globally to illustrate the scope and complexity of the subject. Unfortunately, rigorous data is difficult to obtain because collection capabilities, methods and data collation vary significantly as certainly does the relative currency exchange rates. Beyond that, it is very difficult to separate out the industrial chemical R & D data from overall R & D expenses. Therefore, my information will be much more qualitative than quantitative, and is much more precise for the US than the rest of the world.

In the US in 1989 (*Table I*), a total of \$ 142 billion was spent on R & D. Industry performed \$ 103 B of this work with a sizeable amount of government funding. The chemical R & D segment of this \$ 103 B was \$ 11.9 B or 11 % - of which about half (\$ 5.4 B) was for industrial pharmaceutical R & D, with the remainder on chemicals and allied products.

This \$ 11.9 B total represents an annual growth from 1978-88 of about 11 % with pharmaceuticals showing a 14 % annual growth rate. Correcting for inflation to constant dollars would obviously reduce this growth rate sizably - particularly, in the early 80's. The

TABLE I. - US R & D spending.

\$ Billion	1981	1989
Total spending	72	142
Industrial R & D	52	103
Industrial chemical R & D	5.6	11.9
Pharmaceuticals	2.1	5.4
Industrial chemicals	3.5	6.5

top 15 US chemical companies accounted for about 40 % of this \$ 11.9 B in 1989. US chemical companies in 1989 also spent roughly an additional \$ 1.7 B on R & D outside the US and the growth rate of spending in this category over the last ten years has averaged about 15 %/yr. The US chemicals and allied products industry employs about 77'000 scientists and engineers out of a total of 725'000 engineers and scientists in industry (Table II).

TABLE II. - R & D scientists and engineers US Industry.

('000)	1981	1989
Total scientists and engineers	487	725
In chemicals and allied products	51	77
in pharmaceuticals	23	34
in industrial chemicals	28	43

Globally, in constant 1982 dollars, overall R & D spending in 1988 was roughly \$ 250 B - and this does not include any estimates for USSR, China, or Eastern Europe (Table III). Note that using this basis instead of current dollars, overall US spending drops from \$ 135 B to 112 B.

TABLE III. - 1988 R & D expenses by leading countries (constant 1982 dollars).

Country	\$ B	% of GNP
USA	111.5	2.8
Japan	42.3	2.9
Germany	20.1	2.8
France	14.6	2.3
U.K.	13.7	2.2
Italy	7.9	1.4
Canada	5.3	1.3
Netherlands	3.3	2.2
Sweden	2.9	3.1
Switzerland	2.5	2.9

If the global ratio of industrial chemical R & D to overall R & D was similar of that of the US, then global chemical and allied product industrial R & D would be on the order of \$ 28 B in 1982 constant dollars excluding USSR, China and Eastern Europe, by any standard it is a huge endeavor! Besides spending, another way to perceive the size and global nature of chemical R & D is to consider patents and publications in the chemical literature.

As the Table IV shows, essentially 85 % of all us patents issued in 1981 and 1989 were to corporations, roughly half in the us and half non-US.

On a percentage basis, by country (Table V) here are the countries of origin of us patents in 1981 and 1989. Over the past ten years, these percentages have been very consistent except for a growing share of Japanese origin patents and a corresponding share decrease in us origin US patents.

Looking at papers published in chemical journals (Table VI) provides another view of the global nature of chemical research and development. Comparing 1981 and 1989, we see a 6 %

TABLE IV. - US chemical patents issued.

	1981	1989
<i>US origin</i>	12,790	13,863
to US corporations	11,041	12,069
to US government	367	327
to US individuals	1,306	1,308
to foreign-owned corporations in the US	76	159
<i>Foreign origin</i>	9,660	13,172
to US owned corporations abroad	904	1,131
to foreign corporations	7,882	11,139
to foreign governments	100	175
to foreign individuals	774	727
<i>Total</i>	22,450	27,035

TABLE V. - US patents - % of patents issued.

Country of origin	1981	1989
US	57	51
Japan	13	20
Germany	11	10
U.K.	4	4
France	4	3
Switzerland	2	2
Canada	1	2
Italy	1	2
Netherlands	1	1
Sweden	1	1
Belgium	1	1
Others	4	3
	100	100

increase in total papers, but a very consistent pattern in country of origin. The biggest changes appear to be major growth in papers of Chinese origin and a decline in papers from the soviet union.

After considering this data, I believe one can draw several simple, but important conclusions :

- A. Industrial chemical R & D represents a huge global expenditure - probably on the order of \$ 25 billion globally.
- B. The US will remain as the largest investor in R & D throughout the nineties, although Japan's R & D spending will rise at a much faster rate than that of the US. This growth by japan will continue to be reflected in output measures such as papers published and patents issued.
- C. In all likelihood, growth rates in R & D spending and manpower employed will be similar to those for the period 1981-1989. This is, of course, heavily dependent on global business conditions and major political developments.
- D. Because of the single european market soon to be with US and the aggressive growth in overseas operations by major chemical companies, whether they be of European, Japanese or US origin, industrial chemical R & D will continue to grow in global

TABLE VI. - Chemicals papers published (% by country of origin).

Country of origin	% of total 1981	% of total 1989
US	27.4	27.8
USSR	16.6	12.7
Japan	10.5	11.8
Germany (West)	6.0	6.2
U.K.	6.1	5.7
France	4.2	4.2
China	1.4	3.7
Canada	2.6	3.0
India	3.3	2.8
Italy	2.2	2.3
Polands	2.1	1.6
Netherlands	1.3	1.5
Others	16.3	16.7
	100.0	100.0
Total papers published ('000)	374	397

TABLE VII. - Analytical chemistry. Some of today's tools.

- Fourier transform infrared spectroscopy
- High resolution NMR
- GC/MS
- LC/MS
- MS/MS
- Auger spectroscopy
- Sophisticated thermal analyses
- Gel permeation chromatography

spectroscopy, for example. New and powerful magnets combined with computer technology were opening huge new capabilities in high resolution NMR. For example, here's a graph (*figure 1*) that shows the progress in improving signal to noise ratio in NMR in the period 1960-1985.

The *figure 2* shows the NMR spectra of pyridene using state of the art NMR in 1958 and in 1971 - quite a difference !

Other techniques were opening a far better understanding of surfaces - Auger spectroscopy for example (*Tableau VII*)

Today in 1990, we have an incredible array of powerful tools to help us better understand what is going on in the world of atoms, molecules and macromolecules. These tools are very expensive and sometimes tell us about minute impurities we would rather not know about - but they have made us tremendously more efficient and capable of obtaining precise answers to very difficult questions. These instruments have also evolved into the realm of process control in our plants - the Fourier transform IR that was a state of the art analytical Lab Instrument in 1979 is now commonly used in our plants as an integrated process control tool. On line instrumentation using fiber optics sensing and IR, NMR GC/mass spec. and other exotic tools of a few years ago are common and reliable performers in our plants today.

What can expect in the nineties ? The analytical chemists I work with believe that beside a continuing evolution of the basic tools mentioned (*Table VIII*), we will see a wider use of some relatively new tools such as ESCA and secondary ion mass spectrometry. We will also be able to bring scattering and reflection methods into use with Raman, IR, and X-rays to attack more complex problems on surfaces.

This will be particularly valuable in the polymer field to improve our understanding and aid our modification of surfaces (optical properties and surface tension).

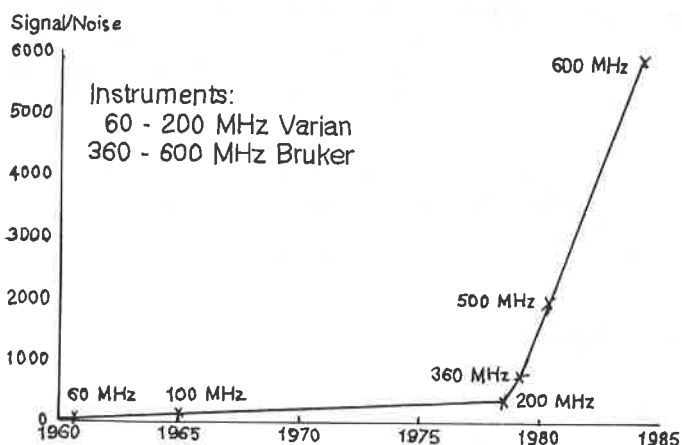


FIGURE 1. - Improvement signal to noise ratio in NMR (period 1960-1985).

integration in the major industrialized countries of the world. The time lag between invention of new technology in the source country and global dissemination and implementation will continue to decline.

Now, instead of talking about overall trends in chemical R & D, I'd like to focus on a few technology segments to give you our views of where R & D is today and where it is headed in the nineties.

Analytical Chemistry

Analytical chemistry is the first area I would like to discuss - and that is not by accident. I believe that much of the progress made in chemical science derives directly from the incredible progress made in analytical chemistry in the last thirty years. I use thirty years because that is my time frame - thirty years ago I was a chemistry student at the university of Illinois. Our state of the art tools then were elemental analysis, infrared, UV and visible spectrophotometry and potentiometry - and at that time at Illinois, professor Gutowsky had put together a huge magnet - so big they had to reinforce the floor below it - and was developing the techniques of nuclear magnetic resonance spectroscopy. Those tools seemed potent and they were - but they seem crude today. Twenty years ago when I was working on brominated flame retardants, our analytical tools were heavily oriented towards gas and liquid chromatography, with areas such as neutron activation analysis emerging. In the mid 70's the linking of computers and chromatographic methods with mass spectroscopy was opening separation and identification capabilities previously unheard of.

And, of course, huge progress was made in microscopy - scanning electron microscopy developed to a level of sophistication that we chemists who were trained to not ever expect to actually see what was happening could indeed do so with growing precision. Ten to fifteen years ago the advent of microprocessors integrated into analytical equipment revolutionized our old standard techniques - Fourier transform brought a whole new dimension to infrared

Neat Pyridine: ^{13}C Spectrum,
 ≈ 1958

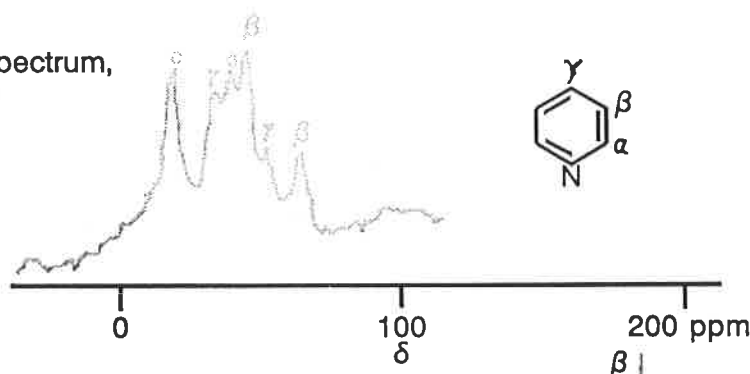


FIGURE 2. - NMR progress.

Neat Pyridine: ^{13}C Spectrum,
 1971

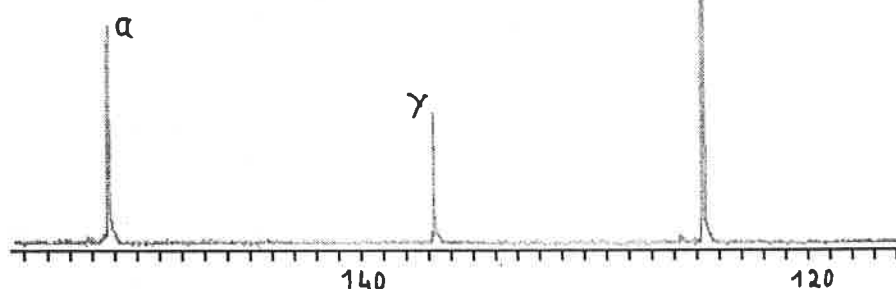


TABLE VIII. - Techniques for the nineties.

Electron spectroscopy for chemicals analysis	(ESCA)
X-ray photoelectron spectroscopy	(XPS)
Auger spectroscopy	(AES)
Secondary Ion mass-spectroscopy	(SIMS)
Scattering/reflection methods	
High resolution electron energy	
Loss spectroscopy	
Infrared spectroscopy	
Raman spectroscopy	
Energy dispersive X-ray analysis	(EDAX)

capabilities being developed today both on "normal computers" and the so-called "supercomputers" will alter the experimental processes that are at the heart of our experimental method. Computational modeling adds a "third leg" to the normal scientific process (fig. 3). In so doing - often with the use of supercomputers because the calculations can be extremely complex and strain normal computers - we can solve very complex problems in a reasonable time frame. For example, *ab initio* quantum mechanical calculations on a complex polymer intermediate that would take an individual 600'000 years to solve manually or 30 hrs. To solve on a VAX - 8650 can be done in 3 hrs on a supercomputer. The use of these calculations allow us to understand reaction pathways and transition states and to predict the effect of substituents. Many weeks of experimental work can be saved via these techniques. They can greatly improve our ability to visualize complex dynamic phenomena such as the positioning of atoms on an active catalyst surface. Another advantage is the ability to

Also, beyond instrument development per SE, we will most certainly see tremendous improvements and innovations in systems to allow communication between instruments and facilitating data analysis and reporting. Networking in the scientific environment will become more important. We will see enhanced possibilities for mathematical applications on large data sets and increased power in data interpretation due to chemometric applications which are possible on the basis of fast data transfer on those networks.

There is an old expression that "a rising tide raises all boats" - I certainly believe that the rising tide of analytical chemistry has raised all the boats in industrial chemical research and the tide will continue to rise steadily throughout the next decade.

Simulation

It doesn't sound chemical, does it ? However, the ability to mathematically model and accurately simulate complex physical and chemical systems will lead us into a far better and deeper understanding of complex phenomena. I believe that modelling

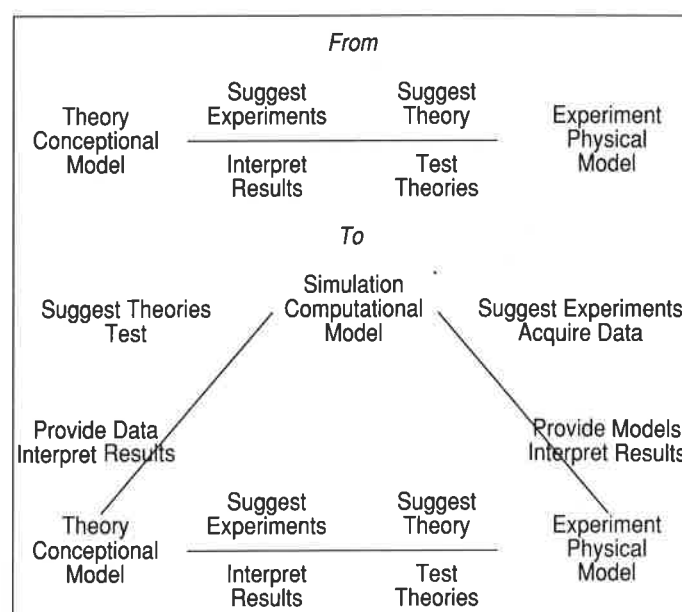


FIGURE 3.

"experiment" when real experimentation is not feasible because of time or experimental constraints - while not a chemical example, the simulation of a severe thunderstorm to study microburst downdrafts is a great example.

There are many areas where this technology is being used today to enhance understanding - such as molecular design, disordered many-body systems, high-temperature superconductor property prediction, polymer crack propagation mechanism studies.

I guarantee in the future you will see a lot more simulation.

Environmental Chemistry

Environmental chemistry is that body of science which focuses on definition of transport and transformation of chemical substances within ecosystems.

Progress in environmental chemistry depends upon :

1. - Advances in analytical chemistry that allow identification of chemical species found at low concentrations in complex solutions and mixtures.
2. - Advances in development of laboratory models to simulate on small scales the environmental degradation (via hydrolysis, biodegradation, etc.) of chemical species - an attempt to experimentally simulate in the laboratory the individual processes taking place in an environmental system.
3. - Development of mathematical models and simulation techniques to predict the spatial and temporal distribution of chemical species and their degradation products in ecosystems - an integration of the multiple environmental processes.

Environmental chemistry (Fig. 4), then is really the convergence of the two previous topics - analytical chemistry and simulation. Because ecosystems are so complex - whether it be the upper atmosphere or a more typical terrestrial/aquatic ecosystem, sophisticated computational and modelling techniques are required to predictively deal with the multitude of variables.

As we globally move towards more emphasis on environmental quality (Fig. 5) in the 90's, these tools will be important in helping us better define and solve environmental problems. In a world of limited resources, it is important that we apply our funds and energy to solving priority problems. These techniques are assisting now, but as the 90's progress they will grow in sophistication and application.

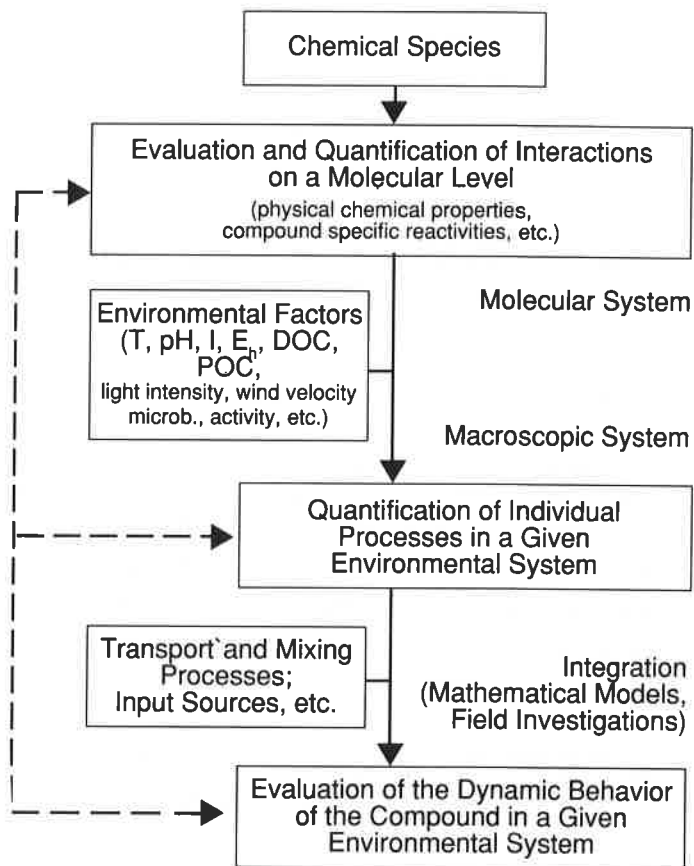


FIGURE 5.

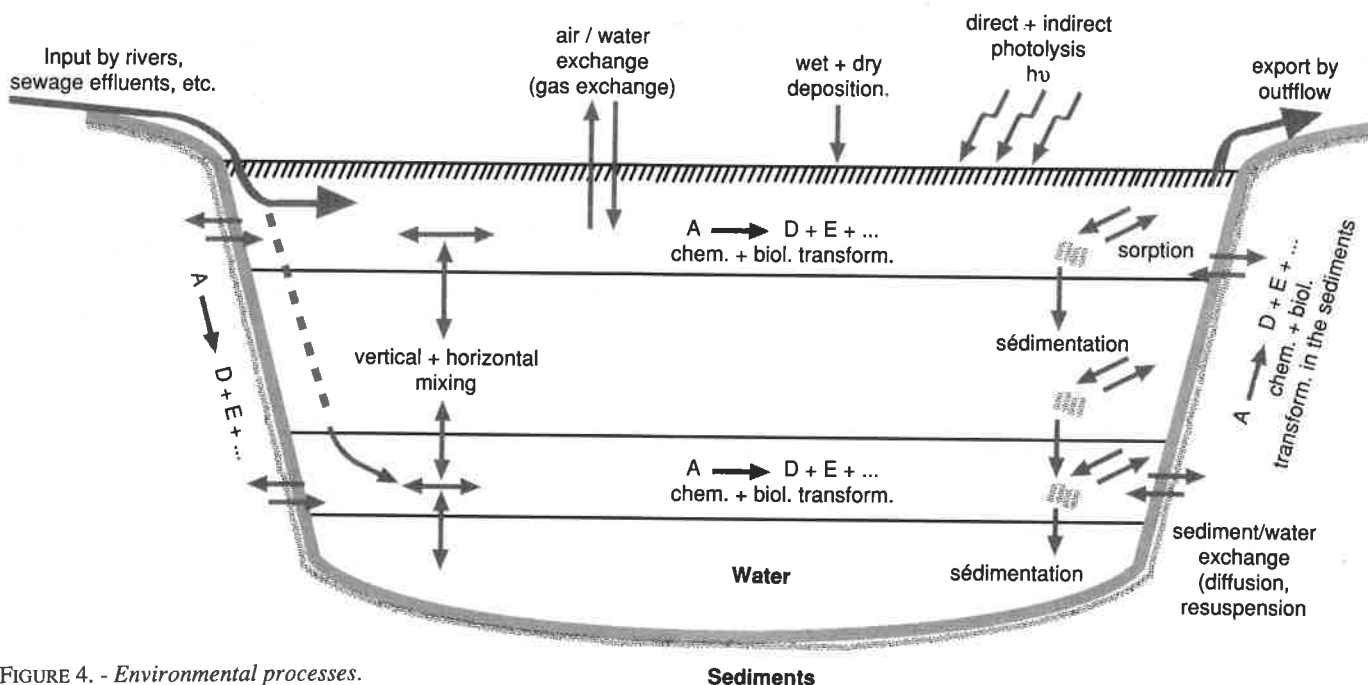


FIGURE 4. - Environmental processes.

Catalysis

Catalysis has played a major role in the rapid development of the chemical, petroleum and petrochemical industries. For the developed economies of the United States, Japan and Western Europe, about 20-25 % of the current GNP is based on the products derived directly or indirectly from catalytic processes. The major petrochemical processes are all catalytic. Also, catalyst technology is changing at a very rapid pace in two basic ways :

First, for the same products, the raw materials and processes changed totally within ten years (1960-70). Second, for the same product and process, the catalyst changes every few years.

In the 1960's, new catalytic petrochemical processes (*Table IX*) based on the cheaper and safer-to-handle ethylene superseded and completely displaced most acetylenic based processes. Thus the same products, made by entirely new catalytic processes, from entirely new, cheaper and safer raw materials.

TABLE IX. - Vinylation before and after 1960.

Product	Before 1960	After 1960
Vinyl chloride	$C_2H_2 + HCl$	$C_2H_4 + HCl + \text{air}$
Vinyl acetate	$C_2H_2 + AcOH$	$C_2H_4 + AcOH + \text{air}$
Methyl vinyl ether	$C_2H_2 + MeOH$	$C_2H_4 + MeOH + \text{air}$
Acrylonitrile	$C_2H_2 + HCN$	$C_3H_6 + NH_3 + \text{air}$

This is not the end of the story. The transition from acetylenics to olefinics has been completed (*Fig. 6*) but now we are in the early stages of the transition from olefinics to paraffinics, syngas and the new C1-chemistry.

The butane-to-maleic anhydride process, the cycloar process to convert propane and butane (LPG) to aromatics, the new ethyl benzene process by alkylation of benzene with ethanol instead of with ethylene, the oxidative coupling of methane to ethane and ethylene, etc., are all typical examples for this second feedstock revolution from olefinics to saturates, occurring in our lifetime. The coming decades in catalysis are full of promise.

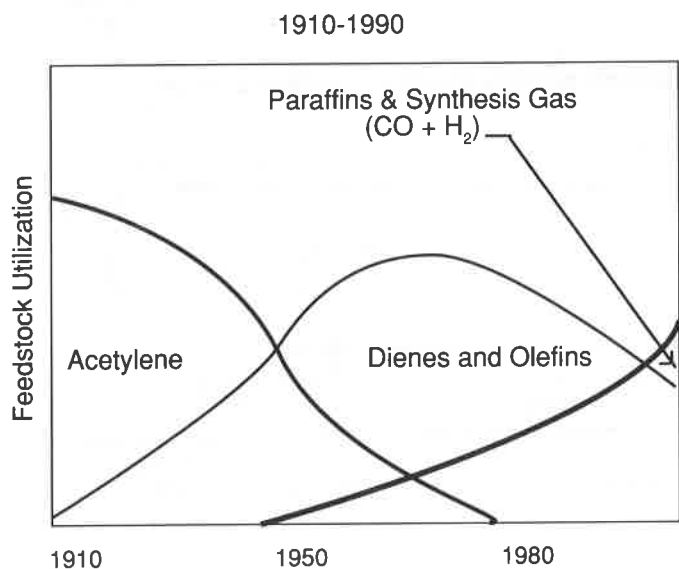


FIGURE 6. - Trends in chemical feedstock.

TABLE X. - Evolution of polypropylene catalysts.

Year	Activity t/kg cat.	Deashing	Isotactic level (%)	Atact. removal	Product shape
I 1972	1-2	Yes	85-92	Yes	Irregular
II 1976	10	No	92-96	Yes	Irregular
III 1989	10-25	No	97	No	Irregular
IV 1983	25	No	97	No	Spherical

The second type of rapid changes in catalyst technology is that, for the same product and the same process, the catalysts are changing every few years.

To illustrate this point (*table X*), let's consider one of the greatest contributions of Italy to modern petrochemical technology : the stereospecific polymerization of propylene achieved by Nobel prize winner Giulio Natta in 1955, and further developed mainly by Montecatini. In 1972, 1 kilogram of catalyst yielded 1-2 tonnes of polymer of lower isotacticity or crystallinity ; this necessitated lengthy and costly unit operations to wash off the rest of the catalyst from the polymer (deashing), to remove the atactic polymer, and finally to shape the material into granules. Ten years later, in 1983, the fourth generation catalyst yields 25 tonnes of higher crystallinity polymer per kilo of catalyst. The concentration of the catalyst in the polymer is now so low that it can do no further harm, hence no deashing is necessary. The atactic polymer is now only 3 % and hence needs no separation. Finally, the fourth generation catalyst provides the polymer product in the form of spheroids ; this eliminates the expense of extruding the polymer and chopping the extrudates to obtain pellets. The number of unit operations or sections in a polypropylene plant was reduced from 16 in the 1972 plant to 9 in the modern plants. The capital investment for a plant was reduced to almost half of what it was ten years ago with the first generation catalyst. This is an outstanding example of how evolution of catalyst technology can influence economics even to the point of eliminating a costly process for pelletizing the product by providing it in a useful shape.

What are the major factors which have accelerated or catalyzed such rapid growth of catalysis science and technology during the last few decades ? There are many. But let me cite three concrete ones which I consider to have been very decisive :

- A multi-disciplinary and truly international approach to make catalysis a science, no longer a black art.
- Development of catalyst characterization techniques, which have reached a stage today so that we can practically see individual atoms on the catalyst surface and their fate during the reactions.
- The development of computers, which have made experiments easier, quicker and more reliable, and which have made mathematical modelling, process simulation and optimization almost routine. Much of the earlier expensive and lengthy pilot-plant work is no longer necessary today.

Such achievements of the past in catalyst technology assure us that the future is going to be still more exciting. In the United States, a few years ago the pimental committee report identified catalysis as one of the crucial thrust areas in the «opportunities for chemistry» in the coming decades.

More recent in the Amundson committee report on «frontiers in chemical engineering research needs and opportunities 1988» highlights four areas in catalysis where significant advances have to be made in the 1990's. These are :

- catalyst synthesis,

- characterization of structure,
- surface chemistry,
- catalyst design.

Some of the major advances in catalyst technology expected in the 1990's are :

- More energy-efficient processes (milder process conditions, fewer process steps, fewer byproducts, little or no recycle).
- New generations of zeolites as shape-selective catalysts.
- Phase-transfer and chiral catalysts to synthesize optical isomers of desired biological or medicinal activity.
- Supported metal catalysts with higher resistance or tolerance to hetero-atoms like sulfur, nitrogen, oxygen, and chlorine.
- Equally active and selective, but much cheaper, substitutes for precious metals like Rh, Ru, Pt, Pd, and Ir, used today in industrial catalysis.
- Cheaper techniques in industrial catalysis regeneration.
- Many more industrial successes for homogeneous catalysis.

Thermoplastics

In general, thermoplastic polymers can be divided into three main groups (*Fig. 7*) covering a performance spectrum ranging from large volume resins like polyvinylchloride (PVC) or polystyrene (PS), through engineering thermoplastics like polycarbonate (PC), polyacetals (POM) and polyamides (PA), to high temperature stable polymers, like polyphenylene-sulphide (PPS), polyethersulphone (PES), polyacrylates (PAR), and liquid crystal polymers (LCP).

Today, 99 + % of the volume of all thermoplastics sold worldwide, is covered by resins developed and introduced before 1980, and true fundamental polymer innovation is declining in favor of modifications of existing polymers by copolymerisation, chemical derivatisation and supplying additives, or by alloying and blending.

The major driving force for this are the enormous resources necessary for development of new polymers, strong intermaterial competition and economics in the final part for the consumer. The use of chemistry and chemical engineering for more efficient use of raw materials for modification and performance upgrading, and polymer application design by computer assisted techniques

indeed allows for an economic application of thermoplastic resins in such diversified markets as foodpackaging, electronics and automotive.

The area of polymer alloys and blends is one of the fastest growing segments of polymer chemistry. Until a few years ago, high academic interest was devoted to the study of thermodynamically compatible polymer systems forming a one-phase mixture with physical and mechanical properties averaging between those of the starting materials. Today, industrial R & D is much more focused towards finding ways to successfully mix two (or more) dissimilar polymers such that the advantageous properties of each individual component are combined into the resulting blend, leading to the commercialization of new price/performance materials.

Key technology developments that help move alloy and blend activities at accelerated rates are :

- Compatibilisers help bridge the interface between polymers that want to separate because of thermodynamic incompatibility.
- Polymeric peroxides to generate covalent bonding between blend components, preventing phase separation.
- Modifiers to provide toughness to polymer blends that would otherwise not be able to withstand mechanical impact.
- Melt compounding equipment with much improved temperature control at high conveying efficiency.
- Continuous reactive extrusion for in-situ generation of grafts for improved compatibility.
- Development of analytical tools to provide better understanding of morphology development and its influence on mechanical properties.

Many high performance thermoplastics are available today (world market 1988 : 34,000 t). Research on high performance materials is geared towards development of products for major markets like aerospace, aircraft, electrical, electronic, and metal replacement. High strength and durability at extreme use conditions over prolonged periods of time are the main motivation actors for their use.

The majority of these new engineering thermoplastics entering the commercial world today (*Fig. 8*) are derived from the condensation of aromatic molecules, providing high heat distortion temperature, high stiffness, good solvent resistance and fire retardancy.

An exciting approach is the use of computer simulation to help predict the physical and mechanical properties of polymers using fundamental properties of atoms, molecules, and groups. The accuracy of such predictions is often within +/- 10 %.

Composites are being used worldwide as light-weight construc-

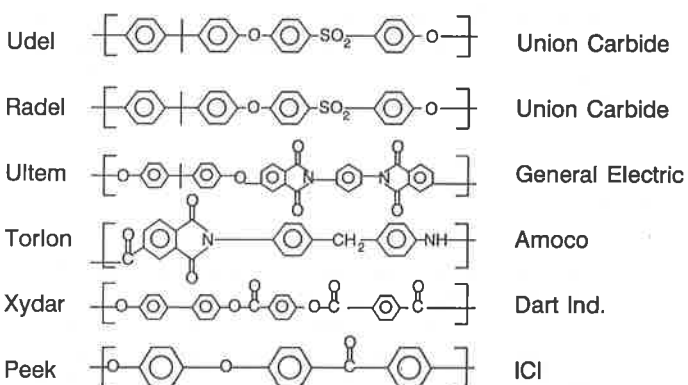


FIGURE 8. - New engineering thermoplastics.

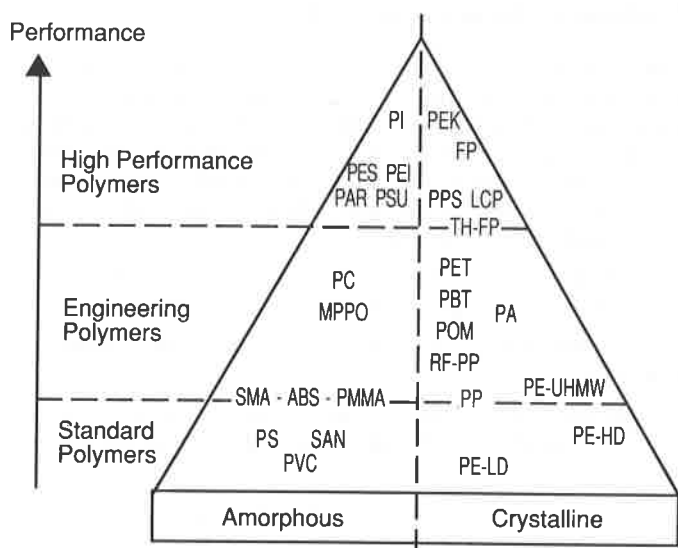


FIGURE 7. - Polymer groups.

tion materials. Traditionally they have been almost exclusively made from thermoset resins. The technologies for processing thermoplastics (injection moulding and extrusion) are very suitable for efficient production of high-volume articles, and much effort is currently devoted to develop composites based on thermoplastic resins.

Various types of reinforcements are being used from particulate fillers, short and continuous glass and carbon fibers to inorganic whiskers. They can be used alone, or in combination with each other. The essence in composites is to transfer the very high tensile modulus and rigidity of the fiber to the polymer matrix to provide a stiff, heat stable material with good dimensional stability and fatigue resistance. To achieve excellent reinforcement, the adhesion between matrix and fiber is very important. Surface treatment, of and the use of coupling agents on the filler, and reactive comonomers in the polymer are being used to increase this adhesion, as well as the ultimate stress transfer potential between the matrix resin and the fiber.

The weak point in thermoplastic composites is their low toughness, and current efforts in industrial research are devoted to improve their impact strength without compromising too much on stiffness - especially by the development of long-fiber reinforced thermoplastic resins.

Thermosetting polymers and composites

Reactive processing to crosslinked networks is an excellent functional definition of this class of plastic materials. Indeed, it covers the 3 main aspects of thermosets : chemical reactivity, processing and performance, linked to the network.

Industrial research programs also concentrate on these three aspects :

- development of new chemistries for reactive processing and curing ;
- new fabrication processes, compatible with the technical and economic factors characterizing an application ;
- development of higher performing materials such as new coating materials with improved durability and corrosion resistance, high temperature and damage resistant composites, or high performance dielectrics in electronics.

Next to these performance materials, the classical thermosetting resins (epoxies, polyurethanes, unsaturated polyesters, phenolics to cite a few), omnipresent in the construction materials, paints, composites for automotive or transformation, and consumer electronics, face the challenge of increased safety for the consumer and the environment.

Research and development programs are already engaged, and it will become increasingly important to develop new technologies for : energy conservation, emission control, post-consumer waste management, and environmental compatibility.

Coatings

The number one industry concerned with emission legislation is the coating industry. The reduction and progressive elimination of solvents, which has already started for general purpose paints, will occur in the more demanding industrial coatings through the development of highsolids, powdercoatings, 100 % solids, and waterbased coatings. Many epoxy or polyurethane solvent based

coatings will be converted either to powder coatings, with the help of new low viscous monomers or new chemistry or water dispersion techniques.

Energy conservation is the driving force for low temperature cure powder coating systems and radiation curing lacquers. New low temperature crosslinking chemistries, a better knowledge of the rheology of water based paints, the understanding of corrosion mechanisms and of interfacial science are fundamental aspects of the research programs engaged.

Other new technologies evolving in the coating industry are :

- microgels with part of the crosslinking already done during the production of the coating polymer,
- IPN's or semi IPN's where linear high polymers are interlaced with thermoset networks to tentatively combine high flexibility and corrosion resistance,
- self-stratifying coatings to reduce the cost of multi-layer application such as for example a corrosion resistant epoxy primer and a decorative weather resistant topcoat, or metallic finishes followed with clear coats.

Foams (polyurethanes)

Besides the escalating cost of energy, global warming is another dictating factor for energy conservation. Demand for insulating construction materials will remain very strong.

The elimination of hard chlorofluorocarbons in polyurethane foams and other foamed thermosets/thermoplastics has drawn considerable resources into industrial research to develop new environmentally acceptable blowing agents, new polyols and foaming technologies for polyurethanes as well as micro - cellular foams to compensate for the reduction of insulating properties associated with the elimination of CFC's.

For maintaining high industrial hygiene standards, the polyurethane industry is also geared towards the elimination of TDI in favor of MDI or other low volatile isocyanates, thus affecting the performance of flexible foams.

Besides the fundamentals of the foaming process, a more fundamental understanding of the fatigue properties in flexible PU foams is needed to serve the cushioning and mattress industry. Improved fire control is also a particularly relevant research area for foamed construction products.

Composites bases on thermosets

Fiber reinforced plastics have been produced exclusively in the past from thermosetting resins. Today, they also face the competition of newly developed engineering thermoplastics composites just described. Their success in large volume applications as replacement of metal parts, for example in automotive, is dependant on a few critical issues being addressed by industry research programs. Those are :

- Recycling technologies (to recovery energy, usable hydrocarbons, or simply for re-use in another form).
- Development of economical and fast fabrication processes for large parts.

Advanced composites for aeronautic, space or military applications have been driven by heavy research funding by governmental agencies.

With much better prospects for profits than a few years ago, and fewer risks involved, industrial corporations are now investing in costly development programs. The increasing acceptance of com-

posite materials in commercial aircraft, including primary structures, and the need to renew large fleets of old planes in the years to come is a good justification. Analysts predict that within the decade the value of composites in commercial aircraft will surpass the value of metal alloys by a factor of three at the horizon 2000.

Technical needs and R & D activities in this area are :

- New toughening technologies such as semi-IPN's with high temperature engineering thermoplastics and controlled particle size polyimides dispersed in bismaleimide resins having adjusted solubility parameters to obtain a gradient of concentration at the interface. In all cases, to be effective, these toughening techniques must be associated with an excellent fiber-resin bond to avoid propagation of cracks at the interface.
- New fabrication processes : RTM (resin transfer molding) is the best technical and economic choice to replace prepregging and autoclaving.
- Fire resistant, low-smoke composites for aircraft interiors. New phenolic resins (such as phenolic-triazine copolymers) show promise.

Electronic Industry

Very large scale integration in electronic components and miniaturization of interconnecting circuitries (multichip modules) will require new high performing resins in terms of :

- higher temperature and oxidative resistance,
- moisture resistant, high purity epoxies for electronic packaging,
- low dielectric constant to minimize signal losses,
- photopolymerizable high performing coatings for imaging and solder resists.

New thermosetting resin chemistries

Finally, to meet the technical challenges for the 1990's and beyond, new chemistries will be needed. Defining thermosetting resins by their function rather than dividing them in the old known categories leads us to the important areas for research and developments :

- Hybrid chemistries. In the future more and more new properties will be obtained by combining in one product the backbone chemistries as well as the functional reactive groups from different resin types. Examples include : polyurethane/unsaturated polyesters, amine functional polyimide oligomers combined with epoxy resins.
- New chemistries for high temperature thermosets such as capped or functionalized polyimides and bismaleimides, benzocyclobutenes and phthalonitrile resins crosslinked via high temperature nitrile polymerization.
- Low polarity resin chemistry for low dielectric constants such as fluorinated hydrocarbons crosslinking via vinyl unsaturations instead of polar reactive groups.
- Molecular reinforcement chemistries incorporating liquid crystal polymers or thermosets containing rigid rods.
- Reduced shrinkage via ring opening crosslinking chemistry.
- Fire-control chemistries eliminating halogens.
- Crosslinkable thermoplastics to close the gap differentiating thermosets from thermoplastics.

Fundamental sciences

- The morphology of high crosslinked thermosets is a science in

its infancy. Publications suggest that topological structural heterogeneities (for instance in epoxy resins) can influence to a large extent mechanical properties, especially toughness, with no effect on glass transition temperatures and modulus.

- The chemorheological modeling of thermoset fabrication processes will help to predict and control properties of composite parts.
- The development of computer assisted molecular design will not quite allow us to practice chemistry without chemicals (!), but help to design resin backbone structures and predict properties.

Agricultural chemicals

The primary role of agriculture is to produce a reliable supply of wholesome food to feed the burgeoning world population, safely and without adverse effects on the environment.

Of the 5.2 billion people inhabiting the world today (1989 est.) approx. 50 % are undernourished or have an unbalanced or inadequate diet, and the world's population is projected to more than double to 11 billion by the year 2050.

Currently it is estimated that 1/3 of the potential world harvest is lost to pests. Without crop protection products, this loss could be twice as high.

These factors, together with the vital role chemical products play in the control of disease vectors such as those for malaria and yellow fever, lead to the conclusion that pesticides are not luxury articles of a technical civilization, but necessities for survival of the world population.

Crop protection products should :

- A - Be highly active, resulting in low rates of use
 - over the past 20 years, typical use rates have declined from kg's/ha to g's/HA as more active products have been discovered. The more active a product, the less has to be applied.
- B - Have no adverse effects on the environment
 - they should not persist in the environment or have the potential to contaminate ground water.
- C - Be selective, giving targeted control with little or no effect on non target organisms.
- D - Possess low potential for the development of pest resistance.

Identification, development and regulatory registration of new agricultural chemicals is a complex, lengthy and very expensive process. While a truly new and outstanding herbicide offers sizeable profit - the risks are high and development must overcome many performance and regulatory obstacles over a period of about ten years. Because of the growing costs of this process and the acceleration of performance of competitive materials, agricultural chemical research has employed many new approaches and new technology in the search for improved pesticides.

Fifteen years ago, new pesticide candidates primarily came from synthesis programs wherein many new compounds were made and these were «screened» or tested in very small scale against a spectrum of pests - insects, weeds, and plant diseases. If activity was found, then a chemically driven search for optimum activity

was undertaken by synthesizing and screening a multitude of chemically related structures.

The primary thrust of the logic though was chemical logic - based upon chemical ways to modify the original molecule showing activity. Since the mid - 70's, this process has evolved to one based far more upon biochemical logic.

Instead of reliance upon random screening of molecules, we are in a much better position to hypothesize based on a knowledge of biochemistry why compounds show activity and how that activity can best be maximized or what non-obvious structural analogues could perform even better.

In this way the focus in agrichemical research has moved from the number and variety of compounds synthesized and screened and discussions of how many new compounds one has to screen to find a new product, to a far more targeted approach of hypothesizing and testing chemical structures that might interfere with a critical life process in the pest organism. The approach involves much more chemical and biochemical sophistication than the previous approach - often employing molecular modelling, quantum chemical calculations, biotechnology based screening tools, separation of enantiomeric species and much more sophistication in quantifying the mechanisms of penetration of the pesticide into the critical parts of the pest.

These new approaches will continue as will the growing demand for products that are ultra-effective on the targeted pest but essentially non-harmful to other species and non-damaging to the environment. The 90's will see fewer new products - because the competition is so difficult and regulatory requirements are so strict - but the products that do evolve will be incredible technology elements with huge value to society. Certainly, also the progress in biotechnological plant modification to improve plant resistant to pests and better cope with environmental pressures will have an impact on agriculture and the use of agricultural chemicals. However, these advances are far more difficult than portrayed earlier in the popular press.

Progress is happening, but it is a longer term process and wide application in the major global crops will be minor prior to the turn of the century.

In terms of the process chemistry needed to produce new agricultural chemicals - suffice it to say that it is state of the art in the area of scaling up from the flask to the chemical reactor. The new pesticides and their process technology resemble pharmaceuticals more than industrial chemicals - both in complexity of chemistry and in production volume of a full scale plant.

In summary, agricultural chemistry will continue to evolve both in chemical and biochemical sophistication to produce more effective yet environmentally friendly products to meet the evolving needs of agricultural production.

TABLE XI. - Advanced ceramics.

Oxides	$\left\{ \begin{array}{l} \text{Al}_2\text{O}_3 \\ \text{BeO} \\ \text{ZrO}_2 \end{array} \right.$
Carbides	$\left\{ \begin{array}{l} \text{B}_4\text{C} \\ \text{SiC} \end{array} \right.$
Nitrides	$\left\{ \begin{array}{l} \text{Si}_3\text{N}_4 \\ \text{AlN} \end{array} \right.$
Spinel	$(\text{Al}_2\text{O}_3, \text{MgO})$
Mullite	$(3\text{Al}_2\text{O}_3, \text{ZSiO}_2)$
For structural applications	
- Machinery and process equipment : nozzles, dies, pump seals.	
- Cuttings tools.	
- Military uses - armor and armor penetration.	
- Nuclear applications - neutron shielding based on B_4C and its alloys.	
For electronic applications	
- Integrated circuit packages.	
- Substrates for printed circuits.	
- Multilayer capacitors.	
- High temperature superconductors.	

In structural applications they offer hardness and incredible resistance to wear, corrosion, and heat. In electronics end-uses, they offer the ultimate in compositional and dimensional stability over a wide range of operating temperatures. The field of high temperature superconductivity is a world in itself - suffice it to say that unique materials based on mixed oxide structures of lanthanum, barium, copper and other metals are being intensively researched throughout the world following the pathfinding work of Bednarz and Muller at the IBM Lab near Zurich.

In terms of properties in the structural and electronic substrate applications, major technical challenges must yet be solved for ceramics to develop to their great potential. And as the potential is great - so are the challenges. In simplest terms, the problems are :

- A. Achieving structure control to obtain high performance.
- B. Improving the synthesis of ceramic compositions.
- C. Significantly simplifying part fabrication.
- D. Reduction of cost of finished articles.

Each of these merits a brief discussion, because the problems are significant.

1. The great hardness and abrasion resistance of ceramics is often offset by their brittleness. Use of high purity raw materials has helped, but control of grain size in submicron particles must improve to improve microstructure and interfacial properties. The strong chemical bonds in these materials often do not reflect in high performance parts because of external defects such as flaws, grain boundaries, secondary phases and pores.

To reach the extreme value of fracture toughness for current ceramics, flaws must be less than 100 μm - and this means one must have structure control on the nanometer scale. Another approach receiving great attention is to use ceramic whiskers and other reinforcing materials to produce composite structures. While this method holds promise, it adds another layer of complexity. Further, it does not appear at this time to reduce the just mentioned need for exceptional microstructure control.

2. These advanced ceramics are produced at very high temperatures ($\sim 2000^\circ\text{C}$) using very pure raw materials in small production

Advanced ceramics

As we consider materials with great promise for the nineties and beyond, the realm of advanced ceramics (Table XI) is full of potential - and many believe sales of these materials could exceed \$ 10 B/year by 2000. Their basis composition is primarily either oxides, carbides, or nitrides of such metals as aluminium, silicon, zirconium and boron. Some materials such as spinel and mullite are combined oxides of several metals such as aluminium and silicon or aluminium and magnesium. Currently Al_2O_3 represents over 80 % of the advanced ceramics material market. These advanced ceramics display properties that offer great promise, both in structural and electronic applications.

facilities. Prices range from \$ 6 to over \$ 100/LB depending on type of ceramic powder purity level, particle size and quantity. To increase volume, prices must come down.

3. Currently, parts made from ceramics are generally simple shapes machined from small blocks or tiles. The direct production of complex shaped parts is a difficult challenge involving high temperature, high pressure compaction. Progress in this technology is absolutely vital to expand the end-use spectrum for advanced ceramics. The challenge is only increased by the previously mentioned need for the ultimate in microstructure control.

4. All of the above factors make the production of advanced ceramics parts a very expensive process. To allow competing for a bigger segment of materials markets, cost reduction in all the above areas will be absolutely necessary.

In summary, advanced ceramics offer truly outstanding properties

- if progress can be made in the reliability, base and cost of production and fabrication. The challenge is big - but so are the potential rewards.

Conclusion

I would like to leave you with the feeling that industrial chemical research has many opportunities as we move into the nineties. We are challenged to meet many economic and societal needs and we have an incredible array of tools to help us. I am excited and optimistic about the 1990's - I see huge opportunities - I hope you do too. I believe industrial chemical R & D is a great occupation - we are paid and supported to change things for the better. We have made great gains in the past and the nineties promise even more excitement.