Catalysis in Transition - II

A key discipline in a new millennium

In Part I of this commentary, published in Cattech 6-3, catalysis was placed in the context of a rapidly changing era of science and technology. The influences range from commercialism, to substantive changes in government policies for funding R&D, to the place of the research university in today's society. Catalysis reflects all of these influences, and represents almost a classic case of metamorphic change in a scientific discipline. This change emerged from the observation that chemical reaction rates could be greatly affected by minuscule amounts of regenerable materials. In the process, catalysis uncovered reaction mechanisms, and indicated some very basic chemistry; some might say that catalysis is about a pure a form of chemistry that one can find.

Petrochemistry ruled catalytic research for many years, to the point that catalysis was often regarded as the handmaiden of the oil business. It struggled to gain a new form with the advent of polymerization technology, and underwent yet another change when the catalytic viewpoint was extended to the manufacture of drugs. Other metamorphic changes have occurred, and along the way the changes were being amplified and varied in great numbers. Many of the changes were technically useful before they were understood, a phenomenon that is frequently illustrated in scientific history.

In the new era of science, computer modeling techniques have become powerful means for understanding and predicting the behavior of matter at the atomic level; nowhere is this better exemplified than in catalysis. Computational models can now illustrate accurate pictures of catalyst structure, of molecular sorption and diffusion, as well as reaction mechanisms. The methodology has also been extended to solid-state synthesis, and, in this context, there is a new, rather close, connection between the design and development of new catalysts with the design and development of new semiconductor materials. The common factor seems to be the pervading influence of surface science.

While computational expertise is proving of great value, the accumulated experience of industry remains of equal value. More than a decade ago, Frits M. Dautzenberg enumerated some guidelines for new catalyst testing. These have become a kind of developmental benchmark. In discussing the guidelines, Dautzenberg noted that companies practice a "sunset strategy," wherein the conservation of the value of the materials is emphasized, with very small R&D budgets. The implication is that ever higher productivity is necessary, with less invested capital. Also, in most organizations, the budgets for catalysis R&D come from profits, the government or outside clients. This presents a very great challenge to the catalysis community.

Within academe, in situ spectroscopy has emerged as a new tool for elucidating mechanisms at the molecular level. Also, the unification of catalysis and reaction engineering with surface physics is pointing to new directions in research and process development. It has now become accepted by most industrial practitioners that catalysis, reaction development, and process development be integrated with the initial considerations of a new product development in a firm. The scientific and technical staffs should be present, with the business and marketing staffs, to ensure economic optimization within the company.

In the tide of globalization, many companies have elected to downsize, or sometimes even eliminate, their internal R&D organizations in favor of an inter-company outsourcing R&D contractor. At the 2001 Toronto meeting of the North American Catalysis Society, Ian Maxwell, the new director of Avantium Corp., noted that much of Avantium's staff and project program derived from the laboratories of Shell-Amsterdam, when the latter downsized its research effort. Avantium now includes Akzo, Eastman, W. R. Grace, Shell, Glaxo and several Dutch universities, further indicating that academe and industry have formed a new and closer association. The reasons for the association are usually given as avoiding duplication of effort by competing companies, and the need to apply the on-site engineering expertise to quick commercialization of promising technology. Although its operations are much broader in scope than only catalytic processing, Avantium is building a large data base on catalysis and catalytic technology.

Elsewhere in Europe, Rhone-Poulenc has evolved into Rhodia, and formed a close association with Hoechst. In the U.S., Dow Chemical Co. and Union Carbide have merged with the corresponding downsizing of the combined development staff. Exxon has merged with Mobil, and British Petroleum has merged with Amoco Oil Co., both resulting in major downsizing of the R&D efforts. A group of ten European companies, and four universities, have formed *Eurokin*, a seven-country consortium to facilitate development work in chemical kinetics and associated areas. The expectation is faster development of products for the marketplace, as well as quicker response from more traditional research organizations in training students and promoting contract research. In Switzerland, the Novartis Group has emerged from several drug and fine chemical firms. Its function is research and development under contract or license, with the expectation that the bench-to-market development period will be drastically reduced.

In Japan, the chemical industry, academe, and the government are associated in close proximity, and there have been numerous restructuring efforts in recent months. In all cases, the purpose is to "cut costs and become more competitive." One of the newest Japanese developments is "integrated microchemistry." This is the Japanese version of the chemical plant on a chip. The prototype is a 3 x 7 cm glass slide etched with channels 100 microns deep. Reactants flow through the channels, mix, react, experience product separation, etc. A dedicated microscope follows the tracks by monitoring the heat produced. It has already been found that chemical behavior in the channels of the chip is different from that in conventional reactors. Rates are invariably higher, associations at the atomic level are greater, and there are very high concentration and energy gradients within the channels. The Japanese Ministry of Economy, Trade and Industry has funded a five-year program for the development of the concepts of integrated microchemistry. Other development programs are underway.

On 16 April 2002, hte Aktiengeselschaft (Heidelberg) announced that it will coordinate a consortium effort to develop catalytic systems to remove NOx and soot particles from diesel exhaust. The consortium consists of Daimler-Chrysler AG, OMG AG & Co., Robert Bosch GmbH, Volkswagen AG, and research centers at the University of Heidelberg, University of Karlsruhe, University of Leipzig, and the University of Stuttgart. The funds are already committed from industry and the German government. This is typical of the newer efforts in directed catalytic R&D.

It should be apparent that catalysis is in the throes of a metamorphic regeneration that includes all of the traditional areas of interest, as well as many new ones, thus broadening the scope and including many new disciplines that may have formerly been outside the realm of catalytic chemistry. The globalization that has gripped much of the world's commerce in the past few years is now being seen as less of a benefit than a developmental impediment. The idea that a country need merely computerize its activities to gain instant world economic status has proven erroneous. It is still necessary to provide goods and services at a profit, and this requires reinvestment of capital, as well as profits. It also requires scientists and engineers to continually modernize their skills and viewpoints. In the chemical business it also constitutes a new era for catalysis.

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