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Problem Solvers and Thinkers

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History shows that strong societal pressure can accelerate scientific breakthroughs. The well-known story of the development of ammonia synthesis in the years preceding World War I provides an excellent example of how an essential threat to society may mobilize scientists and drive discovery. Less well known is how the status of science and technology affected this outcome. At the time of the European continental panic about the nitrate supply, Wilhelm Ostwald had laid the foundation of physical chemistry. Once Fritz Haber discovered the catalytic process, it took only eight years and the genius of Carl Bosch to set up production. Technology progresses through the interplay of science and technology, of thinkers and problem solvers. Both are driven by the perceived urgency of the problem. The current public awareness of the dangers of greenhouse gas emission and the need for new energy resources is comparable to the public debate a century ago on the replacement of natural saltpeter. How can thinkers and problem solvers in chemistry help alleviate the urgent problems of our time?

Catalysis for Change

If we are to answer this question, we need to study the present state of both science and technology. This was the view of the Dutch physicist Hendrik Casimir as formulated 50 years ago, after he had directed research at Philips for many years. He observed that science and technology are intertwined in two interrelated cycles. Existing methods and techniques can solve current challenges. But in realms where no technological answers exist, we need new scientific insights. The two cannot be separated, and each benefits from the other's progress. To have novel technologies available, scientific endeavor is indispensable. With this in mind, a team composed of my colleague Djan Khoe, the science writer Bram Vermeer, and myself interviewed leading thinkers and problem solvers. We asked about potential innovations that could solve the problems of our time. In which areas are we well enough equipped to force a breakthrough? How can the scientific community be mobilized as in the time of Haber? The results of these interviews are documented in the book *2030: Technology That Will Change the World* (see the book review from G. Whitesides in *Angewandte Chemie*).[1]

The book contains many promising innovations outside the realm of chemistry, such as body scans, optical communication, and deep geothermal energy. Yet chemistry plays an important role in our vision for the future. In particular, we note the central role of catalysis in solving the problems of our time. This isn't surprising to anyone who knows the history of catalysis. Ever since the days of Haber, catalysts have proven to be central in improving processes. Catalysts offer better control, increased efficiency, and new ways to use material—all key ingredients in solving problems.

In what areas can we force a breakthrough?

A few examples: the Haber–Bosch catalyst based on iron also turned out to be an excellent catalyst for hydrocarbon synthesis from synthesis gas, which was discovered a decade later by Franz Fischer and Hans Tropsch. This process lessened dependence on crude oil, opening as it did the way to make fuels from alternative sources such as coal, and nowadays also biomass and natural gas. Similarly, other catalytic techniques have been devised to meet societal needs. Complex noble-metal-based catalysts in automotive exhaust reduce harmful nitrate emissions. Nanoporous zeolites, which are synthetic minerals, are applied as solid acid cracking catalysts of crude oil to produce useful fuels with superior efficiencies. As a substitute for clay catalysts, they have improved the efficiency of energy conversion dramatically.

Progress in catalysis technology has always been determined by an urgent demand from society. While the urgency sometimes comes from impending war, the above examples show that concerns about pollution and dependency on oil have also generated sufficient impetus.

Downsizing Production

Today catalysis research and technology offers a new road towards energy efficiency and precision in the use of materials. We have gained incredible insight into the function of catalysts and other complex systems. Single-molecule manipulation, self-organization of complex molecular assemblies, and complex and functional nanoscale materials have become cutting-edge research fields..

This development gives us the possibility of dramatically shrinking products

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and production facilities. As computer technology undergoes a corresponding minimization, we have a unique opportunity to integrate chemistry with intelligence. This leads to a paradigmatic shift in industry: we no longer rely on scaling up to gain efficiency. Downsizing has the advantage of greater precision. It makes it possible to operate processes close to their thermodynamic optimum, and control is faster. So microfluidic processes will lead to more efficient production, may solve many logistic challenges, and will lead to a better use of materials. So why not reverse the size spiral and shrink the equipment?

The challenge is to introduce such new technologies fast enough to carry weight in solving the challenges of our time. Large-scale technological transformation, necessary to introduce microfluidic production, will cost time. Industries have developed networks of symbiotic relationships and long "food chains" of suppliers. Like a natural ecosystem, the complex "chemotope" of interrelated industries can survive small changes. Introducing a new "species," however, such as microplants, may precipitate the entire system's fragmentation and trigger total system change. The economist Joseph Schumpeter called this process "creative destruction," a phase transition reminiscent of the scientific revolutions later described by Thomas Kuhn. We encounter such transitions in other complex systems, such as ecosystems, autocatalytic processes, and the earth's climate.

Dramatic changes on this order need decades to come about. Two colleagues from Shell, Gert Jan Kramer and Martin Haigh, have recently shown that there are physical limits to the rate at which new technologies can be deployed.[2] New technologies that could replace capital goods grow at a rate of one order of magnitude per decade. This is because their introduction involves a lot of testing and the construction of different generations of demo plants. After reaching a market share of a few percent, the exponential growth levels off to match the replacement rate of old installations. This means it will take 30 years for a new energy conversion technology to reach 10 percent of world energy production. Similarly, it may take decades before we buy detergent directly from a microplant in the supermarket.

Intelligent Catalysts

We can't wait that long. If new technology is to be of any help in solving the problems of our time, the time to deployment must be shortened. A massive investment in research will certainly help. This should be directed at finding ways to accelerate the implementation of promising technology. The challenge is to reduce the complexity, cost, and speed of implementation of new technologies for mass production. This is a matter of both science and technology.

Computational tools multiply our capacities.

In catalytic technology we are on the brink of a significant acceleration of discovery and industrial implementation. This is due to pioneers such as Gerhard Ertl and Gábor Somorjai, who have spent most of their lives unraveling the atomic processes on the surface of catalysts. The insights they have won enable us to make computer simulations of new catalytic materials for unexplored reactions, which in turn narrows the experimental search for catalyst discovery. As a result, catalyst discovery is becoming a molecular engineering design skill, bypassing much of the empirical art of "learning by doing." This shortens the development of a new technology and delivers heightened precision. Thus computers replace much physical testing, which gives us the necessary speed to implement new technologies.

This is only the beginning of the profound influence of autonomous computer operation on innovation in the chemical industry. The marriage of catalytic technology with computer technology multiplies our capacities. One example is in automotive exhaust emission control, where sensors and catalysts cooperate. Yet the potential scope is much wider. Catalysts can be considered process multipliers, enhancing energy and material efficiency. Computer technology is a multiplier of intelligence, implying control, feedback, and adaptation and ultimately self-organization. Employed in concert, these could solve the urgent problems of humanity on a time scale of a decade rather than half a century. There is no shortage of problems that demand solutions within one generation. The demands for sustainable energy translate into a need for improved electrocatalytic hydrolysis to supply hydrogen; efficient and high-density batteries to store and transport electricity; different and new conversion systems for carbon dioxide, biomass-related systems, and solar energy; and access to purified surface water, to name a few.

New computational tools will enable a faster implementation of new technology. Yet we can't simply hire computer programmers to create these for us. It is important to realize that these tools are the result of the desire to understand the atomic basis of chemistry and the complexity of the reacting system. Ertl didn't have an application in mind when he set out to understand ammonia catalysis. At the time of his research the process was already near optimum. The new tools he and his colleagues designed for their discoveries are the result of pure science. Therefore, investments are needed beyond merely specific efforts. Science funding organizations should balance application-oriented project funding with research directed at the unsuspected, driven by curiosity and the will to understand. The practical brain of the engineer and the imaginative brain of the scientist complement one another. By providing funding for both, the twin helices of science and technology can evolve and continue to sustain each other. We need both problem solvers and thinkers.

[1] G. Whitesides, *Angew. Chem.*, 10.1002/ange.201106671; *Angew. Chem. Int. Ed.*, 10.1002/anie.201106671.

[2] G. J. Kramer, M. Haigh, *Nature* **2009**, *462*, 568