TECHNOLOGY VISION

2020

The U.S. Chemical Industry

AMERICAN CHEMICAL SOCIETY

AMERICAN INSTITUTE OF CHEMICAL ENGINEERS

CHEMICAL MANUFACTURERS ASSOCIATION

COUNCIL FOR CHEMICAL RESEARCH

SYNTHETIC ORGANIC CHEMICAL MANUFACTURERS ASSOCIATION

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TECHNOLOGY VISION 2020

THE U.S. CHEMICAL INDUSTRY*

The U.S. chemical industry . . .
leads the world in technology development, manufacturing, and profitability.

The U.S. chemical industry . . .
is responsible for breakthroughs in R&D that enhance the quality of life worldwide by improving energy use, transportation, food, health, housing, and environmental stewardship.

The U.S. chemical industry . . .
leads the world in creating innovative process and product technologies that allow it to meet the evolving needs of its customers.

The U.S. chemical industry . . .
sets the world standard for excellence of manufacturing operations that protect worker health, safety, and the environment.

The U.S. chemical industry . . .
is welcomed by communities worldwide because the industry is a responsible neighbor who protects environmental quality, improves economic well-being, and promotes a higher quality of life.

The U.S. chemical industry . . .
sets the standard in the manufacturing sector for efficient use of energy and raw materials.

The U.S. chemical industry . . .
works in seamless partnerships with academe and government, creating "virtual" laboratories for originating and developing innovative technologies.

The U.S. chemical industry . . .
promotes sustainable development by investing in technology that protects the environment and stimulates industrial growth while balancing economic needs with financial constraints.

*U.S. chemical industry is defined as U.S.-based production and R&D

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FOREWORD

In 1994, technical and business leaders in the U.S. chemical industry[1] began a study on the factors affecting the competitiveness of the industry in a rapidly changing business environment and set out to develop a vision for its future. The work focused on needs in research and development (R&D) capabilities, which are directly linked to growth and competitive advantage.

This study was also stimulated by a request from the White House Office of Science and Technology Policy for industry advice on how the U.S. government could better allocate R&D funding to advance the manufacturing base of the U.S. economy. Since then, more than 200 technical and business leaders have investigated the challenges confronting the chemical industry today. (A list of the contributors is on page 67.) The results of this work, contained in *Technology Vision 2020*, emphasize opportunities for advancement in R&D capabilities. *Participants concluded that the growth and competitive advantage of our industry depend upon individual and collaborative efforts of industry, government, and academe to improve the nation's R&D enterprise.*

To assemble these conclusions and recommendations, staff and members of the American Chemical Society (ACS), Chemical Manufacturers Association (CMA), American Institute of Chemical Engineers (AIChE), Council for Chemical Research (CCR), and Synthetic Organic Chemical Manufacturers Association (SOCMA) formed the Technology and Manufacturing Competitiveness Task Group (TMCTG). The charter of the TMCTG was to

- provide technology vision and establish technical priorities in areas critical to improving the chemical industry's competitiveness;
- develop recommendations to strengthen cooperation among industry, government, and academe; and
- provide direction for continuous improvement and **step change** technology.

Over the course of several months, the TMCTG convened 36 formal working meetings and 20 technical sessions to review and establish consensus on requirements within the chemical industry. The task group also polled senior management on the industry's business needs, seeking to link technical recommendations to pressing business issues. Four technical disciplines were selected as crucial to the progress of the chemical industry. They are

- new chemical science and engineering technology,
- supply chain management,
- information systems, and
- manufacturing and operations.

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[1] This report does not focus on the needs of the pharmaceutical industry, but rather examines the chemical industry as the supplier and user of basic chemicals.

In addition to the technical work groups, a study group was put together to research existing concepts of sustainable development, such as those developed by the President's Council on Sustainable Development and the International Council of Chemical Associations (ICCA). The study group provided these concepts to members of the technical groups as major considerations in their future-oriented technology recommendations.

A second study group also reviewed ideas for partnerships among industry, government, and academe. The group concluded that in this age of reorganization, the synergy of collaboration often has a ''multiplier effect'' on our nation's pool of talent, equipment, and capital available for R&D. The conclusions of the four technical and two study groups were reviewed at a public workshop in May 1995 hosted by the TMCTG and attended by 120 leaders from industry, government, and academe. Final recommendations and conclusions are contained in *Technology Vision 2020.*

Technology Vision 2020 is a call to action, innovation, and change. The body of this report outlines the current state of the industry, a vision for tomorrow, and the technical advances needed to make this vision a reality. The vision, like the industry, will evolve as the industry faces new realities and challenges. *Technology Vision 2020* is the first step of a continuous journey—one that will see the U.S. chemical industry continue as a global leader in the next century. We thank you, the reader, for considering our report and are grateful for the outstanding professional contributions of our many working members and reviewers.

Sincerely,
Members of the Steering Committee
John Oleson, Dow Corning
Victoria Haynes, B. F. Goodrich
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ACKNOWLEDGMENTS

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As with any project, there are also people whose contributions merit particular thanks. Special efforts were made by John Oleson, Victoria Haynes, Susan Turner, Diana Artemis, and Hank Whalen to overcome challenges and keep this project on track. Gerry Lederer also helped facilitate meetings during the early part of this project. Leadership for the development of each of the chapters was given by John Oleson, Victoria Haynes, Brian Ramaker, Hank Whalen, and Bob Slough. These people also served as spokespersons for this project during its two-year development. Tom Sciance and Mike Saft wrote separate sections on sustainability and partnerships that were incorporated throughout the document. Other important contributors to the format and content of the report were Mark Barg, John Munro, Dave Rudy, Mike Saft, and Steve Weiner.

The New Chemical Science and Engineering Technology chapter was produced by various team leaders, who led the development of different sections. Special recognition is given to Bob Dorsch, Jim Trainham, Don McElmore, Miles Drake, Jerry Ebner, Francis Via, Chuck Rader, Jean Futrell, and Hratch Semerjian. This chapter was aided by invaluable writing and editorial assistance of Arnold Eisenberg.

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EXECUTIVE SUMMARY

Our Challenges

The chemical industry faces heightened challenges as it enters the 21st century. Five major forces are among those shaping the topography of its business landscape:

- increasing globalization of markets,
- societal demands for higher environmental performance,
- financial market demands for increased profitability and capital productivity,
- higher customer expectations, and
- changing work force requirements.

How the industry meets these challenges will affect the entire American economy. The U.S. chemical industry is the world's largest producer of chemicals (value shipped, $367.5 billion in 1995), contributing the largest trade surplus of any non-defense-related sector to the U.S. economy ($20.4 billion in 1995), representing 10 percent of all U.S. manufacturing, and employing more than 1 million Americans. The chemical industry, faced with an ever-changing business environment, must work individually and collectively to remain a world leader.

Meeting the Challenges

We believe the chemical industry in the United States must confront these new market pressures head-on. With the goal of creating a technology "roadmap" for the chemical industry to follow, we examined the technical disciplines of new chemical science and engineering technology, supply chain technology, information systems, and manufacturing and operations. From our assessment of the industry's needs in these areas, we determined that the chemical industry must accomplish five broad goals over the next 25 years. It must

- improve operations, with a focus on better management of the supply chain;
- improve efficiency in the use of raw materials, the reuse of recycled materials, and the generation and use of energy;
- continue to play a leadership role in balancing environmental and economic considerations;
- aggressively commit to longer term investment in R&D; and
- balance investments in technology by leveraging the capabilities of government, academe, and the chemical industry as a whole through targeted collaborative efforts in R&D.

Steps to Getting There

To meet its goals, the U.S. chemical industry should accomplish the following.

Generate and use new knowledge by supporting R&D focused on new chemical science and engineering technologies to develop more cost-efficient and higher performing products and processes.

Capitalize on information technology by working with academe, federal and national laboratories, and software companies to ensure compatibility and to integrate computational tools used by the chemical industry. Develop partnerships for sharing information on automation techniques and advanced modeling.

Encourage the elimination of barriers to collaborative precompetitive research by understanding legislation and regulations that allow companies to work together during the initial stages of development.

Work to improve the legislative and regulatory climate by the reform of programs to emphasize performance rather than a specific method of regulatory compliance, and a greater consideration of cost, benefits, and relative risk.

Improve logistics efficiencies by developing new methods for managing the supply chain and by sponsoring an effort to shape information technology and standards to meet the industry's manufacturing and distribution needs.

Increase agility in manufacturing by planning manufacturing facilities capable of responding quickly to changes in the market-place using state-of-the-art measurement tools and other technologies for design, development, scale-up, and optimization of production.

Harmonize standards, where appropriate, by working with governments within the United States and internationally, and with independent standards groups on nomenclature, documentation, product labeling, testing, and packaging requirements.

Create momentum for partnering by encouraging companies, government, and academe to leverage each sector's unique technical, management, and R&D capabilities to increase the competitive position of the chemical industry.

Encourage educational improvements through the advancement of strong educational systems and by encouraging the academic community to foster interdisciplinary, collaborative research and provide baccalaureate and vocational training through curricula that meet the changing demands of the industry.

Technical Recommendations

TECHNOLOGY AREA 1: NEW CHEMICAL SCIENCE AND ENGINEERING TECHNOLOGY

Chemical science is the most fundamental driver of advances within the chemical industry. Maintaining and improving the competitiveness of the U.S. chemical industry requires advances in three areas of chemical science: chemical synthesis, bioprocesses and biotechnology, and materials technology.

Chemical Science

CHEMICAL SYNTHESIS

The traditional tools of chemical synthesis in use today are organic and inorganic synthesis and catalysis. Synthesis is the efficient conversion of raw materials such as minerals, petroleum, natural gases, coal, and biomass into more useful molecules and products; catalysis is the process by which chemical reactions are either accelerated or slowed by the addition of a substance that is not changed in the chemical reaction. Catalysis-based chemical syntheses account for 60 percent of today's chemical products and 90 percent of current chemical processes.

To take full advantage of the potential offered in chemical syntheses, industry should work to (1) develop new synthesis techniques incorporating the disciplines and approaches of biology, physics, and computational methods; (2) enhance R&D collaborations in surface and catalytic science relevant to commercial products and processes; (3) promote enhanced understanding of the fundamentals in synthesis, processing, and fabrication for structure control of complex molecular architectures; and (4) support fundamental studies to advance the development of chemistry in alternative reaction media (gas phase, water, supercritical fluid, etc.).

BIOPROCESSES AND BIOTECHNOLOGY

Humans have used biologically based processes (bioprocesses) since they first made cheese, leavened bread, and brewed spirits. Systematic exploration of biological catalysts (biocatalysts) began approximately 100 years ago with initial studies of enzymes, protein-based catalysts found in living organisms. Bioprocesses are increasingly used to produce chemical products, and there is a whole world of potential biocatalysts to be discovered.

Each sector of the chemical enterprise has a role to play in advancing the use of biotechnology. (1) Industry should define R&D necessary to discover, develop, and provide more powerful and efficient biocatalysts, more effective process technology, and low-cost raw materials for bio-processes. (2) Academe should broaden the knowledge base relevant to industrial bioprocesses (such as metabolic pathway engineering, enzyme discovery and optimization, and efficient reaction and separation technology) and use results of biotechnology research in health and agriculture to seek discoveries in bioprocessing. (3) Government should encourage, support, and participate in precompetitive biotechnology R&D, while supporting long-term, high-risk technology development and demonstration.

MATERIALS TECHNOLOGY

The development of new synthetic materials has fueled the growth of the chemical industry and revolutionized our society in the 20th century.

Replacement of traditional materials such as metals, wood, glass, and natural fibers with synthetic polymers and composite materials has resulted in products with lower weight, better energy efficiency, higher performance and durability, and increased design and manufacturing flexibility.

Further improvements in the design, fabrication, and quality of materials can be made only if industry (1) works together with academe to promote interdisciplinary approaches to materials science, including the integration of computational technology; (2) defines key needs in structure–property understanding and fundamental information, which can be used to design and tailor materials; (3) works with federal laboratories and academe to develop practical materials synthesis and processing technologies that focus on efficient manufacture of advanced materials systems; and (4) promotes efforts to define common approaches for disassembly and reuse of materials.

Enabling Technologies

PROCESS SCIENCE AND ENGINEERING TECHNOLOGY

Process science and engineering technology (PS&ET)— which includes engineering technologies; engineering science; and engineering design, scale-up, and construction— dates back to the 1930s and is the foundation for the development, scale-up, and design of chemical manufacturing facilities. When effectively integrated with basic science and enabling technologies, PS&ET offers great potential for bringing science and quantitative understanding to the service of the chemical industry, permitting much higher capital utilization, improved yields, reduced waste production, and improved protection of human health, safety, and the environment.

To exploit the potential of PS&ET, industry should (1) work with government and academe to develop relevant process software and real-time measurement tools; (2) support engineering research in nontraditional reaction and separation systems (e.g., plasma, microwave, photochemical, biochemical, supercritical, cryogenic, reactive extraction and distillation, and membrane reactors); and (3) pursue the development of new concepts in flexible manufacturing, process technology for high-performance materials and structures, disassembly and reuse of materials, solids processing, and “smart” processes.

CHEMICAL MEASUREMENT

Chemical analysis is a critically important enabling technology essential to every phase of chemical science, product and process development, and manufacturing control. New knowledge and insight provided through chemical measurement greatly accelerate progress in chemical science, biotechnology, materials science, and process engineering by providing reliable data to evaluate current and emerging technologies.

To ensure that chemical measurements meet the needs of the chemical industry in the future, the industry should (1) promote centers of excellence focused on chemical measurements and process analytical chemistry in order to probe molecular processes; (2) establish a task force to assess the chemical process industry’s measurement priorities and related modeling and database needs; (3) develop instrumentation interfacing standards to enable use of distributed analytical networks and more efficient data acquisition and control systems; and (4) support development of high-performance spectrometers, as well as robust measurement techniques for real-time analyses.

COMPUTATIONAL TECHNOLOGIES

Computational technologies have a broad range of applications, from molecular modeling to process simulation and control. Today, these technologies are embodied in almost every aspect of chemical research, development, design, and manufacture. Those most critical to the chemical industry include computational molecular science, computational fluid dynamics (CFD), process modeling, simulation, operations optimization, and control.

In the area of computational technologies, industry should (1) assess and assign priority to its CFD simulation needs and explore software paradigms for CFD tools; (2) support further development of high-performance desktop workstations, large and fast vector-processor machines, and highly parallel processors; (3) encourage improvements in national networks to allow high-speed communications, on-line collaborations, and efficient data transfer; (4) support experimental validation of, or challenges to, computational results; and (5) pursue public–private partnerships for illustrative implementation of larger advisory systems.

Technology Area 2: Supply Chain Management

The chemical industry has concentrated on science and production and also has given substantial attention to manufacturing. But it has given less attention to the supply chain, defined as the critical link between the supplier, the producer, and the customer. Supply chain management comprises

- planning and processing orders;
- handling, transporting, and storing all materials purchased, processed, or distributed; and
- managing inventory.

Today, many estimate the costs associated with supply chain issues to be approximately 10 percent of the sales value of delivered products domestically and as much as 40 percent internationally. To improve its efficiency in managing the supply chain, and thus increasing its competitiveness, the industry should

- encourage implementation of the Chemical Manufacturers Association's Responsible Care® initiatives throughout all logistics operations, including third-party service providers;
- encourage the preparation of a benchmarking study to identify best practices and define performance targets in supply chain management;
- develop the logistics function to include the use of operations optimization tools on a worldwide basis;
- work with government to harmonize supply chain issues of packaging, labeling, documentation, handling, storage, and shipping; and
- encourage the development of information systems having compatible communications, data transmission, and information processing to support global supply chain activities.

Technology Area 3: Information Systems

Throughout the chemical industry, the ways in which data are turned into information and used, managed, transmitted, and stored will be critical to its ability to compete. Improved and enhanced information systems are at the very heart of our vision, which sees the chemical industry operating highly efficiently and economically. To facilitate the advances in information systems required for its future, the industry should achieve the following:

- Encourage technology providers to develop open systems, focusing on the capability of integrating specific sets of information into larger systems. This will require improvements in data security, quality, and reliability, as well as data compression technologies.
- Work with government to improve knowledge of molecular modeling and simulation as they apply to the chemical process industry by encouraging the government to enhance the transfer of process simulation and modeling techniques to the private sector.
- Encourage the development of standards for transferring models and model parameters to facilitate the use of modeling and simulation technologies.
- Encourage the development of expert systems and intelligent decision-support tools that are flexible enough to model multi-national, multiproduct enterprises for use in business decision making.

Technology Area 4: Manufacturing and Operations

The revenue-generating capability of the chemical industry is derived from its capability to deliver chemicals and materials that satisfy customer needs. Manufacturing operations play a key role in that activity. Maintaining and improving the competitiveness of the U.S. chemical industry will require advances in six areas of manufacturing operations: (1) customer focus, (2) production capability, (3) information and process control, (4) engineering design and construction, (5) improved supply chain management, and (6) global expansion. To achieve improvements in these areas, the industry should

- Encourage customer and supplier focus in a partnering fashion with emphasis on reliability of supply, continuous improvements in product quality and consistency, and responsiveness to change.

- Encourage improvement in production capabilities to continuously improve process safety, reduce the impact of manufacturing processes and products on the environment, and speed up access to product and process information, thus enabling quick response to change and easing management of improvements.
- Develop the technology to build plants in a shorter time and at lower cost to allow reconfiguration of plants as markets change.
- Enhance the supply chain enterprise system by giving it a chemical industry focus.
- Expand the capability for global operations and commerce.

Chapter 1

INTRODUCTION TO THE CHEMICAL INDUSTRY AND ITS CONTRIBUTIONS TO U.S. SOCIETY

The chemical industry is more diverse than virtually any other U.S. industry. Its products are omnipresent. Chemicals are the building blocks for products that meet our most fundamental needs for food, shelter, and health, as well as products vital to the high technology world of computing, telecommunications, and biotechnology. Chemicals are a keystone of U.S. manufacturing, essential to the entire range of industries, such as pharmaceuticals, automobiles, textiles, furniture, paint, paper, electronics, agriculture, construction, appliances, and services. It is difficult to fully enumerate the uses of chemical products and processes, but the following numbers give some indication of the level of diversity[1]:

More than 70,000 different products are registered. More than 9,000 corporations develop, manufacture, and market products and processes. The U.S. government uses eight standard industrial classification codes to categorize chemical companies:

- industrial inorganic chemicals;
- plastics, materials, and synthetics;
- drugs;
- soap, cleaners, and toilet goods;
- paints and allied products;
- industrial organic chemicals;
- agricultural chemicals; and
- miscellaneous chemical products.

In short, a world without the chemical industry would lack modern medicine, transportation, communications, and consumer products.

World Position

The United States is the world's largest producer of chemicals. In 1995, some $367 billion worth of products was shipped. This represents about 24 percent of the worldwide market, which is valued at $1.3 trillion. Countries that rank next in total production are Japan, Germany, and France. In terms of exports, Germany is currently the global leader. The United States ranks second, with approximately 14 percent of total exports worldwide, valued at $60.8 billion in 1995.

National Position

The U.S. chemical industry runs one of the largest trade surpluses of any industry sector ($20.4 billion in 1995), and it ranks as the largest manufacturing sector in terms of value added. The more than one million employees in the chemical industry enjoy a relatively high standard of living, with salaries in production roles averaging approximately one-third higher than in other manufacturing industries. Overall, the chemical industry is the third largest manufacturing sector in the nation, representing approximately 10 percent of all U.S. manufacturing.

Research and Development in the Chemical Industry

The outstanding success of the chemical industry is largely due to scientific and technological breakthroughs and advances, making possible new products and processes. The chemical industry now

[1] Chemical Manufacturers Association. CMA Statistical handbook; Washington, D.C., 1995, p. 7.

spends about $17.6 billion annually on R&D[2]. In fact, according to an Institute for the Future study, the chemical industry is one of the eight most research-intensive industries. The scientific and technical research of these industries makes our lives as Americans safer, longer, easier, and more productive.

Through significant investment in R&D, the U.S. chemical industry has led the way in developing and supplying products that have made our lives better. When one reviews the contributions of the chemical industry to our civilization, it becomes clear that rather than any single individual invention or technological breakthrough, it has been the industry's overall commitment to R&D that has represented its most significant legacy.

Investment in R&D is the single greatest driver of productivity increases, accounting for half or more of all increases in output per person[3]. Research and development is the source of new products that improve the quality of life and new processes that enable firms to reduce costs and become more competitive. As we look to the future, it is apparent that a continued investment in technology is necessary for industry to meet the needs and expectations of the next generation. Reaching the goals of *Technology Vision 2020* will require appropriate levels of support for R&D, the wellspring of future growth.

Compared with R&D investment levels (as a percentage of gross domestic product, GDP) in leading industrial countries, the United States is currently only slightly ahead of Germany and France and just behind Japan. In terms of nondefense-related R&D, which has more impact on the chemical industry, the United States outspends only France. Moreover, federal expenditures on nondefense-related R&D have actually fallen as a percentage of GDP over the past three decades. This reduction is a serious threat because government is the primary source of support for basic research. Government expenditures, in turn, influence the level of private support for applied research and development. Applied research can only proceed in directions indicated by basic research, and commercialization follows from applied research. Exacerbating this situation is that companies appear to be shifting their R&D investments to shorter term R&D.

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[2] U.S. Department of Commerce, *Meeting the Challenge: The U.S. Chemical Industry Faces the 21st Century*; January 1996.

[3] Material in this section is drawn from The Council of Economic Advisers, "Supporting Research and Development to Promote Economic Growth: The Federal Government's Role," October 1995.

Chapter 2

BUSINESS ISSUES FACING THE U.S. CHEMICAL INDUSTRY

A Time of Dynamic Tension

Looking ahead to the 21st century, we see six forces changing the topography of the business landscape: increasing globalization, sustainability, financial performance (profitability and capital productivity), customer expectations, changing work force requirements, and increased collaboration.

Within this changing landscape, the industry continues to both improve its ability to meet customer needs and develop pathways for continued growth and improved profitability. It is certain that some paths will lead to new levels of success, and others will take us to the “dead end” of declining competitiveness. The critical question today is, “Which is which?”

All paths have barriers, but the leadership of the chemical industry is confident that the United States has or can develop the resources necessary to get from where the industry is today to where it must be in 2020.

Privately financed scientific R&D conducted by chemical companies has built a strong and vital chemical industry. Nevertheless, as other nations enter the global marketplace and major producers become more competitive, the current level of investment in R&D may be insufficient to maintain a competitive edge. Companies alone will be unable to meet the new realities of the 21st century. Partnerships can help to leverage R&D resources in the interest of industry needs.

The following sections provide a more detailed examination of the challenges and opportunities created by the forces shaping the chemical industry and the increasingly important role technological leadership plays in the outcome.

Chapter 3

ROLE OF TECHNOLOGY

Technology holds promise for positively shaping the U.S. chemical industry as it adapts to the new global business environment requirements for sustainability, financial performance, expanded customer expectations, and a more highly skilled work force.[1]

INCREASING GLOBALIZATION

We define globalization as the accelerating interdependence of nations and private firms.

Opportunities

Technological innovation will provide many new market opportunities. As industry advances toward our *Technology Vision 2020*, people, technology, capital, information, and products will move freely across international boundaries, minimizing, and sometimes equalizing, past economic and technological disparities. Worldwide economic growth offers many new opportunities for selling products and services in countries previously inaccessible because of geography. To compete effectively in foreign markets, local manufacturing is important and will increase the potential markets for U.S.-owned foreign affiliates, which generated sales of $186 billion in 1992.

[1] For further details on trends affecting the chemical industry, refer to the U.S. Department of Commerce Report, *Meeting the Challenge: The U.S. Chemical Industry Faces the 21st Century*, January 1996.

Impact of Technology

Success in capturing new, emerging markets will depend on the industry's ability to compete in different environments. Threatened by what some economists forecast as an inevitable decline in the U.S. share of world output and trade, the chemical industry can develop competitive, advanced manufacturing technologies, improve logistics and management of supply chains, and create new products that support the needs of customers globally.

SUSTAINABILITY

We define sustainability as technological development that meets the economic and environmental needs of the present while enhancing the ability of future generations to meet their own needs.

Opportunities

While the challenges of sustainability are significant, there are also major opportunities for growth as the chemical industry advances through the next quarter-century. As world population increases, the chemical industry can serve more customers with higher quality, higher performing products and services, while demonstrating responsible stewardship of our planet.

With the U.S. chemical industry's commitment to Responsible Care®, the nation is ideally positioned to bring into reality the technology vision of an industry that is a welcome neighbor—one that protects environmental quality, improves economic well-being, and promotes a higher quality of life.

Impact of Technology

The chemical industry now has the opportunity to accelerate its development of advanced manufacturing technologies and new chemistry and related technologies that use materials and energy more efficiently.

U.S. companies also have an opportunity to build on their current dominance in the relatively new field of environmental technology. Environmental technologies make sustainable development possible by reducing risk, enhancing cost effectiveness, improving process efficiency, and creating products and processes that are environmentally beneficial or benign. The world market for environmental technologies is growing rapidly, forecasted to increase from $300 billion in

1992 to $425 billion in 1997. U.S. companies make up the largest portion of the industry, with approximately 45 percent of the global market.

FINANCIAL PERFORMANCE

Companies are increasingly being judged by their ability to create products that generate revenues to satisfy stockholder's profitability expectations. The emphasis on short-term profitability has improved stockholders' satisfaction, but is a significant barrier to funding long-term R&D.

Impact of Technology

The chemical industry now has the opportunity to devise strategies to achieve targeted short-term returns while at the same time attracting the capital needed for investment in longer term projects and facilities. Appropriate, strategically driven investment in R&D and new technologies, such as those described below, will continue to drive the industry toward unprecedented levels of productivity and return on capital.

R&D is the single greatest driver of productivity increases. Investment in advanced manufacturing technologies, logistics and management of the supply chain, information technology, and new chemistry and engineering technologies are vital for achieving our goal of leading the manufacturing sector in profitability.

CUSTOMER EXPECTATIONS

Responding to needs of customers in real time increasingly defines financial success for both the customer and the chemical producer.

Opportunities

As the values and structure of business shift, the chemical industry has unprecedented opportunities to develop new markets and forge even stronger relationships with its customers.

Realizing the technology goals of *Technology Vision 2020* will require that the industry relates to its customers in new ways. These changes include

- improved business relationships developed through new partnerships between suppliers and customers,
- cooperation to remove inefficiencies in both supplier and customer operations,
- collaboration to reduce environmental impact, and
- enhanced performance for customers and for society as a whole, through commitment to continuous improvement.

The companies that gain and retain market share will be those companies that meet changing customer expectations by

- increasing responsiveness, especially in terms of reduced product cycle time, focused on adding value to customers' products;
- continuously improving product quality; and
- continuously improving service.

As customers aggressively expand and unify their operations globally, chemical producers in the United States must meet constantly evolving material specifications. From "just-in-time" delivery to higher quality and increased technical support, customers are requiring more from their chemical suppliers.

Impact of Technology

To meet expanding customer expectations, the industry needs to apply innovative technology throughout all phases of R&D, production, and distribution. Improvements in logistics and supply chain management will enable manufacturers to deliver products to customers more efficiently and at lower cost. New operations and manufacturing technologies will ensure highest product quality, and more sophisticated information systems will link companies to their customers. New chemistry and engineering will provide products that add value for customers and, in turn, for their customers. Over all, technological advances will reduce product development response times and help industry meet customers' rising expectations.

CHANGING WORK FORCE REQUIREMENTS

Because of all the forces creating change in industry, particularly having to do with the nature of the manufacturing process and facilities (as we will detail below), more highly skilled workers will be required for tomorrow's work force.

The influx of computers and automation will make plants easier to run but will require a more technically advanced understanding of the process.

The increasing complexity of technology and the rapid pace of technological change places increasing demands on employees across the work force, from the scientist at the laboratory bench to the operator on the plant floor.

The hallmark of the future work force will be flexibility, not an assault on jobs. Worker training will be an ongoing part of every employee's career. This dynamic has implications for educational curricula and programs of the future.

THE PATH TOWARD TECHNOLOGY VISION 2020: TECHNICAL ISSUES

This section looks closely at four disciplines that will determine the progress of the chemical industry: new chemical science and engineering technology, supply chain management, information systems, and manufacturing and operations.

Twenty-five years ago, few people could have imagined many of the technological advances that have led to tools taken for granted today, from the omnipresent microwave oven to the immediacy of electronic mail. We are confident that during the next 25 years, similarly dramatic new technologies will emerge, as the needs and challenges are met and the challenges associated with them are overcome.

Here are some glimpses of the future, as we look ahead to the year 2020, when chemical science and engineering technology will have become the driving force for creating sustainable value and growth in the U.S. chemical industry.

We describe current technological conditions, identify research needs and challenges, envision optimal future conditions, and offer recommendations to achieve these advances in each area. The sections delineate not only the new capabilities required to reach this vision of the chemical industry's future, but also the step change improvements and enhancements that are just as crucial in moving forward.

Chapter 4

NEW CHEMICAL SCIENCE AND ENGINEERING TECHNOLOGY

The Three Areas of Chemical Science

CHEMICAL SYNTHESIS

Current State

The traditional tools of chemical synthesis in use today are organic and inorganic synthesis and catalysis. *Synthesis* is the efficient conversion of raw materials such as minerals, petroleum, natural gases, coal, and biomass into more useful molecules and products; *catalysis* is the process by which chemical reactions are either accelerated or slowed down by the addition of a substance that is not changed in the chemical reaction.

Advances in core strategies, such as those in synthesis or catalysis, can have huge impact. For instance, a major breakthrough in catalysis was the discovery of coordination anionic catalysis, which won Karl Ziegler and Guilio Natta a Nobel Prize in 1953 and opened up the possibility of developing materials based on olefins. This catalytic discovery led to the creation of a multibillion-dollar-per-year market, predominantly in two polyolefins—polyethylene and polypropylene—including the production of everything from common garbage bags and children's toys to high-tech internal automotive parts and life-saving medical devices.

What may be surprising to many nonscientists is the fact that the vast majority of products made today are being produced with traditional synthesis methods developed between 40 and 50 years ago. Though classical organic and inorganic syntheses are used widely to support much of the chemical industry, catalysis-based chemical syntheses account for 60 percent of today's chemical products and 90 percent of current chemical processes. Given this dominance, catalysis has emerged as the primary focus of development in chemical synthesis. In fact, innovations in catalysis have driven many incremental improvements in synthesis.

Needs and Challenges

To advance chemical science, the industry must move beyond the current state-of-the-art in synthesis and catalysis. A summary of industry needs and challenges follows.[1]

Develop new synthetic techniques incorporating the disciplines and approaches of biology, physics, and computational methods.
Meeting this need will require the further development of synthesis tools that permit rapid creation of unique molecules, using

- a variety of new combinatorial techniques,
- new computational techniques to guide synthesis by theory and molecular modeling,
- techniques to conduct molecule-specific measurements, and
- further development of chemistries using natural processes such as photochemistry and biomimetic syntheses.

Develop new catalysts and reaction systems to prepare economical and environmentally safe processes with lowest life-cycle costs.
This includes the need for new and improved catalysts that can be applied to existing processes, such as

- viable solid acid and base catalysts to replace the toxic and corrosive mineral acids and bases for organic syntheses,
- methods of synthesis and catalysis to convert product molecules and polymers back to useful starting materials, and

[1] See the "Computational Technologies" section (pg. 34) and the Information Systems chapter (pg. 43), which describe the impact of computational technologies, and specific "Needs and Challenges" sections on product and process development.

- catalysts with increased molecularity, and catalysts with long life and self-repairing abilities.

Develop chemistry for the use of alternative raw materials.
This will require the development of new catalysts and systems for carrying out reactions in alternative reaction media, specifically new catalysts for the efficient conversion of biomass and unused byproducts into useful raw materials, and new chemistries based on abundant materials, such as CO_2.

Develop new synthesis tools to efficiently create multifunctional materials that can be manufactured with attractive economics.
Cost-effective techniques are needed to synthesize organic- and inorganic-based materials, allowing control at the molecular level, using

- new catalysts for customizing polymer properties (composition, stereochemistry) during synthesis;
- molecular self-assembly methods, chemistries, and techniques;
- new inorganic/organic hybrid chemistry;
- use of biologically based pathways; and
- new organometallic compounds and clusters, inorganic polymers, metal alloys, metallic glasses, and sol-gel-based materials.

Develop techniques for stereospecificity, or precision in spatial arrangements of molecules.
Achieving this will require catalysts for reaction pathways focused on ultrahigh selectivity, higher molecularity, higher regio- and stereospecificity, and asymmetric and chiral syntheses.

Develop new cost-effective techniques to create a broader variety of molecular architectures in alternative reaction media.
New chemistry and fundamental understanding is needed for application in

- water-based systems,
- gas-phase systems,
- reactions carried out in bulk, and
- supercritical reaction media.

New Capabilities
Interdisciplinary activities will create new fields of technology.

Final product performance can be developed through control of structure and properties at the molecular level.

Multiple product functionalities will be routinely coupled in single, or perhaps complex, molecules or molecular architectures.

Chemists will apply natural processes, including photo- and biomimetic chemistry, to industrial chemicals and materials, achieving widespread economic efficiency and improved process safety.

Surface science and supporting engineering sciences will be able to define, control, and manipulate chemistries of active sites at the single-site level.

How to Get There
Research can be conducted by scientists working in industry-wide collaborative research teams involving scientists and engineers from companies, universities, and government laboratories in joint efforts reflecting levels of unprecedented collaboration. Advances will depend on enhanced collaboration among scientists and engineers working in fundamental and applied research in surface and catalytic science relevant to commercial processes and products.

Research can become more interdisciplinary, integrating knowledge from surface, biological, catalytic, and traditional chemical sciences to develop manufacturing technologies for ultrahigh selectivity and chirally, stereo-, and regio-selective products.

Similarly, education and training for chemists can become more interdisciplinary. Curricula for training research chemists can be restructured, refocused, and intensified to highly integrate the disciplines of biology, biochemistry, physics, and computational methods.

Research can accelerate the understanding and development of novel synthesis techniques using processes such as biomimetic synthesis and photochemistry.

Research in computational chemistry can be supported by supplying fundamental knowledge of structure–property–performance relationships through the development of accurate predictive tools and timely incorporation of these tools in testing and validating models.

Improvements and Enhancements

Advances in chemistry will be characterized by a shortened and enhanced value-adding chain, the control of chemical reactions and structure development at the molecular level, and fewer steps for processing.

Engineered systems will support the adoption of nontraditional synthetic pathways.

Scientists will be able to synthesize and manufacture catalysts and their products with little or no postprocessing for separation, purification, or isolation.

Chemists working in the area of synthesis will have ready access to newly applicable combinatorial techniques.

Life-cycle concepts will be integrated into product and process selection criteria. When favorable, highly selective natural processes will be translated into analogues for versatile commercial processes.

Plans for disassembly and reuse will be an integral part of product development.

HOW TO GET THERE

Centers of excellence are needed to promote development of fundamentals in synthesis, processing, and fabrication that result in the ability to control structures at the molecular level in economically efficient ways.

Research will focus on the translation of knowledge and techniques from the biological sciences, among others, to apply combinatorial methods in the broader field of chemical synthesis.

Scientists can develop a set of life-cycle concepts that can be accepted nationally and industry-wide.

Investment in new engineering technologies, such as reactor design and separations systems, should be cost-effective and environmentally protective.

BIOPROCESSES AND BIOTECHNOLOGY

Bioprocesses and biotechnology is the second area in the chemical sciences where advances are critical to the industry if it is to maintain and improve competitiveness.

Current State

Humans have used biologically based processes (bioprocesses) since they first made cheese, leavened bread, and brewed spirits. Systematic exploration of biological catalysts (biocatalysts) began approximately 100 years ago with studies of enzymes, the protein-based catalysts found in living organisms. A wide range of bioprocesses are now used, sometimes complementing traditional process chemistry and sometimes offering alternative process chemistries.

Currently, bioprocesses account for commercial production of more than 30 billion pounds per year of chemical products, including organic and amino acids, antibiotics, industrial and food enzymes, fine chemicals, as well as active ingredients for crop protection, pharmaceutical products, and fuel ethanol. These products account for almost $10 billion in annual sales at the bulk level, but are largely unrecognized by consumers, who buy them as ingredients or components of products with other names. Examples include additives to motor fuels that reduce air pollution, enzymes that clean clothes better or make fabrics softer, food ingredients and packaging that keep food fresh and safer, and the active components in drugs that restore health.

The potential for discovering new biocatalysts is largely untapped, since 99 percent of the microbial world has been neither studied nor harnessed to date.[2] Recognized today through their genetic code (DNA sequence), these members of the Archaeal and Eubacterial domains[3] are expected to provide biocatalysts of much broader utility as this microbial diversity is further understood.

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[2] DeLong, E. F.; Wu, K. Y.; Prezelin, B. B.; Jovine, R.V.M. *Nature* 1994, Vol. 371, p. 695. Amann, R.; Ludwig, W.; Schleifer, K-H. *Microbiol*. 1995, Vol. 59, p. 143.

[3] Woese, C. R.; Kandler, O.; Wheelis, M. L. *Proc. Nat. Acad. Sci*. 1990, Vol. 87, p. 4576. Barnes, S. M.; Fundyga, R. E.; Jeffries, M. W.; Pace, N. R. *Proc. Nat. Acad. Sci.* 1994, Vol. 91, p. 1609.

Needs and Challenges

Given the breadth of possible research, setting priorities in biotechnology may be most critical. The improved performance of bio-catalysts and improved biochemical processing are two areas holding great promise for the chemical industry.

Improved performance of biocatalysts

Improved biocatalysts are needed for biochemical routes to higher performance chemical products made by lower cost bioprocess alternatives. More powerful enzymes will provide the basis for improved biocatalysts; increasing the yield, rate, and selectivity of bioprocesses while retaining the advantages of sustainable chemistry. That is, in addition to increasing productivity and speed of bioprocesses, these improved catalysts will better target the desired chemical reaction. They will also allow better use of lower cost feedstocks from biomass and greater stereochemical specificity. This ultimately results in bioprocesses that improve protection of human health, safety, and the environment.

Achieving these advances will involve overcoming challenges in the following areas:

- New enzymes must be isolated from the currently unexplored realms of microbes being discovered through studies of biodiversity.
- Substrate specificity (a biocatalyst's preference for a specific molecular structure, from among many similar structures, as its raw material) and activity of known enzymes must be enhanced. Using the techniques of molecular biology and targeted molecular evolution, researchers will achieve analogous improvements that increase the robustness of the catalysts, permitting a broader operating range of pH, temperature, and media composition that is both water- and nonwater-based.
- Sequential enzymatic pathways (metabolic pathways) that perform multiple synthetic steps in industrial microorganisms must be engineered to make new products through lower cost and more efficient processes. The increased yields, reaction rates, and final product concentration in the production media will be key elements for achieving these enhanced processes.

Improved biochemical processing

Improvements in biochemical processing will depend on enhancements in fundamental biochemical engineering capabilities and applied engineering skills. Such improvements would include

- on-line measurements and process control models for combined biological and chemical processes;
- fully effective continuous processes for the biological reactions;
- better processes at the interface between the biological and chemical operations within a bioprocess;
- more effective separation processes that, for example, address the acid– base–salt use challenges faced in the production of charged molecules; and
- successful biological reaction and product extraction processes yielding greater productivity and lower investment.

TECHNOLOGY VISION 2020

New Capabilities

The DNA of all industrially important microorganisms and plants will be sequenced and gene structures defined, thereby permitting optimal efficiency of metabolic pathways.

High-value-in-use molecules and structures will be designed, some of biological or biochemical origin.

Metabolic pathways will be thoroughly understood and fully functional; quantitative models will be available.

Very low cost raw materials for bioprocesses will be derived from agricultural and forestry wastes and, to an increasing extent, cultivated feedstock crops.

New capabilities, including biotechnology-based processes, will enable the manufacture of chemicals with greater energy efficiency and environmental stewardship.

How to Get There

Fully automated sequencing of very large genes will be complemented by information systems that offer easy access to the data obtained.

Molecular biology will have gained exquisite control of the magnitude and timing of activating genes to produce enzymes. The coordinated function of genes and enzymes in forming a pathway will be well understood.

Quantitative models will be constructed based on the knowledge derived from this work.

Very low cost raw materials for bioprocesses will require coincident improvements in disparate fields, such as

- plant biology and stock improvement technology for farm and forest,
- science and engineering for separating feedstock values from plant-based materials; and
- recovery of feedstock energy values from residuals of the plant materials.

Improvements and Enhancements

Bioprocesses for chemical manufacture will play a more prominent role as we approach 2020.

Known biocatalysts will be improved through the application of molecular biology, genome sequencing, metabolic pathway engineering, and directed molecular evolution. These improvements will lead to further use of biological processes, based on domestic and renewable materials.

Bioprocesses will increasingly be used to produce a broader range of chemicals.

HOW TO GET THERE

Research teams will integrate basic sciences to conceive, design, synthesize, and manufacture high-value-in-use molecules and structures, some of biochemical origin and others based on a fundamental understanding of biology.

Scientists and engineers will develop better strategies in several areas, including

- highly efficient processes for converting biomass or cultivated feedstock crops into very low cost raw materials for bioprocesses;
- more efficient concepts and designs for microbial bioprocess reaction steps such as media sterilization, oxygen transport, agitation, and temperature control; and
- robust techniques for separating biocatalysts (whole-cell or supported enzymes) from process media and separating the desired product from the spent medium. The separation must be characterized by high levels of purity and relatively low cost.

Industry, academe, and government must together support the research and educational efforts that will lead to broader economic viability and public acceptance of bioprocesses as the source of sustainable, higher performance chemical products and a globally competitive chemical industry. This will require that scientists in industry clearly define the challenges in precompetitive science and technology that, when met, will provide more powerful and efficient biocatalysts, more effective process technology, and very low cost raw materials, particularly domestic and renewable ones.

Companies can sponsor and pursue the proprietary research that will yield higher performance products and processes.

Scientists and engineers in universities should broaden the knowledge applicable to industrial bioprocesses. This would include work in the following areas:

- metabolic pathway engineering and the quantitative modeling of fluxes through the pathways,
- enzyme discovery and optimization through biodiversity and directed evolution, and
- more efficient reaction and separation technology.

Government can encourage, support, and participate in the precompetitive efforts described above, while supporting long-term, high-risk technology development and project demonstration.

MATERIALS TECHNOLOGY

Materials technology is the third area in the chemical sciences where advances are important.

Current State

The development of new synthetic materials has fueled the growth of the chemical industry and revolutionized our society in the 20th century. Replacement of traditional materials such as metals, wood, glass, and natural fibers with synthetic polymers and composite materials has resulted in products with lower weight, better energy efficiency, higher performance and durability, and increased design and manufacturing flexibility.

Biomedical polymers have enhanced health, with uses in diagnostics, medical and prosthetic devices, and membranes. Synthetic materials are an important component of the chemical industry and are critical to the aerospace, automotive, construction, electronics, energy, metals, and health care industries.[4]

Recent examples of progress in materials are noteworthy. During the past several years, advances in composites, including mixtures of polymers and fibers, and metals and ceramics, have extended the range of performance and applications of these materials. New advances in catalysis are upgrading common polymers into materials offering uncommon performance. Tailored blends of polymers and other materials have expanded their applications beyond the range accessible with single-polymer systems.

Emerging concepts in materials R&D include increasing the functionality of materials, extending their performance range, and using new synthetic techniques. Smart or triggered materials are increasing materials functionality, and their properties include the ability to self-repair, to actuate, and to transduce.

Examples of smart materials include electrochromics, controlled-release devices, electro- and magneto-rheological materials, and shape memory alloys.

Advances in modifying materials surfaces and interfaces are also being achieved through new coating technologies, film, self-assembly, or reactive approaches using ion beams, among other methods. Also under development are materials that have special attributes, such as the ability to withstand superhigh temperatures, photovoltaic capabilities, and superconductivity.

Additionally, bioengineering with plants and bacteria, microwave-enhanced chemistry, and new compositional concepts—such as hybrid organic–inorganic systems and self-reinforcing systems—have emerged recently as routes to higher performance.

These recent developments will lead to higher performing materials produced at lower cost. New approaches to the design and fabrication of materials will facilitate the incorporation of life-cycle considerations into materials design and will enable the reuse or disassembly of many materials used today.

[4] National Research Council. "Materials Science and Engineering for the 1990's," National Academy Press, 1989.

Needs and Challenges

Prediction of materials properties

The highest priority challenge is the prediction of materials properties from the molecular level through the macroscopic level. This includes the development of a fundamental understanding of structure– property relationships and computational techniques.

Advances needed include the ability to

- rapidly develop new products with desired performance at lowest cost,
- develop tools to integrate material performance needs with emerging process and raw material alternatives, and
- develop new ways to use natural and other renewable sources to create materials that can achieve the required performance.

Synthesis technology for precise manipulation of material structures

Develop new practicable synthesis technology for precise manipulation of material structures—including bulk, surface, and interfaces—from nanoscale to macroscale for the economical synthesis, processing, and manufacturing of lower cost, higher performance materials. These technologies may include

- molecular self-assembly,
- net shape synthesis,
- biomimetic synthesis, and
- materials catalysis.

Enhanced performance in materials

Find new ways to improve and develop enhanced performance in materials in the following categories:

- sensors for chemical process industry use;
- materials with enhanced environmental stability and durability and strength-to-weight ratios;
- electrical and optical materials;
- triggered or smart materials (for disassembly, self-repair, self-indication, actuation, transducing, etc.);
- biocompatible systems;
- higher temperature systems for intermaterial replacement, including composites;
- materials for separation processes; and
- membranes for chemical processing, packaging, medical, and other separations applications.

Develop routes for step change improvements in performance of materials systems with the use of new additive technology.
We can look for improvements in these areas:

- new nontoxic additives for the polymer industry, including plasticizers, flow aids, colorants, flame retardants, etc.;
- additives for the polymer industry that can tolerate high temperatures, including plasticizers and flow additives; and
- alternative approaches to additive technology that include increasing functionality and using low-cost synthesis routes.

Develop technology in integrated materials and processes for reuse and disassembly.

TECHNOLOGY VISION 2020

New Capabilities

Scientists will be able to design materials, and predict their properties, from the molecular level through the macroscopic level, relying on easy-to-use computational tools.

Scientists will be able to manipulate materials precisely—from nanoscale to macro-scale—for the economical synthesis, processing, and manufacturing of lower cost, higher performance materials.

New chemical structures have been developed that meet requirements presently provided using additives, mixtures, blends, etc.

There is increased acceptance of methods for disassembly and reuse, and life-cycle considerations are part of materials development.

HOW TO GET THERE

Companies can collaboratively define fundamental structure–property needs to guide academe toward increasing scientific understanding and control of the functional properties of materials.

Industry can increase collaboration in guidance of current development platforms or create new ways to accelerate the collaborative development of tools for modeling and prediction in materials systems.

Academe and industry should create and support interdisciplinary programs or centers focused on synthesis of novel materials with controlled bulk, surface, and interface structures, from nanoscale to macroscale.

Research programs that develop alternative pathways to enhancing materials performance, currently achieved with additives, should be supported.

Industry, academe, and government should work collaboratively to define protocols for disassembly and reuse and support molecular design and synthesis programs oriented toward these protocols.

Companies should consider early integration of disassembly and reuse concepts in new materials development programs.

Early integration of bioresponse models (for example, toxicity predictions) should be incorporated with molecular, systems, and synthetic modeling.

Improvements and Enhancements

Enhanced education will ensure the availability of critical tools and integrated resources and programs that respond to industry's needs.

Industrial organizations focus on cross-disciplinary teams and their abilities to rapidly translate and assimilate new knowledge and tools.

Specialty materials are cost competitive with lower functioning materials on a systems basis.

HOW TO GET THERE

Scientists in universities should integrate mathematics, physics, and chemistry curricula to develop an interdisciplinary approach for a new materials curriculum focused on the development of structure–property relationships and the design and synthesis of both new and existing materials. This new materials education should integrate computational methods with traditional curricula.

University researchers should develop appropriate science for a mechanistic understanding of new features of materials science.

Companies should restructure industrial organizations to accommodate an appropriate cross-disciplinary ability to translate new interdisciplinary knowledge.

New processing technologies that focus on economic bulk-processing technologies applied to a variety of new and traditional materials systems should be developed.

Enabling Technologies

The industry's future will be shaped, in part, by advances in its enabling technologies that improve the application of its fundamental sciences. These include (1) process science and engineering technologies, (2) chemical measurements, and (3) computational technologies.

Process Science and Engineering Technology

Process science and engineering technology (PS&ET) dates back to the 1930s and is the foundation for the development, scale-up, and design of chemical manufacturing facilities. PS&ET consists of engineering technologies; engineering science; and engineering design, scale-up, and construction. Taken together, these provide the basis for manufacturing excellence and sustainable competitive advantage.

Engineering technologies include environmental processing, hazards evaluation and control, materials engineering, particle processing, process control, and unit operations. Although an understanding of the first principles of the science underlying these technologies is beginning to mature, the technologies are generally applied using empirical, semiquantitative techniques that permit the safe development, design, and operation of our chemical processes. Engineering science includes thermodynamics, kinetics, and mechanisms; transport phenomena; and reaction engineering. Engineering design, scale-up, and construction include process synthesis and conceptual design, process development and scale-up, and engineering facilities design and construction. A continuum extends from process synthesis to production design and construction.

Current State

The application of PS&ET is somewhat fragmented, often sequential, and frequently driven by immediate business needs. These technologies are also applied to operating manufacturing facilities to reduce the operating costs, to incrementally increase capacity, and to comply with ever-changing federal, state, and local regulations. Integration of basic science and enabling technologies with PS&ET offers great potential for bringing science and quantitative understanding to the service of the chemical industry, permitting much higher capital utilization, improved yields, reduced waste production, and improved protection of human health, safety, and the environment. All this results in greater international competitiveness.

The supporting tools that would permit a more fundamental application of these technologies are just becoming available. A wealth of science underlies the fields of engineering science, and the measurement, modeling, and simulation tools needed to apply this knowledge to engineering problems are generally available. Industry and academe have collaborated effectively to develop both the science and the tools. Advances in computational technology, coupled with new measurement techniques, have provided the support for simulation and analysis of problems of ever-increasing complexity and commercial importance. However, as described in the Information Systems chapter (pg. 43), improved systems integration capabilities are needed to effectively apply these technologies.

The current state of engineering design, scale-up, and construction technologies varies from embryonic to very mature. Process synthesis is a relatively new development that is permitting early assessment and evaluation of the manufacturability of products resulting from potential new chemistries. While much of the work in this area is still focused in academe, some companies are using the techniques effectively.

The basic approach to process development and scale-up remains much as it was a decade ago except that new computational and simulation tools are being employed to accelerate the rate of commercialization. Facilities design and construction is a relatively mature technology, but is benefiting from advances in logistics management. Since most of the cost of a manufacturing facility is incurred during development, design, and construction, significant effort is underway to improve the effectiveness of these activities and the capital productivity of the resulting manufacturing facilities.

Beginning to emerge are concepts in nontraditional chemical processing, such as bioprocessing, recycling, expanded use of water-based processes, cryogenic processing, and new reactor and separations technologies.

Needs and Challenges

Future advances in PS&ET will require collaborative efforts of interdisciplinary research teams focused on the following "Needs and Challenges." Refer to the Information Systems and Manufacturing and Operations chapters of this report for additional insight on PS&ET needs.

The development of appropriate design principles, tools, systems, and infrastructures to accommodate a variety of improvements to meet current and emerging needs

- Reduction of the commercialization process for new products and processes to less than three years (from product synthesis through plant construction)
- Development of an economically viable process technology for high-performance materials and structures such as ceramics, composites, and electro- and photoactive polymers
  Improvement in solids-processing efficiency
- Integration of process control and optimization for plantwide and multisite implementation
- Integration of reactor and separation systems such as reactive distillation or extraction, membrane reactors, and supercritical fluid systems
- Development of production planning, scheduling, and optimization tools that cover any business's value-adding chain
- Production of reactors for new, emerging process chemistries including nontraditional media, such as plasma, biochemical and microwave media, and supercritical fluids
- Development of smart processes that include biomimetic control schemes
- Improvement of manufacturing process flexibility
- Production of existing and new products that reduce significant overall waste, optimize cost, and minimize environmental impact
- Development of disassembly procedures for recovery or reuse of materials

Meeting these needs will require advances in computational technologies in combination with new measurement techniques to meet the demands of increasingly sophisticated simulation and analysis of technical problems.

Incomplete knowledge of the particulate process

A major area of weakness is the current incomplete knowledge of the particulate process, which is extremely important because a high percentage of the chemical industry's products and processes involve handling solids.

Improving manufacturing flexibility

Process engineers and scientists are facing the challenge of improving manufacturing flexibility while reducing the capital investment needed to build effective manufacturing facilities.

TECHNOLOGY VISION 2020

In the future, process design will be viewed more comprehensively and will focus on the principles of concurrent engineering, designing from first principles, improved energy efficiency, and the protection of human health, safety, and the environment.

New Capabilities

Open architecture software tools will be developed to permit rapid "plug-in'' integration of tools and data from a variety of sources, along with a consistent user interface for

- rapid selection of chemistry;
- physical property databases (thermodynamic, kinetic, and transport) or ways to compute values for commercially important systems;
- rapid product and process development that optimizes technology options, manufacturability, environmental and safety issues, and financial performance;
- solids processing;
- plantwide process control and multisite optimization; and
- production planning, scheduling, and optimization of value-adding chain.

Traditional quality control laboratories will be replaced by real-time, continuous, in-process measurement of composition and properties.

Improvements and Enhancements

Many new commercial processes will use recycled raw materials as feedstocks.

Much of industry's production capacity will be characterized by new, economic, high-yield and high-quality processes with improved environmental impact.

Many new commercial processes will be based on nontraditional chemistry. They will include plasma, microwave, photochemical, biochemical, supercritical, and cryogenic processes.

HOW TO GET THERE

The development of relevant software and real-time measurement tools can be supported by funding for broad-based consortia, coordinated among industry, commercial vendors, federal laboratories, and university researchers.

Fundamental engineering research can be supported on nontraditional reaction and separation systems, such as plasma, microwave, photochemical, biochemical, supercritical, cryogenic, reactive extraction and distillation, and membrane reactors. This research can be supported on flexible manufacturing, high-performance materials and structures, disassembly of materials, solids processing, and smart processes.

CHEMICAL MEASUREMENT

Current State

Chemical analysis is a critically important enabling technology essential to every phase of chemical science, product and process development, and manufacturing control. New knowledge and insights about existing and new systems, developed as a result of advances in chemical measurement over the past two decades, have greatly accelerated progress in chemical science, biotechnology, materials science, and process engineering.

Impressive achievements have been made in the resolution, sensitivity, and specificity of chemical analysis. The conduct of analytical chemistry has been transformed by advances in high-field superconducting magnets, multiple-wavelength lasers, multiplex array detectors, atomic-force and scanning–tunneling microscopes, non-scanning spectral analysis (for example, Fourier transform), and the integration of computers with instrumentation.

The recent extension of these methods to the detection and spectral characterization of molecular structure at the atomic level shows that the ultimate limit of specificity and sensitivity of chemical measurements can actually be reached in tightly specified experiments.

More broadly, the inclusion of analytical specialists as full partners has been shown to greatly enhance the efficiency of research teams in chemical synthesis, surface science, catalysis, nanostructure science and technology, and environmental chemistry. Real-time control and refinement of process variables can be achieved with sophisticated analytical instrumentation.

Comprehensive compositional analysis is seldom used in chemical manufacturing process control. Multistep protocols, requiring skilled technical labor, are required to obtain accurate compositional data for process monitoring. Real-time analytical measurements are not generally available, either on-line or off-line. Most compositional measurements are used to provide postproduction quality control assessment and demonstrate waste discharge compliance.

Needs and Challenges

While significant progress has been made in moving process analytical measurements from the laboratory to the manufacturing line, more real-world chemical measurements are still conducted off-line. Most of the more spectacular recent achievements in this area have been made by highly skilled scientists using one-of-a-kind instruments. The isolation of sophisticated methods of chemical analysis from the environments in which they are most needed—ranging from R&D laboratories through manufacturing facilities—is a major limitation in present-day chemical measurements. Both state-of-the-art research-grade instruments and laboratory proto-types often lack the robustness, sophistication, and general utility required for effective, widespread use by nonspecialists. Advances are needed to meet challenges in three distinct, but related, areas of PS&ET measurement.

Highly sensitive, precise, and accurate measurement technology needed to probe molecular processes in the laboratory

- Nanotrace analysis. These chemical analysis techniques will provide information at nanometer-scale spatial resolution with ultra-high sensitivity and selectivity, using electron beam, ion beam, and surface spectroscopies. To conduct nanotrace analysis, non-scanning (transform, array detector) spectrometers are required. Also needed are methods for sampling and characterizing heterogeneous materials in

small sampling volumes, including characterization of interfacial phenomena, particulates, and aerosols.
- Time-resolved measurements. These are needed for detailed studies of the dynamics of reactions, interfaces, adsorption and desorption phenomena, catalysis, and drug release using spectroscopic techniques capable of detecting single molecules and molecular-scale aggregates and following the time dependence of chemical reaction, molecular motion, and configuration change with picosecond resolution.
- Macromolecular characterization. Materials characterization to the level of macromolecular architecture is needed. The fabrication of designer materials is currently limited by challenges involving cross-linking, networking, branching, composition of copolymers, and terpolymers, etc.
- Characterization of minute amounts of biopolymers and biomolecules. These measurements provide high selectivity analysis of micro- and nanoliter volumes, providing information on tertiary structures of biopolymers and assays of optical activity and/or bioactivity.
- Techniques to support combinatorial chemistry in cellular systems. These will aid discovery efforts in pharmaceuticals and agro-chemicals.

For instance, research in drug discovery and pharmaceutical efficacy can be facilitated by stereospecific analysis for monitoring enantiomer-specific catalysis.

- Improved separations techniques. These include
— stereospecific methods of analysis and separations, including process-scale chiral techniques,
— techniques for isolating specific groups of compounds from complex mixtures of organic constituents removed from the bulk matrix, and
— chromatographic stationary phases that provide function-selective separations of organic compounds with similar chemical properties.
- Advanced methods for matrix-independent chemical analysis. These will provide techniques for completely extracting analytes, with minimal optimization of conditions, from a wide range of matrices (e.g., supercritical fluid extraction, microwave-assisted solvent extraction, and accelerated solvent extraction) using on-line flow injection.
- Accurate and comprehensive databases and models for chromatographic retention and spectroscopic data. These will aid identification of compounds and minimize the need for reference compounds.

Robust measurement techniques for real-time, highly reliable analyses in practical environments

The techniques required include the following:

- On-line and real-time analysis will aid process control and environmental monitoring.
- Separation-free analyses that have reduced cycle time and low error rates must be incorporated.
- Multielement, temperature-programmable, solid-state sensor arrays that are low cost, self-correcting or calibrating, and nonfouling are important.
- Temperature-programmable sensor arrays that provide sufficient selectivity and sensitivity should be integrated into applications in multiphase, multicomponent process streams.
- On-line combination of extraction, group isolation, chemical separation, and detection systems will provide rapid and accurate measurements of individual compounds.
- Integration of modeling tools and information such as artificial intelligence (AI), neural networks, on-line data reduction, and high-order analysis into instrumentation is essential to managing the profuse data required to characterize systems of high complexity.
- Sensitive, selective, distributed, multiplexed, and integrated instruments are needed for on-line process and environmental analysis. The needs include multifunction chemical sensors, fiber-optic probes, miniaturized mass spectrometers, optical spectrometers, and chromatographs.
- Automated analytical laboratory systems—remote device control and data interchange protocols and standards—are needed to make chemical analysis systems more reliable, accurate, and cost-effective. Given the large number of instrumentation manufacturers, industry-wide interfacing standards will have to be developed for efficient and accurate analyses of complex analytes, especially those involving extractive methods. Interfacing of automatic analytical systems with control systems will be critical to full implementation of process analytical methods for process control.

Theoretical models for guiding and optimizing chemical analysis in laboratory and plant–process environments
This will include addressing two issues: First is integration of information theory, AI, neural networks, and model-based chemical analysis with chemical measurements. This may include the use of computers for designing analytical strategies that minimize the number of measurements required for definitive laboratory measurements and process control.

Second is the need for new theories for defining the relationship of measurements at the single-particle level with those for ensembles representative of bulk properties. We must apply statistics to validate analytical methods for limited data and small numbers of particles, and develop new predictive capabilities for spectroscopy, kinetics, and thermodynamics based on quantum mechanics.

Development of the collaboratory concept so that scientists and engineers at one location can do experiments on the best equipment even if it is located at a physically remote site
This technology will also enable staff at central research organizations to do experiments and acquire data promptly at remote manufacturing facilities.

TECHNOLOGY VISION 2020

New Capabilities
Nonspecialists in the scientific community will be able to use research-grade analytical measurement instruments.

Improvements and Enhancements
The capability, speed, and accuracy of measurement techniques will improve.

- All critical-process chemistry will be measured accurately on-line in a manufacturing environment.
- Measurement will be matrix independent in a majority of measurements taken.
- Interfaces, particulates, and aerosols will be accurately and precisely characterized.
- identified and measured, including their conformation with changing physical and chemical states.
- Large, combinatorial chemicals will be routinely measured and characterized.
- The most sophisticated measurement techniques of the mid-1990s, once used only in the laboratory, will become automated analytical procedures that will be commonly used throughout the industry.
- Sample preparation will no longer be needed for routine analytical measurements.
- Analysis cycle time will be reduced by a factor of 10 over what it was in the 1990s.
- On-line measurements will become an integral part of the process control scheme.
- Crystallography and resonance spectroscopies will be used routinely to determine macromolecular structures.

HOW TO GET THERE
Use by nonspecialists of research-grade analytical measurement instruments will require a new paradigm of collaboration between scientific innovators, computer and chemical information specialists, instrument manufacturers, and chemical technologists.

Centers of excellence can be promoted to advance research programs focused on chemical measurements and process analytical chemistry. Cooperative research efforts between industry, instrumentation companies, universities, and federal laboratories can be developed to advance the state-of-the-art of measurement science.

Instrumentation interfacing standards can be established to enable the use of distributed analytical networks and more efficient data acquisition and control systems.

The development of high-performance spectrometers can be supported using technology advances in superconducting magnets, high-performance lasers, and faster and higher capacity computers.

An industry–academe–government task force to prioritize the chemical process industry's simulation needs can be formed, followed by a general state-of-the-art assessment of available codes and current technology.

COMPUTATIONAL TECHNOLOGIES

Current State
Computational technologies have a broad range of applications, from molecular modeling to process simulation and control. Today, these technologies

are embodied in virtually every aspect of chemical research, development, design, and manufacture. Those most critical to the chemical industry include computational molecular science, computational fluid dynamics (CFD), process modeling, simulation, operations optimization, and control.
Within the past five years, computer hardware capable of handling more computationally intensive applications has become available to support the development and use of software tools. The tools today are far better than those available just a few years ago and much easier to use. However, computer architectures are changing rapidly, and software for the newest, highest performance (lowest cost/processing unit) applications does not keep up with these architectures.

Recent advances in computational molecular science have made it possible to accurately and reliably study systems of a few tens of atoms, although less accurate methods can be applied to a few hundred atoms. The cost of the most rigorous of these methods grows extremely rapidly (n^7) as more atoms are considered. Computational methods can now calculate selected physical, chemical, and kinetic properties needed to simulate and design products and processes. For most of these properties, empirical knowledge of similar systems is necessary to approach experimental accuracy of ±1 kcal/mol.

Current single-phase fluid dynamic modeling tools, initially developed for other industries, are being adapted and extended to permit the modeling of more complex, multiphase, fluid dynamic systems. However, the modeling of reactive flows is still in its infancy.

Steady-state process simulation is now indispensable in designing chemical plants. Dynamic process modeling is applied widely in research and process development, but less often in plant operations. The use of more fundamental mechanistic models for nonlinear process control is emerging.

Operations simulation and optimization may be defined broadly as the use of modeling and optimization technologies, tools, and methods to improve operations. Aspects of operations modeling and optimization are used in a variety of business functions, including manufacturing, technical, finance, logistics, production scheduling, capacity planning, distribution network planning, and other supply chain activities.

Commercial software exists for implementing expert systems, neural networks, and fuzzy logic for process monitoring, control, decision support, and heuristic inference in general. Other technologies, such as generic algorithms and database mining, as well as hybrids of AI, are developing rapidly.

Needs and Challenges

The principal challenges in developing computational technologies are to ensure that these tools and methods are tailored to meet the needs of the chemical industry. Doing so will require effective collaboration among those with technology (industry, national laboratories, and others), those with resources (industry and the federal government), and those who can provide the essential support infrastructure (commercial software vendors). Access to cost-effective, high-performance computing systems, software, and database architectures that do not require custom interfaces between complementary applications will be useful in fulfilling the promised benefits of parallel and distributed computing.

Renewed effort in experimental validation is required. The development and application of computational methods are now largely separated from experimental testing of results; discrepancies and limitations are still sometimes discovered by accident rather than by design.

In the area of computational molecular science (CMS), several improvements are necessary to make the tools more useful in modeling. Major improvements are needed in user interfaces for molecular modeling and design, including guidance in problem specification, method selection, computing platform selection, results visualization, and performance of ancillary computations to relate these results to observable physical and chemical properties.

Integration of CMS with statistical thermodynamic and continuum methods is required for full treatment of many problems.

Development of kinetic and thermodynamic modeling will allow prediction of long-term stability and performance of materials.

For scientists and engineers to better model more complex fluid dynamic systems (coupling chemical reactions with multi-phase, multidimensional, simultaneous fluid, heat, and

mass transfer dynamics), CFD programs can be developed to incorporate emerging advances in physical models and property databases and to provide a readily adaptable architecture.
In addition, advancement in CFD will depend on the development of tools for more complex systems such as high-temperature gas-phase systems, multiphase mixing, polymer processing, non-Newtonian rheology, dense multiphase turbulent flow (with or without chemical reaction), and crystallization with particle nucleation and growth.

Scientists and engineers need support to go beyond current constraints of a narrow range of operating conditions, enabling them to model complex, multisite, multiproduct, international environments.
Software tools are needed that bring together a complete modeling environment, including simulation, parameter estimation from experimental data, optimization, graphical representation of results, and statistical measures of uncertainty. See the Information Systems chapter for additional discussion.

Some of the specific challenges that can be met in this area include the development of

- simulation tools that integrate combinatorial optimization and ways to deal with uncertainty in simulation and optimization, such as sensitivity analysis and deterministic modeling;
- whole-site business production models, that move beyond individual plant modeling; and
- more robust fundamental models that are broadly applicable and reduce empiricism.

Large-scale integration of smart systems need to be incorporated into the guidance of operations with more significant advances in AI for scientists and engineers to move beyond the small scale or limited scope of current advisory systems.
Accomplishing this will require

- an information infrastructure that permits data to be shared regardless of geographical location with sufficient safeguards to protect proprietary information,
- a knowledge representation that is independent of the software system or inference engine that uses that knowledge, and
- cost-effective combinations of heuristic inference, discrete-event simulation, real-time optimization, dynamic simulation, and computational modeling in single, real-time, on-line advisory systems.

See also the Information Systems chapter.

TECHNOLOGY VISION 2020

In general, the application of computational technologies will lead to

- shortened product–process development cycles,
- optimization of existing processes to improve energy efficiency, and
- efficient design of new products and processes.

New Capabilities
Through the ability to model atomistic systems with high reliability, computational molecular science will allow chemical companies to rapidly design new materials and chemical processes that protect human health, safety, and the environment.

CFD tools will guide experimental optimization and scale-up.

Process modeling and optimization will be an integral part of the development and implementation cycle, from the early stages of research through process operations.

Advisory systems employing AI technologies will play a significant role in the integration and management of the entire chemical enterprise, including business systems, process flow sheets and unit operations, and computational simulations.

Coupling process science and engineering with the basic sciences will ensure the rapid development, design, scale-up, control, and optimization of existing and new processes for safely manufacturing chemicals and the products made from them, as well as their disassembly, recycle, and reuse.

Improvements and Enhancements
While experimental methods will become more efficient and reliable through the integration of computation, they will not be made obsolete.

Modeling and simulation will be used at every step of the value-adding chain—including scientific, engineering, and business processes—from discovery through commercialization. Measurement science will provide understanding and control of essentially all key process variables, compositions, and product properties in real time.

Intelligent systems will be applied to operations as the chemical industry advances.

Computational technologies will play an increasing role in the design, construction, and operation of plants.

Successful accomplishments of these advances will be marked by widely available, user-friendly modeling environments that are comprehensive, cohesive, well supported, and affordable. Such environments will provide tools that couple

- chemistry with fluid dynamics,
- modeling with experimentation,
- process models with business models, and
- structures with material properties.

Measures of accuracy and usability will show that the energy of a molecule or reaction transition state of 20 to 30 nonhydrogen atoms can be calculated cost effectively to an accuracy of 1 kJ/mol, comparable to the best achievable experimental accuracy.

Relative energies of weak intermolecular interactions (e.g., hydrogen bonds, van der Waals complexes, and nonidealities in liquids and gases) can also be calculated to accuracies comparable to the best experimental methods.

A host of other molecular properties are more readily computed than measured. Well-designed, effective user interfaces will make the most sophisticated and demanding methods accessible and effective for nonspecialists.

Well-maintained national databases and high-speed networks will make it easy to share results and avoid duplication.

Success will be marked by widely available, cost-effective, user friendly commercial software for implementing advisory systems that can provide operational support for an entire enterprise, including plant operations, supply and distribution chains, and business decisions.

How to Get There

Noted above (in the discussion of issues related to chemical measurement, "How to Get There," pg. 34) is the recommendation that a task force be formed to give priority to the chemical industry's simulation needs in general. A high-priority activity of this task force would be to focus on those simulation needs specific to CFD. Such an investigation can be followed by a general state-of-the-art assessment of available codes and current knowledge, theory, and methods relative to these needs. At the same time, flexible software paradigms can be explored and new, modular base codes developed. The results of these tasks can permit a clearly defined development path to be defined for new CFD tools.

Support and further development is essential for three types of computing platforms:

- high-performance desktop workstations, which give the individual scientist direct, personal means of solving a useful range of small and midsize problems and visualizing the results of larger problems;
- large, fast vector-processor machines, because many of the more rigorous methods have not yet been efficiently programmed for parallel computing, and commercial packages have favored this type of architecture;
- highly parallel processors, which require major advances in support tools for system operation and programming; parallel numerical algorithms and template applications; and fully developed, optimized, and supported end-user applications.

Further development of the national network is required to improve communication speed, to develop tools for on-line collaboration, and to meet a variety of needs in sharing, archiving, and retrieving results.

Increased support is required for experimental validation of (or challenges to) computational results. The technology would benefit greatly from a large coordinated program combining work on theoretical and computational methods with experimental programs designed from the beginning to challenge those methods.

Public–private partnerships can be developed to use expertise from the chemical industry, national laboratories, and AI software companies for illustrative implementation of single-system AI.

Chapter 5

SUPPLY CHAIN MANAGEMENT

While the chemical industry has concentrated on science and production and has accorded substantial attention to manufacturing as well, an area that has received less attention than it merits is that of the supply chain, defined as the critical linkages between the supplier and the producer, and the producer and the customer. Supply chain management focuses broadly on three areas:

- planning and processing orders;
- handling, transporting, and storing all materials purchased, processed, or distributed; and
- managing inventory.

As the chemical industry becomes increasingly global, issues related to the supply chain are increasingly critical to industrial competitiveness.

Current State

Today, many estimate that the costs associated with supply chain issues represent about 10 percent of the sales value of delivered products domestically and as much as 40 percent internationally. Clearly, this represents an area of opportunity for increasing competitiveness.

Circumstances are emerging that demand greater responsiveness to rapidly changing customer requirements across a global network.

Customers for chemical materials are aggressively expanding and unifying their operations globally, particularly as free trade expands. With this expansion, tariffs on chemicals generally are being reduced or eliminated. Because of increased carrier safety and efficiency, permitted materials will find easier entry at border crossings. Related to this easing of trade restrictions, and creating a synergy with the free-trade agreements, is the realization on the part of citizens of various countries that imports of higher quality may be available at lower cost in the international marketplace.

Managing the supply chain effectively involves not only the manufacturers, but also their trading partners: customers, suppliers, warehousers, terminal operators, railways, barge operators, motor carriers, airlines, customs house brokers, freight forwarders, port operators, and many other businesses central to the U.S. economy. Coordinating these efforts globally to ensure continuous order and product integrity, as well as protection of the environment, is a major task requiring specialized expertise.

Managing the supply chain today also requires an understanding of and conformance with regulations, laws, and other requirements that govern the storage, handling, shipping, packaging, labeling, and documentation of products and shipments. Today, such requirements vary within and among the local, state, national, and international levels of trade.

The state of packaging varies from well standardized to completely idiosyncratic. On the one hand, international containers for bulk materials are well standardized through the International Maritime of Dangerous Goods (IMDG) requirements and are well accepted by importing countries. On the other hand, packaging containers are specified through United Nations performance-oriented packaging standards that do not specify packaging materials. As a result, a wide variety of packaging materials and designs are used, with the burden on the shipper to satisfy performance standards. Because of this complexity, some countries (e.g., France and Germany) require that packaging materials be returned to the country where the shipment originated.

In the United States, there are inconsistencies in labeling requirements among the Occupational Safety and Health Administration, the Environmental Protection Agency, the Department of Transportation, the Federal Insecticide, Fungicide, and Rodenticide Act, and state laws and local ordinances. One example is the confusing array of definitions and labels for flammable, combustible, corrosive, and toxic materials, to name a few. Such confusion is greatly compounded when viewed along with other countries' symbols, definitions, and interpretations. Thus, misunderstandings about labeling can easily become a significant barrier to trade. Furthermore, the methods used to certify materials vary from country to country (e.g., flashpoint certification using Pensky–Martins, closed cup, open cup, or other methods).

The sizes of packaging containers also vary globally. For instance, a standard "gallon" drum in the United States is 55 gallons and 41 gallons in Japan. The content, format, and even symbols used on labels vary globally. Furthermore, no single language is required for labeling in international trade.

Complicating the operating environment is the need to share massive amounts of information among participants in the global supply chain, using systems and data that most often are technically incompatible and inefficient. To an ever increasing degree, the efficiency of supply chain functions are more and more dependent on proliferating information technology—hardware, software, and communications products. There is also a strong trend toward compatibility in information technology, allowing connectivity among various manufacturers' hardware, software, and communications products. Taking advantage of these trends, trading partners in the chemical industry are investing significantly to upgrade their information-processing capabilities. The result is a massive growth of interconnected global networks and cultural acceptance of the global information superhighway.

The supply chain needs to protect the environment and the people involved in handling, storing, and transporting chemicals. The Responsible Care® Distribution Code of Management Practices provides guidance for safe industry practices. The industry's drive to extend environmental stewardship to all operations is creating a model for safety and environmental protection among participants in the global supply chain.

To understand what will be involved in reducing time and costs associated with supply chain activities in the global marketplace, we will look at six drivers of supply chain efficiency as they relate to increasing competitiveness:

- market globalization;
- growth of free trade;
- regulatory restrictions;
- transportation;
- environmental, health, and safety concerns; and
- information processing.

Needs and Challenges

Market globalization

As customers of the chemical industry aggressively expand and unify their operations globally, chemical producers are increasingly able to supply materials with common specifications, regardless of where the materials are made or used.

Challenges that represent significant barriers to globalizing supply chains include the need to

- balance the demographics of chemical production locations relative to their feedstock sources and customers,
- rationalize undepreciated assets in facilities that cannot compete on a global basis,
- obtain the capital needed to globalize operations,
- overcome the disadvantage of low-cost feedstocks from offshore sources, and
- ensure compatibility of supply chain inventory systems among trading partners.

Growth of free trade

While the expansion of free trade is generally positive insofar as it is accompanied by reduction or elimination of barriers to trade, each country's situation is still different in terms of tariffs, specific border restrictions, and registration requirements. Exacerbating this is the fact that this information is dispersed, as well as difficult to access and understand. For a production site to be based on free-market forces—such as economics or customer need—tariffs, border restrictions, and registration requirements should be reduced or eliminated where appropriate.

Regulatory restrictions

As noted above, inconsistencies abound in packaging materials, design, labeling, and measurement. Test methods for certifying materials also vary from nation to nation.

Transportation

Challenges in this area focus on safety, efficiency, and cost-effectiveness. Often there is a lack of economic incentives to place vessels and ports into service to handle large volumes of bulk chemical products. Specific challenges lie in the areas of fuel consumption, lading capacity, and equipment utilization.

Environmental, health, and safety concerns
The ability to successfully meet environmental, health, and safety challenges depends largely upon our success in clearly identifying the problem. Without some degree of consistency, problem identification becomes extremely difficult. A lack of harmonization in international transportation regulation schemes, tariffs, border instructions, and documentation and information technology implementation introduces variables that exacerbate the problem and lead to the inconsistencies that limit the effectiveness of environmental, health, and safety strategies.

Information processing
Managing the vast amounts of information needed to operate the supply chain among global trading partners poses a great challenge to the chemical industry. Improvements can be made in communications to allow quick and accurate connectivity among parties interconnected to the global supply chain.

TECHNOLOGY VISION 2020

New Capabilities
The supply chain functions will operate in an environment of seamless coordination of orders, production, and distribution across countries and continents.

Definitions of chemical classifications will be harmonized.

HOW TO GET THERE
The chemical industry can structure its marketing, manufacturing, and distribution operations from a global perspective, harmonizing manufacturing and distribution operations as its customers globalize and harmonize their requirements.

Chemical producers can form global partnerships with their customers, feedstock suppliers, coproducers, and third-party service providers, both domestically and abroad, to remain competitive.

The U.S. government can support, wherever possible, efforts to harmonize multinational and domestic tariffs, border restrictions, registration requirements, regulations, and standards. These efforts can be made in conjunction with trade associations and international business units that deal in chemicals and chemical materials.

Discrepancies within regulations regarding chemical product shipments can be addressed.

Risk–benefit analysis can be incorporated when defining standards and revising regulations.

Improvements and Enhancements
The safe and efficient distribution of chemical products will continuously improve, thereby generating major benefits to the U.S. chemical industry and economy, as well as the environment.

Chemical companies' responsiveness to the changing requirements of their customers throughout the world will increase dramatically. Overall response time will be reduced. They will thus be able to support their customers' product needs several times faster than in the 1990s.

Supply chain operations will be more cost-effective and require less investment. Inventories could be reduced by as much as 50 percent and storage and handling costs reduced by as much as 20 percent of what they were in the 1990s.

Consequently, profits in chemical companies may increase, adding to the potential revenues of the U.S. government and permitting chemical manufacturers to make the investments needed to reconfigure their global manufacturing and distribution facilities, develop the required information systems, and train their workers to meet the demands of an evolving global industry.

The global environment will benefit from worldwide implementation of the Responsible Care® initiatives.

HOW TO GET THERE
The chemical industry can initiate a benchmark study to identify the best practices in supply chain management. Such a study should

- review current surveys of best practices across multiple industries;
- develop detailed measurements of contributions of the total logistics and supply chain to establish benchmarks for assessing industry improvements;
- compare the chemical industry with others in terms of these measurements;
- define targets for the industry;
- promulgate the comparisons, benchmarks, and objectives throughout the industry; and
- provide assistance to companies seeking to improve their performance.

To improve its international competitiveness, the chemical industry can develop the logistics function to better manage its supply chains and achieve such efficiencies as sharing of facilities, operations, and services. Toward that end the industry should

- formally recognize the value of logistics in managing supply chains;
- structure marketing and distribution operations from a global perspective;
- develop global partnerships with customers, carriers, feedstock suppliers, coproducers, and third-party service providers to share facilities, operations, and services;
- streamline and standardize business practices;
- develop better methods and equipment for shipping faster and managing “waiting to ship” times more successfully.

The federal government can partner with the chemical industry to harmonize global packaging, labeling, documentation, handling, storage, and shipping requirements that protect the environment and are cost- effective. Some necessary measures are to

- encourage global harmonization of packaging, labeling, documentation, handling, storage, and shipping requirements;
- work with industry to ensure use of best available practices and risk–benefit concepts in establishing standards;
- promote communications networks that provide direct access to different countries’ regulatory requirements in standardized format; and
- support the reduction of barriers to trade.

The chemical industry can sponsor an effort to drive information systems toward harmonized communications, data transmission, and information processing in support of global supply chain activities. Steps toward that end include

- surveying the chemical industry to determine the most important functional and technical requirements for global systems;
- working with the software industry to determine the best software and hardware packages available to support the chemical industry’s requirements;
- working with the information technology community to meet the global needs of the industry for harmonized formats;
- through consortia and other cooperative efforts, participating in the development of large, integrated, computer networks for the chemical industry; and
- working within the educational community to establish training programs and curricula that meet the industry’s need for skilled workers.

Chapter 6

INFORMATION SYSTEMS

Information Systems in the Chemical Industry from Three Perspectives

Throughout the chemical industry, the ways in which data are turned into information and used, managed, transmitted, and stored will hold the key to increasing competitiveness. Improved and enhanced information systems are at the very heart of our future technology vision, which sees the chemical industry as operating in ways that are highly efficient and economical.

To this end, we consider information systems from three perspectives:

(1) infrastructure issues and the development of open systems;
(2) the use of information systems in business/enterprise management; and
(3) the use of sophisticated information systems in product and process design and development.

From each of these three perspectives, we review the current status of information systems, identify the needs and challenges, and look to the future, articulating our *Technology Vision 2020* and outlining the recommendations that will move the industry ahead.

Information systems are also key to advances in manufacturing, engineering design, and plant construction, and we discuss these systems in the following section.

INFRASTRUCTURE AND OPEN SYSTEMS

Significant technological advances will require significant growth in the infrastructure of current systems. Therefore, progress from closed to open systems is essential.

Current State

The current state of information systems stems from the proprietary nature of the computer industry and the highly competitive way in which the industry has matured.

Data compression techniques are not adequate for transferring and storing large quantities of data. Computer systems remain that do not communicate with other systems. Electronic communications are limited by the data-transfer infrastructure.

Many software applications operate from proprietary databases that are not widely available and often not transferable to other uses.

A company using an internal database system, without adequate transfer methods, will not be able to use many commercial software products. Some companies that developed early versions of common databases were forced to develop many software systems in-house to meet their database requirements.

Companies using different database systems often have difficulty exchanging information. Without effective data transfer, they must often reenter data into systems manually. Reentering data increases costs and serious risk of error.

Document management today involves many formats, from electronic to microfilm to paper. In general, document management plans have yet to be developed for the complete business cycle. The ability to support work-flow through these systems is important. Operating procedures are being converted from paper documents to electronic formats that can be viewed on-line. Information-transfer techniques can be improved to ensure more efficient integration of material safety data sheets (MSDSs), vendor documentation, and computer-aided drafting and design (CADD) information.

Needs and Challenges

Advances in several areas must take place in order for the chemical industry to fully enjoy the benefits of information systems technologies.

Changes in policy

There can be an industry-wide commitment to changes in and improvement of data management.

- Computer systems and networks must be available when needed.
- The use of paper in the workplace can be significantly reduced.
- Process control systems can be used to automatically input data into the systems. Customer and supplier data can be transferred between computer networks in both directions. Consequently, data will never have to be entered more than once into any computer.
- Data exchange must be transparent to the user, and software enhancements to make this possible must be developed.
- The protection of proprietary information must be enhanced through the continuous improvement of computer security systems.

Improvements in software and hardware

Appropriate software and hardware can be developed to support more sophisticated functions, including development of the following:

- Interfaces and gateways can be developed to support database connectivity.
- Data compression technologies or large bandwidths will permit transfer of large packets of information with improved system reliability.
- Automated devices, such as on-line or automated data collection devices or scanner–bar code readers, can help enter data accurately into the system.
- Computing hardware and software can be developed to the point that the most complex calculations are accessible via intuitive user interfaces. These interfaces should cost the same or less than today's systems.

Improvements in networking, communications, and data exchange

Advances in networking and communications will be required.

- Low-cost, reliable, and secure worldwide telecommunications are needed.
- Enabling technologies, such as desktop video-conferencing and wireless communications, can be widely used. For instance, such technologies would enhance communication from the plant floor to the sales and marketing departments.
- Communication, including data transfer between suppliers and customers, can be timely.
- Fast, reliable, cost-effective data networks must be available.
- Electronic data interchange (EDI) would enhance "just-in-time" material management systems, helping to integrate inventory systems throughout the entire manufacturing process. This could reduce inventory costs and improve overall manufacturing performance.

TECHNOLOGY VISION 2020

In the future, our investments in information management will reflect their importance as corporate assets.

New Capabilities

Individuals with the need to know will have reliable, instantaneous access to information and decision-support tools via intelligent, intuitive interfaces that help them do their jobs regardless of their location—virtual offices without borders.

Data will be managed as a corporate asset with the owners assuring accuracy, timeliness, and validity. Data will be entered only once into the system and will be accessible to all programs or individuals on a need-to-know basis. This will greatly improve the efficiency of the staff who today spend significant time gathering, verifying, and moving data around for various applications. Data centralization and replication techniques could be used to develop cost-effective data exchange methods.

Critical information will be managed through document management plans, with important information in electronic format.

How to Get There

All manually accessible documents can be scanned by optical character recognition (OCR) devices to convert it to electronically readable, searchable, and compatible formats. The cost of scanning and correcting can be reduced to the point of cost-effectiveness.

To protect data, security techniques are needed that ensure the authenticity and traceability of documents. Also needed are techniques for automatically capturing and retaining operating knowledge.

Data compression, transfer, and storage technologies can advance so that large packets of information may be rapidly transferred.

Eventually, there could be no practical limitations to transfer and storage capabilities. Cost-effective data compression and transfer technologies can be developed to achieve these technology goals.

Technology that bridges the gap between islands of automation can be developed, ultimately creating open systems from which data can be delivered vertically and horizontally.

Techniques for improving reliability of software and hardware can be developed. Standards for exchanging information via document management systems in an open environment using common database structures and formats can be developed.

Consistent, international protocols for process, plant, and business database formats can be developed.

Improvements and Enhancements

All applicable literature, regulatory information, and scientific data will be available on-line.
Individuals will be able to do literature surveys through personal computers.

HOW TO GET THERE

The capability of worldwide network communications can be improved so that it operates more consistently.

BUSINESS AND ENTERPRISE MANAGEMENT

Information and timeliness of access to information are critical to competitiveness in business. Opportunities for growth in the area of business information systems will focus on accelerating access and personalizing system use and training. Information systems can be widely implemented throughout all levels of the organization to aid decision making. Instantaneous access to data means faster, more accurate decisions.

Current State

While information systems have dramatically increased productivity, a lack of integration continues to limit their contribution to organizational effectiveness. For instance, top management has limited on-line access to sales, distribution, and plant operation information needed for business decisions. Data reside in multiple, disconnected databases. The ability to perform “What if?” evaluations is limited. On-line executive information systems are only now becoming available.

For management to be able to make sound analyses of business performance, timely access to information on performance of individual product lines, business units, and plants is required.

Many software packages are not designed to facilitate communication across platforms, departments, sites, or with other systems.

Older, or legacy, software is usually proprietary. Because vendors do not always offer complete-enterprise systems, system integrators—external or in-house—develop special software, hardware, or a combination of both to bridge the gaps among systems. Often, the result is a one-of-a-kind system requiring heavy maintenance. Upgrades are difficult and expensive. Inadequate end-user involvement and needs assessment during development often leads to difficult-to-use applications that require additional resources for modifications and patches before the software can be used.

Many process control systems are isolated from production planning and business decisions, and the same is true of financial, sales, and distribution information. Inadequate networking of computers results in repetitious data entry. Limited electronic data transfer makes businesses less responsive to the needs of customers.

Needs and Challenges

Improvements in hardware and software

Systems that provide information on production costs, inventories, profit-and-loss statements, costs of sales, and volume of business need to be developed.

For decision support systems to become optimally useful to management, they require accurate, current exchange of information between the operating plant, the laboratories (for quality assurance), and the maintenance system. Support systems that analyze productivity, reduce cycle time, and aid in trouble-shooting and improving safety will need to be developed in addition to decision-support tools that assist in analyzing data and creating and verifying business models. Tools such as neural networks, artificial intelligence (AI), and expert systems can be used in all functions of the enterprise from process analysis to business analysis.

To optimize business utility, separate functional modes—such as those for manufacturing, purchasing, and maintenance—can be combined. Computer-integrated enterprise models with traditional functions are often of limited utility because they have been over-taken by new requirements and approaches to data organization and management.

Consistent labeling and tracking systems will need to be developed to support the use of computerized logistics systems that minimize cost and delivery time for products.

An automated auditing system can be developed that reduces the time and effort spent on ensuring compliance with external and internal standards and requirements.

Users need to be able to select from a number of possible visual formats, such as raw data, charts, and graphs, and to view data according to any selection criterion they wish, such as by country, by customer, by region, or by product. To accommodate these needs, information systems must advance to the point where they are characterized by sequential viewing capacity.

Changes in networking, communication, and data exchange

Plant floor and production planning systems should share information with order entry systems to better meet customer requests.

Quality assurance information can be shared with business centers to achieve efficient control.

Safety information can be immediately accessible to operations people.

Changes involving information users

Since each information system user has different skills levels, learning systems based on artificial intelligence and neural networks will identify the skills of the user and adapt the interface to the user's specific level.

Management can have access to personnel training as well as health and safety information.

On-line interactive training for use of information systems needs to become available.

New Capabilities

In the future, automated systems will support business and enterprise management's decision-making processes, and both customers and suppliers—internal and external—will have timely access to the information they need. This means that individuals will gain access to the information and tools they need to help them do their jobs. For instance, information for all parts of the supply chain will be available, along with the capability to track materials and products at every stage.

Improved forecasting tools will be available to support business decisions.

Information management will be based on electronic storage rather than on paper, and the paperless factory will become a reality.

How to Get There

Information systems that provide data on demand and in real time for planning and scheduling functions can be developed.

Information systems can be developed to accommodate management of a business portfolio with an expanding set of products.

Standards for infrastructure and data exchange can be developed.

To develop better business strategies, industry can fund the development of intelligent information–agent tools that collect information.

Search tools can be developed to efficiently scan all sources, external and internal, for information pertinent to the business or enterprise, and make that information readily accessible.

Information integration can be the first goal for a plantwide information system.

Information can be presented in a variety of formats that accommodate users of differing skills. Software can be developed to facilitate user-specific interfaces for information.

Improvements and Enhancements

Information will flow freely throughout the enterprise and supply chain, both vertically and horizontally.

Knowledge-based systems will be developed to the point where they have decision-making capability.

Real-time data on operating costs and use of resources will improve accuracy of financial analyses.

Speed of communication within an organization will improve.

Little or no inventory will be required due to "just-in-time" deliveries and real-time product tracking.

HOW TO GET THERE

Vendors can be encouraged to provide information in a form that permits it to be integrated into a larger system.

Government and industry can fund the development of technologies for business and enterprise management, including expert systems and intelligent decision support tools.

Business models can be flexible enough to incorporate multinational business practices and cultural diversity.

PRODUCT AND PROCESS DESIGN AND DEVELOPMENT

Current State

Although computer-aided simulation and modeling of products and processes have been used extensively in the aerospace, automotive, electronic, and pharmaceutical industries, the use of such techniques in the chemical process industry is still emerging.

The development of new industry practices, the use of techniques adopted to other industries, and the emergence of new modeling and simulation technologies specific to the chemical industry will allow companies to shorten product and process development time. These advancements are integral to maintaining global competitiveness.

The chemical industry increasingly uses new, more productive computational approaches to product design and development. Advances in simulation, modeling, hardware, and software are enabling this change and will accelerate the pace at which technological change will take place.

In product development, product designs are scaled up from bench-level quantities to production-level processes. As detailed process design proceeds, steady-state and dynamic simulation are used to model pressures, temperatures, and flow rates. Safety and regulatory concerns are factored in, and elaborate "What if?" scenarios are investigated by modeling before the first factory valve is turned. Over the past two decades, steady-state and individual process-unit modeling have evolved.

Simulation of chemical reactors and both batch and continuous processes has been improving rapidly, although more research and development is needed in these areas. Such simulation and modeling techniques are rapidly becoming the chemical process engineer's most powerful tools.

In product design, molecular modeling and computational chemistry are evolving to the point where they can be applied to larger molecules, such as polymers.

Modeling is compressing the time between hypothesis and experimental outcome. New materials and their properties can be predicted and visualized before the materials are synthesized. Similarly, complex molecular interactions and information on chemical reactions can be modeled.

Scientists also are beginning to prototype information on chemical intermediates and reaction byproducts. In addition to reducing design cycles, modeling eliminates material acquisition and disposal costs and improves safety by reducing exposure to chemicals and intermediates in the laboratory.

Needs and Challenges

Changes in policy

The culture of the chemical industry's research community needs to shift away from empirical design toward computational design.

Health and safety needs should be further explored in both product and process design and the development process.

Improvements in modeling and application of information technology to specific needs of the chemical industry

Easy-to-use modeling tools can become available.

The information and assumptions used in modeling should become accurate.

Research is needed in specific areas of interest to the chemical process industry (CPI):

- simulation and modeling techniques as they apply to the CPI;
- prediction of the chemical properties of new materials based on those of existing materials; and
- reaction and separation dynamics.

Improvements in hardware and software
Safety and regulatory information can be integrated with design tools.

Property-prediction databases that contain a wide selection of compounds can become available. Databases need to be expanded and verified through comparison with experimental results. In the longer term, techniques need to be developed for predicting properties of future products from the properties of similar products. Pattern recognition and forecasting techniques, such as statistical analysis and neural network technology, are just beginning to be used. However, the bulk of the near-term work lies in gathering information on the properties of current materials and making it readily accessible.

Reasonably priced high-performance work-stations and computer hardware are needed.

High-speed hardware can become available at a reasonable cost.

Changes in communication, networking, and data exchange
Separate cells of information are of little value if they cannot be effectively transmitted throughout an organization to those proceeding with the next step in commercializing a product. Design, development, operations, and quality control groups lose value when time is lost reentering information gathered previously by another group. Information and models must become readily available and easily passed from one group to the next.

Adequate computer network speed and bandwidth are required to support transfers of large quantities of data.

Reliability of data can be increased through improvement of data interfaces.

Communication can be improved between design and development groups and development and operations groups.

Data transfer standards can be developed and used industry-wide.

Changes involving information users
Key to the implementation of more sophisticated modeling techniques will be the development of easier-to-use interfaces, such as tools based on virtual reality.

TECHNOLOGY VISION 2020

Improvements in information systems, particularly in modeling and databases, will radically change the way the chemical industry conducts R&D.

New Capabilities— Properties Prediction

The properties of new materials will be predicted by the use of databases on the properties of existing materials.

How to Get There

The expansion and development of databases for predicting the properties and performance of chemicals can be fostered.

New Capabilities— Product and Process Modeling

Models will move easily between various software packages and hardware platforms.

Technology for modeling and optimizing safety, fluid dynamics, multiphase flow, and viscoelastic flow in chemical processes will be used throughout the CPI.

Dynamic simulation tools will be used for product development.

The cost and time-to-market for new products will be reduced dramatically through improved modeling technology and more extensive use of new modeling tools for computational chemistry.
The need for pilot plants will be reduced through the use of process modeling tools, and modeling will guide experimentation and scale-up.

Product stewardship will have been improved through modeling of safety, recycling, and reuse factors for chemical intermediates.

User interfaces to semi-empirical and quantum mechanical molecular modeling tools will be improved for use in product and process design throughout the chemical industry.

How to Get There

The chemical industry can be encouraged to compare its modeling practices against those in other industries and adopt best practices.

Protocols can be developed for transferring models and model parameters within an organization.

Government and industry can undertake a concerted effort to enlarge common knowledge of molecular modeling and simulation as applicable to the chemical process industry. Specific efforts can be devoted to process modeling, particularly with regard to dynamic simulation.

Models that can interact and exchange data, such as the Project for Process Simulation Data Exchange, can be developed.

Safety-related modeling of chemical processes can be improved.

Government can enhance mechanisms and interactions that enable the transfer of process simulation and modeling techniques to the private sector. Two primary sources of such techniques would be the U.S. Department of Defense and the U.S. Department of Energy.

Computers in Manufacturing

MANUFACTURING AND OPERATIONS

Current State

Manufacturing and operations will require continual infusion of the newest information and process control technologies if the chemical industry is to maintain the ability to reliably deliver products that best serve the customer and are delivered at the lowest cost available in a global market.

Knowledge of process operations and process information and control methods is found too often in separate, functional groups within a company. Dismantling these functional silos will be necessary to enable U.S. industry to become globally competitive by 2020. Companies must invest not only in process automation, enterprise-wide networks, and standard manufacturing software systems, but also in human resource systems (both physical and educational) that make possible the capture and maintenance of the maximum economic return from each manufacturing facility. Process automation will require a highly skilled operating and maintenance staff to take full advantage of dynamic business opportunities. Support from knowledge-based operations and maintenance adviser systems will be available, but the need for cause-and-effect analyses in unusual situations will still require human intelligence for chemical plant operations.

Currently, the chemical process industry has an existing base of computer systems that perform the manufacturing tasks of

- process control,
- process information,
- modeling,
- statistical process control,
- equipment monitoring and maintenance,
- document management, and
- laboratory systems.

Frequently, these systems were purchased from numerous suppliers or were developed internally. In either case, they were likely installed individually and not designed to communicate with each other. Movement is underway toward networking individual computer systems and integrating the various applications into plantwide or company-wide information networks. Legacy systems that do not use open systems concepts impede these efforts. However, the dependence on these systems and the investment in them are such that it is difficult to throw away and design the ideal system.

Many companies have started on the path to facility-wide networks (typically connecting major concentrations of manufacturing staff with fiber-optic cables) and the transition to commercially available plug-and-play software systems for manufacturing support. This drive results from several factors. Internal resources available to develop and maintain point-to-point device and component application interfaces are often limited with the reconsolidation of corporate engineering and information systems functions. At the same time, manufacturing management is demanding more functionality from process information and control systems to meet customer’s quality requirements and government regulations; and commercial management is demanding that manufacturing and other business support functions provide information that is integrated enterprise-wide to support business planning.

Laboratory systems in the chemical process industry range from stand-alone equipment using manually entered results to integrated analytical equipment and information systems. The applications are as varied as the numbers and types of materials analyzed—from raw material, to in-process, to final product.

Efforts are underway to improve process data availability in electronic form among company personnel. More data are available, or soon will be, than staffs have time to analyze, and the need to convert data into information and advice is broadly recognized. Data are being analyzed using tools such as process graphics of past and present conditions, trends in historical data, and custom-built tools in spreadsheets. The statistical technology used most often today in manufacturing is statistical process control. This technology is used to monitor chemical processes against control limits and calibration of analyzers. Statistics are also used to design process sampling procedures, reconcile data, and illuminate process capability and variability.

Steady-state models are used in manufacturing to design processes, plan and schedule plant operations, and occasionally to achieve on-line optimization. Dynamic models have been used for operator training, control studies, and “What if?”

scenarios. Developing models takes time, especially if they are matched up to operating plants. The accuracy of the models is questionable over the full operating range of a plant. Modeling of distillation operations is fairly well understood, while reactor models are still custom built. Just becoming available are dynamic modeling systems that have model libraries and point-and-click interfaces for model building.

Equipment systems today are mainly in the monitoring mode. Some of the data are read electronically, but much is entered by hand. Vibration is being monitored on most large motors, compressors, and turbines, but the systems are not networked into the plant information systems.

Control is mainly on/off. Machines experiencing a disturbance are backed off to a clearly safe operating speed because minimum changes needed to control the machine are not known. Maintenance data systems are still in the development stage, with much of the data being hand-entered. These systems are used to store maintenance and inspection records and to schedule maintenance activities.

Needs and Challenges

A high degree of automation and decision making will be achieved when statistical diagnosis of process information becomes an integral part of the enterprise's information system. Process control information will need to be communicated upward, to identify raw materials consumed and products made and being made, and downward, to identify products to be produced and how to do so.

Open systems and integrated applications

Integrating numerous and diverse computer systems geared to individual manufacturing tasks presents major barriers to full automation. For the industry to overcome these barriers, standard-setting groups can encourage and support vendors in their progress toward openness in digital control system architecture and applications.

Control components, both hardware and software, will advance so that they can plug-and-play, easing costly barriers to integration and support that limit manufacturing advances today. Once plug-and-play is achieved, a complete control system will no longer need to be changed to take advantage of a different vendor's technology. High-speed, reliable, wireless communications integrating audio, video, and data will be essential. Changes in architecture will not require costly wiring, rewriting, and support.

Plug-and-play modules and openness decrease reliance on custom devices and components, freeing engineers to focus on development of new applications, expert systems, knowledge-based systems, neural networks, and simulation modeling. Advances in analytical and modeling technology are needed that will support highly accurate on-line and real-time decision making. Long cycle time for results will be unacceptable. In addition to smarter instrumentation, instrument suppliers will provide standard communications.

Process control

Advanced process control technology can be developed to handle the full operating range of a plant, from start-up to shutdown. Advanced control can run all the time to ensure meeting product specifications all the time. The plant must be able to eliminate as many process disturbances as possible and to handle the nonlinear behavior of process units. Advanced process control technologies can continue to develop until very specialized methods typically associated with off-line use become on-line parts of everyday operation. These techniques will enable plants to run optimally.

To support advanced control capabilities, the use of in-line measurements (analysis) will grow, as will inference and prediction of stream composition. The development of soft sensors using models and neural net technologies to predict stream compositions will minimize the need for costly analyzers. Where inference and prediction cannot be used, the alternative in-line analytical devices will need to be simple and rugged, which will require advances in analytical technology. Sample systems will be eliminated so results will be available instantaneously to support decision-making. Analyzers will be self-recalibrating. They will do preventive recalibration when measurements are different, but still in tolerance, rather than when product is off-specification, rework is required, and downtime is necessary to recalibrate.

Equipment and monitoring

Reliability of rotating equipment must be improved. Data systems for rotating equipment need to progress from mere monitoring to the point where they offer control and, eventually, prediction. Such performance will require accurate on-line measurements of machine conditions, external and internal.

Performance accuracy of real-time mapping needs to be improved to allow machines to be run at their true permissible speeds rather than within overly conservative limits that may reduce efficiency. Control of the machines can improve so that backing off from critical operating regions requires movement back to the real limit and not overcorrection.

Techniques for predicting the optimum time for maintenance and predicting system performance must be developed.

Rotating equipment can be designed to allow needed performance to be dialed into the machine by the control system. Maintenance database systems can evolve from the repository of data today to the repository of knowledge of all equipment at a manufacturing site.

Virtual reality will evolve to the point that on-line visual inspection of the inside of equipment will be possible, with accurate measurement being the key to success in this area. Corrosion monitoring will be available to continuously monitor all parts of the equipment, not just selected points.

Data on equipment will need to enter the database automatically. Wireless systems will give maintenance people in the field access to data, diagnostic tools, and maintenance procedures. Once problems are diagnosed, parts will be ordered automatically from the vendor's warehouse; a local stock of spare parts will no longer be needed. By the time the faulty equipment reaches the shop, the spare parts will have arrived. The computer will help the mechanic with repairs as necessary. Shut-down of units will be predicted from equipment conditions, and shutdown planning will be completely automated. The need for specialists will be greatly reduced.

Process modeling

Processes can be understood well enough to build steady-state and dynamic models that accurately represent the plant over the full operating range.

Dynamic process models can be run at 50 to 500 times real time. This goal can be met with computer speed, calculational efficiency, or both.

Models for any use can be derived from a single source. Dynamic models can be an extension of steady-state technology. Building models can entail only simple selection from libraries of existing models. One day can be enough time to model any process unit. Models can be robust and insensitive to starting conditions and can match the full operating range of the plant. Models can shadow dynamic plant operations. Standard data exchange is needed so that models in the library can come from different sources.

Advisory systems

Better advisory tools are needed for situation management, such as alarm avalanche and knowledge retention. Advisory systems can move beyond custom-built to off-the-shelf applications.

Detailed process understanding, dynamic models, and multivariate statistics are keys to success in this technology area.

Advisory systems that convert raw data into information and advice for use by operations and plant support staff can be developed. Such systems can cover unit profitability, equipment performance, situation management, knowledge retention, and operator training. These systems will progress over time from providing information through calculations, to providing advice for consideration and possible action, to taking action and informing personnel of results.

Future advisory systems need statistical techniques to reduce large volumes of data into diagnostic information. Multivariate statistical techniques are needed to determine why dynamic process models do not match plant operations.

Many applications of advisory systems will require dynamic data reconciliation. This can become a generic tool that can be broadly used. Sophisticated pattern recognition techniques, such as neural networks, need to be developed to convert raw process data into useful information.

Hardware and software

Computers must be able to handle large volumes of data and calculate fast enough for real-time uses. Hardware speed and capability to store and retrieve large quantities of data are critical to handling process information.

Computers in Manufacturing—General

The manufacturing operation will be an agile, reliable, reproducible, clean, efficient, responsive, and productive component of the chemical industry's supply chain. Continuous improvement will remain a way of life as automation advances.

Management and workers will be familiar with manufacturing processes and automation.

Manufacturing operations will be guided in accord with completely integrated information from sales, marketing, R&D, and supply. Data will flow seamlessly along the supply chain, from raw materials suppliers through manufacturing operations to the customer. The three layers of automation—process, plant floor, and supply chain—will be connected so that data need be entered only once.

The automation will not only connect the parts of the supply chain, but also will connect the process on the plant floor to the commercial operation of the supply chain, which extends from raw materials suppliers through manufacturing operation to the customer. Distribution and shipping will be considered parts of manufacturing operations.

Manufacturing operations will respond to customer demand that comes either by pull or by make-to-order. This demand drives scheduling, raw material supply, distribution, deployment of manufacturing resources, and production. The system operates automatically without manual intervention; logic and expert systems will make the routine decisions.

Implied in this technology vision are computer networks, wireless communication capability among all components of the supply chain, and plug-and-play software well beyond the capability of the 1990s.

Also, in the factory of the future, individuals who need to know will have instantaneous, reliable access to information and decision-support tools that will help them do their job regardless of their location. Data security will be adequate to allow global communication of process data. Intelligent, intuitive, person–computer interfaces, often voice activated, will be the norm.

Computers in Manufacturing—Operations

Manufacturing processes will be operated under fully controlled conditions. Automatic process control will be practiced from plant start-up to shutdown.

The processes on the plant floor will be fully controlled and always produce what is needed. Reproducibility of products will be improved. The system will compensate for variability in raw materials or control it within the desired range.

Use of automation will greatly increase. Clean-out will also be automated, with proper attention to cleaned-out material. Expert systems and logic will make these units run according to command.

Manufacturing performance will meet conversion, quality, reproducibility, and cost requirements. Process understanding will have developed to the point that unit operating conditions are based on predictions from dynamic plant models accessible to the control room. Manufacturing inventory costs will be minimized by scheduling production campaigns that closely match (and in some cases anticipate) customers' needs. This degree of automation will make the productivity of capital and people very high.

The software and process equipment will be plug-and-play, with standardization and validation improving their interface. Improved reliability and redundancy of computer hardware will assure very high availability of manufacturing control through information systems. Expert systems and logic will be built into the software with no adaptation required. The materials-handling systems will adapt easily to changes. Process equipment will be automated to produce a broad range of materials.

Plants will operate with only rare, unscheduled outages caused by equipment failures. Maintenance databases will contain full knowledge of all equipment, with knowledge-based computer assistants coaching plant staff in making routine repairs. Specialists will be needed only for first-time problems. Analytical results will be available on-line instantaneously, as required to support a fully automated manufacturing facility.

Operations will be informed of plant conditions and corrective actions that have been taken by the computer. Diagnostic techniques using statistics will facilitate this capability.

The plant floor will instantly respond with the latest input to schedules to meet production requirements. The plant floor also will inform the integrated system of the status and availability of equipment, people, materials, maintenance needs, and other elements needed to support automated scheduling.

Batch operations of the larger manufacturers will be fully controlled. The integrated and transactionally current automated information system will direct scheduling and production. Products will be changed using information just an instant old, which will permit very short lead times and excellent response to customers.

Batch operations of small manufacturers may not justify full automation, but will use robotics to assist operators in tasks such as loading catalyst into the reactor. Teleoperation will allow the operator to handle field tasks without leaving the control room.

Both continuous and batch processes will have fully automated handling systems for raw materials, package components, and finished products. Robotics will be used. This activity, combined with complete process automation, will mean a reduced need for manual intervention.

How to Get There

Open systems and standards

Development of standards for open systems can be encouraged, and vendors can be encouraged to create products that meet these standards and the needs of the CPI. These needs offer an opportunity for academe, industry, and vendors, with government support, to jointly develop the necessary technology.

Standards for product labeling can be developed, including identification and hazard information.

Standards for computer-aided drafting and design can be developed to ease integration and operation.

Process control

Statistical process control can be expanded into multivariate systems.

Digital control systems can be on all units where they are economically justified, allowing implementation of advanced control concepts.

Advanced controls can optimize plant operation under most conditions.

A capacity for wireless transmission of process data within plant boundaries can be developed.

Equipment and monitoring

Rotating equipment can be broadly monitored, with improved analysis to indicate how to move machines out of critical speed ranges.

Maintenance databases can have automated data entry.

Monitoring data can allow equipment performance to be predicted six months in advance.

Real-time performance maps of rotating equipment can be able to be created with 1 percent accuracy.

Maintenance databases can have full analysis to pinpoint maintenance problems and full on-line help for equipment repair.

Process modeling

Modeling tools can address dynamic and steady-state technologies.

Dynamic and steady-state models can exist for all processes and be capable of shadowing plant operations.

Advisory systems

All manufacturing data can be available at the desktop computer and reduced to information and advice for routine situations.

Key product quality results can be available on-line, and manual entry of laboratory data can be minimized.

Operations people can be informed of plant conditions by advisory systems, which will be used widely.

Statistical techniques can be used extensively for data reduction and diagnosis front ends for advisory information systems.

Product quality inference techniques will be used on-line; key components will be analyzed on-line; and key entry of laboratory data will be eliminated.

Hardware and software

Industry can communicate to hardware and software vendors the criticality of computer speed, the ability to handle large databases, and the need to provide open systems.

Improvements and Enhancements

Process understanding can have developed to the point that units will be run on the basis of dynamic models.

Full automation can exist and can include control from start-up to shutdown.

COMPUTERS IN PLANT ENGINEERING AND CONSTRUCTION

Current State

Some relationships between facility owners and engineering contractors reflect a time when billing for time and materials or a fixed-price contract were the only available paradigms for payment.

One of the factors that limits communication and partnering is that electronic linkages between owners and contractors have not been developed.

In terms of engineering, old approaches are being executed with high efficiency, thanks to the use of computer-aided design (CAD) and computer-aided engineering (CAE) to help engineers and designers work efficiently.
Underlying engineering practices, however, have changed little during the past half-century.

While technological advances are necessary in engineering and plant construction, change in this area will be evolutionary, rather than revolutionary, as it is throughout the manufacturing sector. The rate of change will be driven by the industry's success in meeting several needs and challenges, as outlined below.

Challenges

We predict that facility owners will frequently partner with engineering firms, construction companies, and major equipment suppliers to design and construct chemical plants with many standardized, prefabricated modular components that meet industry-wide requirements.

Continuing investment in engineering automation will be necessary if firms are to remain cost-effective suppliers of engineering and construction services. The application of concurrent engineering approaches will also require innovative approaches to integrating input from all potential customers.

Most of these enhancements can take place with current technology, and many sophisticated methods have already been achieved. The need to validate designs before construction will lead to increasing use of computer-generated models that provide holograms and other three-dimensional CAD tools. Also, the use of robotics in plant construction and operation will be expanded. Integration of the measurement and information systems in each component will only be practical when standard communication protocols become available and are widely used by the industry.

TECHNOLOGY VISION 2020

Changes in Business Relationships

Contractor relationships will focus on value added, rather than time and materials. Joint ventures or partnerships between engineers, construction companies, and owners will become routine.

Data, model sharing, and exchange among owners, contractors, and subcontractors will be highly developed.

A limited number of very large international firms will be in the plant construction business, supplemented by small, highly specialized firms.

HOW TO GET THERE

To forge the partnership, the following changes are necessary:

- An industry-wide commitment to collaborative demonstration projects for automated technologies.
- The use of economic incentives to encourage contractors to automate their operations.
- The development of incentives that encourage engineering contractors and CAD/CAE vendors to collaborate on ways to shorten the design and construction cycle.
- The dissemination of sample partnership agreements with government research laboratories for developing and using automated technologies.

Technical Aspects

Automated design and modular construction of chemical plants in 2020 will cost the chemical industry significantly less than comparable facilities built in the 1990s.

Standard protocols, formats, and transfer techniques permit process design, development, simulation, and regulatory information to be translated into mechanical design and physical plant layout.

Lower operating costs, lower total invested capital per innovation, and shorter times from concept to manufacturing will add to the global strength of the chemical industry.

Automated design technologies will replace CAD technology and greatly improve time needed for design over what it was in the 1990s.

Comprehensive engineering and construction database systems will be in place. Many engineering steps will also be automated. Use of materials (piping, steel, concrete, etc.) will be highly optimized. Automated design technologies will replace CAD.

CAE techniques will become much more sophisticated, and only those tasks that demand atypical engineering judgment will not be highly automated.

Time and costs for the project cycle, including construction, will be greatly reduced over what they were in the 1990s.

Generally, data will flow smoothly from concept through design to construction and on into plant maintenance and operation, with-out any need for data reentry.

Automated engineering and design systems will create a highly detailed virtual plant capable of

- simulating plant start-up;
- verifying procedures, including material flow, energy needs, and emergency response plans; and
- training operators.

The quality of engineering and design will improve, with plant procedures verified in the virtual plant.

All information developed during design will be available to operations during the start-up and running of the facilities.

Construction activity sequences will be developed, and many tasks in construction, such as quality assurance and inspection, will be assisted by robotics.

How to Get There

Standard protocols, formats, and transfer techniques will be developed that permit process design, development, simulation, and regulatory information to be translated into mechanical design, and physical plant layout.

Comprehensive engineering, design, and construction database systems will be developed and put in place.

The use of materials, such as piping, steel, and concrete, will be highly optimized.

Intelligent systems will be developed and refined so that knowledge-based and cognitive systems become the norm.

Standards necessary for common industry information to be shared can be developed.

Chapter 7

MANUFACTURING AND OPERATIONS

The revenue-generating capability of the chemical industry is derived from its ability to deliver chemicals and materials that satisfy customers' needs. Manufacturing operations plays a key role in that activity. Maintaining and improving the competitiveness of the U.S. chemical industry will require advances in six areas of manufacturing operations: (1) customer focus, (2) production capability, (3) information and process control, (4) engineering design and construction, (5) integration of suppliers, and (6) global expansion

CUSTOMER FOCUS

Current State

The U.S. chemical industry has made significant improvements in its relationships with its customers. This has been brought about by increased awareness of the importance of the customer and greater efficiency in the order, supply, and payment functions. Improvements in customer demand forecasting, however, need to be made to ensure that inventory more correctly matches the customer's needs.

Needs and Challenges

To enhance supply chain focus on the customer, the industry should move toward improvement in (1) the reliability of supply, (2) the quality and consistency of products, (3) responsiveness to changing customer requirements, and (4) partnering for innovation.

Improvements in the response to customer demand

The industry should tailor its manufacturing and delivery systems to customer demand, rather than mere replenishment of capability inventory. This will require new technologies.

- Because of marketplace variability, the customer's demand forecast will not likely improve in accuracy, so the industry's capabilities must be improved to respond rapidly once an order is received. One of the new technologies required will be software that can rapidly convert customer orders into production and delivery actions that operate in parallel.
- To meet customer needs, different process units must be brought into use quickly. This may require new technology to make process units that are dedicated to product families, rather than individual products. These units will need to be designed to be easily cleaned and quickly supplied with raw materials. Unused capacity will need to be shared across a very large product base so that variations in customer orders can be managed economically.
- Improving the flow of products from the chemical industry plant to the customer requires delivery technologies that respond to needs quickly and economically. Flexibility and agility in the delivery system is essential and must be developed.

Products of high quality and consistency

A new level of quality and consistency will be required. New manufacturing technology needs to be developed so that products can be made with a much narrower band of variation.

Advances in testing and understanding chemistry and process technologies are necessary to achieve needed improvements. The goal will be to have parametric-based acceptance of all products and intermediates. A significant challenge will be to apply new technology and science to products and processes developed in the past.

Partnering for innovation

Partnering with the customer to bring forth innovation will become normal business practice. New products with related process technologies must be driven by the customer and the industry member.

New concepts of joint work at each stage of the innovation cycle will be required. Research will need to be undertaken with the customers and suppliers. It may be necessary to develop concepts like "shares'' that are based on the research investment that entitles the provider to a certain share of the revenue generated. It may require the establishment of joint ventures to effectively exploit the opportunity. In the simplest form, it involves a customer and supplier jointly developing a new product.

PRODUCTION CAPABILITY

Current State

As the industry evolves, retrofitting and new plant construction are occurring. Prioritization is a requirement as new technologies become available for new products and processes. In addition to new chemical and process technologies that improve the manufacturing capability, there are new manufacturing practices and concepts that enable the producer to better serve the customer.

Needs and Challenges

To advance the industry's production capability, new technology is needed in several key areas. These include: (1) reduced variability in the way chemicals are produced, (2) improved manufacturing processes to protect health, safety, and the environment, (3) agility to quickly respond to change, (4) reconfigurable manufacturing plants, (5) continued need for skilled workers, (6) integrated management of the production capability, and (7) a capability to access product and process information quickly and then manage the improvements.

Reduced manufacturing variability
A key challenge to the chemical industry is to continuously improve the consistency and predictability of operations.

Improved impact of manufacturing processes on the environment
Improvement in material and energy balance closure is an important activity of the industry that requires new technology. Analytical methods will allow the industry to better understand products at the molecular level. Types of technology required include on-line frequent measurements and the development of scientific risk assessment methodologies.

The ability to respond with agility to unexpected or anticipated change
The rate at which change is occurring within the U.S. chemical industry is gradually increasing. Shorter product life cycles and new product development present continuing challenges. This will require a continuous infusion of new technology to cope effectively.

New technology requirements are varied and difficult to assemble. Some examples of technology requirements are

- process equipment that can be easily reconfigured to make other products,
- support equipment that can quickly adapt to new production requirements,
- a management system that facilitates change as an integral part of production capability, and
- systems that increase agility among raw and packaging material suppliers.

Manufacturing reconfiguration
Process plants have often been built for a single purpose or product. However, it is more economical to design and build plants so that they can be easily converted to other purposes as needed. In addition, new technology is needed in understanding the chemistry and chemical engineering involved and harmonizing the requirements of the process. Ultimately, production of different chemicals at the same plant could shift seamlessly in response to customer needs.

Continued need for skilled workers
The depth and understanding of chemical, product, and process technology will require a highly skilled workforce. The integration of production capabilities will make the concept of teamwork more important than ever. Industry can work with high schools, colleges, and vocational schools to ensure meaningful courses are developed that correspond to actual industry needs.

Integration of production capability
Chemical companies are increasingly investing in new technology to integrate all aspects of business operations. Improved production capability is a critical goal of this new technology. The production process also needs to support the customer focus of these integrated systems. The systems will be people-oriented with computer software providing the connectivity. Connectivity will link the plant floor, the maintenance shops, and the analytical laboratories to purchasers and suppliers. With the

establishment of inter-connectivity and integration, more sophisticated technologies will be possible that will greatly enhance the industry's competitiveness.

A capability to assess historic process and product technology and use it to manage improvements
New technology that better uses knowledge about a product and its manufacturing process is essential if next-generation improvements are to build upon previous accomplishments.

Databases will be required that contain drawings, documents, prints, videos, and other forms of data that can be easily accessed through quick information retrieval.

The technology to access historical data as a basis for additional improvement is vital. Both continued and step change in products and processes improvement will be facilitated.

INFORMATION AND PROCESS CONTROL

Current State
Manufacturing operations will require a continual infusion of the newest information and process control technologies if the chemical industry is to maintain its global ability to reliably deliver products that best serve the customer at the lowest cost.

The chemical process industry will have computer systems that perform the manufacturing tasks related to process control and information, modeling, statistical process control, equipment monitoring and maintenance, document management, laboratory systems, scheduling, etc. In the past, systems were often purchased as stand-alone entities. As the industry works to achieve integration of systems, it creates new software requirements.

Needs and Challenges
The agility provided by new integrated systems needs to be exploited to improve the competitiveness of the U.S. chemical industry.

Elements required for improvements in computer capabilities include the following: (1) the use of data and an integrated system to allow the rapid implementation of new product and process technology globally, (2) the availability of current information to support global strategies to enhance company competitiveness, (3) significant improvements in make-and-deliver systems.

The operations of the make-and-deliver system will have a significant improve-ment in effectiveness.
Integrated systems that improve the effectiveness of the make-and-deliver system of a company will be a requirement in the future. Customers will continue to be the focal point and a company's ability to satisfy their requirements will be enhanced. Technology will advance through improvements to individual modules in the integrated system. These advances will enhance the capability of the overall make-and-deliver system. Furthermore, new technology to globally integrate systems capabilities will require greatly improved multilingual capability that can handle idea complexity and technical information and language.

The use of data and the integrated system will allow the rapid development and implementation of new-product and process technology globally.
The time required to bring new products and processes on-line will be significantly reduced by improved effectiveness of the product development process. Better definition of the potential application, fitting the available or new technology to the application, building the model materials or chemicals, and establishing the manufacturability will be enhanced. This will occur by increasing the availability of information and data relevant to the commercialization process. Access to pertinent information established the capability to deploy the technology globally in a rapid fashion. The whole process will stress speed to market and the rapid development of the application.

A major focus should be the development of the application requirements with the customer in mind.

The changing requirements in manufacturability will require companies to increase their agility.

Real-time availability of global transactional information will enhance U.S. chemical company competitiveness.
The global availability of integrated and current information and the discipline of routine transactions will allow a more strategic approach to global product line management. It will also allow the effective execution of the global supply chains in a routine fashion.

A significant improvement in the discipline needed to effectively execute make-and-deliver processes will occur.
A key element of successful make-and-deliver processes is an effective method to deliver consistent and reliable products. Harmonizing computer information systems with process control systems provides for this ability. New technology is needed to ensure the harmonization of integrated systems with process control practices and systems.

BUILDING NEW PLANTS

Current State
Electronic links allow plant designs to be done in any part of the world with the contractor and the owner simultaneously involved. Drafting boards and linen prints are being replaced by electronic design and CAD systems. CAE helps engineers and designers be more efficient.

Needs and Challenges
The building of new plants continues to be in a state of change. Improvements will result from both innovations and the better application of old technologies. Future conditions will cause this change to continue. (1) Owners will often partner with the engineering firms, construction companies, and major equipment suppliers when building new plants. (2) Standard, prefabricated modular components designed for industry-wide requirements will be increasingly used. (3) Pressure to shorten the time needed to design and build a plant will force significant change in the way this process is carried out. (4) The design of a plant will be done globally to minimize the cost. (5) The use of electronic footprints of existing plants will enable plant designs to be done more quickly.

The use of standard, prefabricated modular components designed for industry-wide requirements will increase.
This trend is driven by the need to shrink the time to market, as well as to reduce engineering and construction costs. Use of electronic media for the design process allows the adaptation of a standard design to specific situations. Owners will partner with engineering firms, construction companies, and major equipment suppliers to make this a standard operating procedure.

Pressure to shorten the time needed to design and build plants will force significant changes in the design and construction process.
Plants will need to be designed and built in a much shorter time. Technology is needed to automate the design process through modular concepts in easy-to-use software. In addition, compatible communications systems between major equipment suppliers and their design firms will allow for rapid translation of concepts into innovative plant structures. Partnering is required to get adequate response from the supplier to cut the building time. Dynamic simulation will allow for integrated design with verification of structural integrity. This will shorten start-up time and eliminate overdesign.

Plant designs will be centrally stored and available for worldwide use.
This technique is being used now on many international projects with less expensive labor in various parts of the world. As electronic networking increases, this activity will expand and the capability of these design shops will improve. New technology is required to enhance the speed at which the design can be done. Much can be learned from the software industry, where designing occurs worldwide.

The use of electronic footprints of existing plants will allow the designs to be completed more quickly.
Databases for the designs of current plants are often electronically accessible. The next step is to develop new technology to use the footprint of an existing plant and modify it so that it meets the needs of a new plant of a different size or changed product distribution.

SUPPLIER RELATIONSHIPS

Current State
The suppliers that support the commercial operations of the U.S. chemical industry are instrumental to the success of the industry. Suppliers are diverse and use many technologies to provide the industry with key ingredients. Their variety extends from crude oil and gas-based materials to silicon. These materials also include packaging components, catalysts, inorganic materials, fillers, etc. Additionally, the energy that the industry uses comes from suppliers that provide electricity, natural gas, and other fuels. All are vital to the success of the industry.

The industry uses contracts, spot purchasing, sole sourcing, and partnerships to obtain critical resources and products. In some cases, the relationship is an electronic connection that allows for monitoring the use of the supplier's product and "just-in-time'' delivery. In other cases, inventory is reserved at the user's site to assure a supply. Pipeline supplies are also common. Maintaining quality relationships with suppliers is very important to the success of the U.S. chemical industry.

Needs and Challenges

Out-sourcing of activities will continue in the industry, requiring the development of special relationships. Everything from cafeteria food to maintenance materials management is being done by suppliers. Companies will increasingly focus on core competencies. This involves developing strong partnership relationships with suppliers focusing on expertise relevant to the specialty.

GLOBAL OPERATIONS

Current State

The U.S. chemical industry operates with a global focus. Extensive operations are conducted offshore. For a company to be global, a significant understanding of the local market conditions must be gained.

Needs and Challenges

Two major trends will continue to enhance the global operations of the U.S. chemical industry: sourcing strategy will be integrated and executed globally, and information systems will need to be globally compatible.

A significant challenge that requires improvement is the ability to effectively ship and move materials in a global fashion with increased speed. With present oceangoing shipping, the cost of sea travel and the inventory value that is tied up are detriments to agility that could significantly assist in optimizing global economics. Shorter staging times and faster transit times will be required with no loss in safety or security.

Integrating and executing sourcing strategies globally

As product volumes increase in a particular country, product designs are required that use common intermediates and, at the last step of production, are tailored to a family of products and packages that suit local needs. This last step in product identity is a vital part of doing business globally and needs to be a key part of the strategy for enhanced industry competitiveness.

Global compatibility of information systems

For U.S. chemical companies to improve their capability to operate globally, an information system that is capable of supporting the activity is needed. The characteristics of this system must be aligned with the needs of a global product, application, and delivery team. Without this information system, the time for transaction will be much too long for a competitive activity.

Ability to quickly and effectively ship and move materials worldwide

Improved efficiencies in shipping materials by air, sea, and land continue to challenge the industry. The costs of moving chemical goods must be considered in light of the costs of warehousing. An improvement is needed that reduces both the total inventory time and cost-to-market. Technology for faster ships seems to be emerging. This technology must be combined with a supply chain that moves chemical materials to the ship from the producer and then from the dock to the user or customer. This will greatly facilitate the global transport of chemicals.

TECHNOLOGY VISION 2020

Manufacturing Operations

The *Technology Vision 2020* for manufacturing and operations in the U.S. chemical industry combines six areas for advancement. The vision assumes continued advancement of the industry in a world that experiences continued industrial development and improvement.

In 2020, manufacturing and operations are an agile, reliable, reproducible, clean, efficient, responsive, and productive component of the U.S. chemical industry's supply chain. Continuous improvement is a way of life. Customers receive a consistent supply of reliable products that satisfy all requirements. The industry responds to the customers' needs in an agile fashion. New products are introduced from technology platforms with a significant reduction in introduction cycle time.

Advances in shipping management and equipment allow for rapid movement of chemicals and materials from country to country. This capability is a integral part of the sourcing strategy.

Management and workers are familiar with manufacturing processes, automation, customers, and suppliers. Manufacturing and operations are guided in accordance with completely integrated information from sales, marketing, research and development, customers, and suppliers. Data flow seamlessly along the supply chain from raw material suppliers through manufacturing operations and finally to the customer. The three layers of automation—process, plant floor, and supply chain—are connected so that data entry need occur only once.

These capabilities are supported by computers, software systems, networks, and all other wireless communications, all with plug-and-play features. This seamless system links all customers, sites, and suppliers worldwide. Security systems to protect proprietary information have evolved to meet user needs.

Process control is highly automated, as are plant start-up, operation, and shutdown. Models with more than 100,000 equations are routinely solved to provide dynamic simulation-based control. Statistics play a key role in determining the quality of the signals.

Raw material efficiencies are significantly improved. Process clean-outs are automated with monitoring as a routine and frequent part of the process.

Manufacturing performance meets conversion, quality, environmental, reproducibility, and cost requirements. Process chemistry and engineering knowledge has developed to a state where unit operating conditions can be based on dynamic models available in the control room.

Partnering for innovation exists with the industry's customers. Definition of application requirements is a critical part of the partnership. New products with appropriate manufacturability are developed with customer involvement.

Partnerships also exist to improve the existing product lines so that products and intermediates are protective of public health and safety and environmentally sound. Interaction with the government and regulatory agencies is facilitated by a sense of shared mission and partnership in protecting human health, safety, and the environment.

Maintenance of the chemical plant will advance and be integrated with operational activities. Sophisticated tools have continued to improve reliability. Maintenance databases will contain full knowledge of all equipment, and knowledge-based computers monitor routine and preventive repairs. The maintenance system will be an expert system that prevents failure through the proper level of maintenance. The process plant will be a truly continuous operation with enhanced reliability.

The plant floor responds to schedules that meet production requirements using raw materials made available in tandem with the plant floor's response. Because information is transactionally current, scheduling systems are optimized with real-time input. The plant floor informs the integrated system of the status and availability of staff, equipment, materials, maintenance needs, and other information to support scheduling.

Batch operations have various degrees of automation. These operations are a part of the integrated supply chain activities. They will operate according to the changing needs of the customers. Lead times are short, and responsiveness and agility are high. Batch operations are a critical capability in the chemical industry. The batch equipment provides a very broad product line for the industry and its customers.

Both continuous and batch operations have automated handling systems for raw material, packaging components, and finished products. These support systems are agile to handle a wide array of products. The principle of delaying product identity to the latest possible time operates within these production capabilities.

Technology for plant design and construction will cost significantly less than in the past. Standards will be developed where appropriate, with modularity a common practice. Design and construction improvement will allow plants to come on-stream in significantly less time. Plants will be designed using electronic footprints of past plants with automated conversions to existing needs. Engineering automation will be used extensively. Plants will be easily convertible to other products as economies change. Users, engineering and design firms, construction companies, and major equipment suppliers will work in partnership to improve the system.

HOW TO GET THERE

The industry could form a consortium to develop agility models for manufacturing processes.

Individual companies could partner with customers in meeting their needs by the joint development of new product technology.

The industry can develop the technology to build reconfigurable plants that are easily converted in response to changing market demands.

The industry can work with academia to develop training for the professionals who develop, design, build, operate, and improve facilities.
Software groups can work with industry to improve operations.

Partnerships or consortia can be created with engineering firms to develop the technology to shorten significantly the lead time from concept stage to operation.

The industry can work with transport and logistic firms to develop more efficient means of global transport that protect human health, safety, and the environment.

CONCLUSION

The chemical industry has been a driving force in supporting a healthy U.S. economy in terms of providing jobs, a healthy trade surplus, and key products for other U.S. manufacturers. There will be growing challenges for the chemical industry over the next 25 years as global competition, technology advances, public health and environmental concerns, and new markets and products shape the future.

The U.S. chemical industry is ready to meet these challenges, and it is committed to continuing to be a world leader. The vision out-lined in this report highlights where the industry wants to be in the year 2020. It wants to lead the world in technology development, manufacturing, and profitability, while optimizing health and safety and ensuring environmental stewardship.

Technology Vision 2020 outlines a wide range of recommendations that will assist the chemical industry in advancing toward its vision. Involvement by a broad spectrum of groups—such as government, academic researchers and teachers, suppliers, standard-setting groups—individually or in cooperation with the chemical industry itself will be crucial. We challenge all who see roles for themselves in the advancement of these recommendations to do so. Not only the chemical industry will benefit, but more importantly, our nation itself, of which the industry provides much underlying support.

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AMERICAN INSTITUTE OF CHEMICAL ENGINEERS (AIChE), founded in 1908, is a non-profit, professional association that provides leadership in advancing the chemical engineering profession. Its membership of approximately 60,000 is made up of individuals who work in industry, government, academia, and consulting, as well as students and retirees. Its members are creative problem solvers who use chemistry, physics, and mathematics to develop processes and design and operate plants that alter the physical or chemical states of materials to make useful products at a reasonable cost and in the safest manner possible. AIChE, 345 E. 47th Street, New York, NY 10017-2395, (212) 705-7336.

The **CHEMICAL MANUFACTURERS ASSOCIATION (CMA)** is a nonprofit trade association whose member companies account for more than 90 percent of the basic industrial chemical productive capability in the United States. Founded in 1872, CMA is one of the oldest manufacturing trade associations in the Western Hemisphere. CMA, 1300 Wilson Boulevard, Arlington, VA 22209, (703) 741-5000.

The **COUNCIL FOR CHEMICAL RESEARCH (CCR)** seeks to advance research in chemistry-based sciences, engineering, and technology that benefits society and the national well-being through productive interactions among industrial, academic, and governmental research sectors. CCR's membership comprises more than 200 industrial companies, universities, government laboratories, and research institutes that collectively perform more than $7 billion annually in chemically related R&D. The member organizations are represented by more than 450 of the top chemical R&D managers in the country. CCR, 1620 L Street, NW, Suite 825, Washington, DC 20036, (202) 429-3971.

The **SYNTHETIC ORGANIC CHEMICAL MANUFACTURERS ASSOCIATION (SOCMA)** is the leading association representing the batch and custom chemical industry. This industry produces 95 percent of the 50,000 chemicals manufactured in the United States while making a $60 billion annual contribution to the economy. SOCMA's 260 member companies are representative of the industry and are typically small businesses with fewer than 50 employees and less than $50 million in annual sales. SOCMA, 1100 New York Avenue, NW, Suite 1090, Washington, DC 20005, (202) 414-4113.