A. 21C New Paradigm in Chemical & Energy Industries

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1. Introduction

1.1. Our Challenge

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.

We believe the chemical industry in the Korea 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. 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.

1.2. Steps To Getting There

To meet its goals, the Korea 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.

2. Role of Technology

Technology holds promise for positively shaping the Korea 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.

2.1. Increasing globalization

We define globalization as the accelerating interdependence of nations and private firms. Worldwide economic growth offers many new opportunities for selling products and services in countries previously inaccessible because of geography. Success in capturing new, emerging markets will depend on the industry's ability to compete in different environments.

2.2. 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.
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.
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. The Korea 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.

2.3. 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.
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.

2.4. Customer expectation

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

2.5. Changing work force requirement

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.

3. New Chemical Science and Engineering Technology

3.1. 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 down by the addition of a substance that is not changed in the

chemical reaction.
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.

= 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
· 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.

3.2. Bioprocesses and biotechnology

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

3.3. Material technology

Material technology is the area in the chemical science where advances are important.

= 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.

3.4. 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.

Future advances in PS&ET will require collaborative efforts of interdisciplinary research teams focused on the following needs and challenges.

= 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.

3.5. COMPUTATIONAL TECHNOLOGIES

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.
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.

4. 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.

= 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.

5. Information Systems

5.1. 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.
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.

5.2. 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.

= 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.

= 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.

5.3. Product and process design and development

= Change of 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.

5.4. Manufacturing and operation

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.

= 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. 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.

5.5. Computers in plant engineering and construction

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.