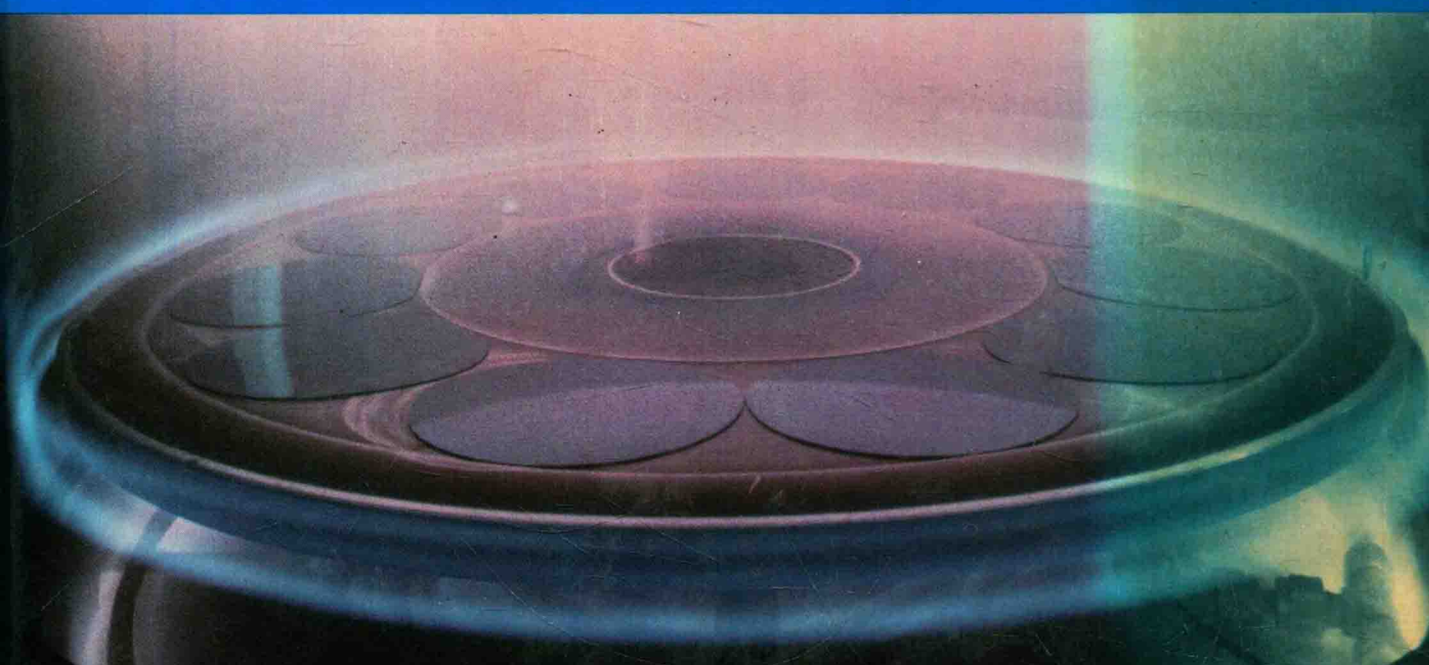
FRONTIERS IN CHEMICAL ENGINEERING



RESEARCH NEEDS AND OPPORTUNITIES

NATIONAL RESEARCH COUNCIL

FRONTIERS IN CHEMICAL ENGINEERING

RESEARCH NEEDS AND OPPORTUNITIES

Committee on Chemical Engineering Frontiers:
Research Needs and Opportunities
Board on Chemical Sciences and Technology
Commission on Physical Sciences, Mathematics, and Resources
National Research Council

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This report has been reviewed by a group other than the authors according to procedures approved by a Report Review Committee consisting of members of the National Academy of Sciences, the National Academy of Engineering, and the Institute of Medicine.

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FRONTIERS IN CHEMICAL ENGINEERING

RESEARCH NEEDS AND OPPORTUNITIES

Contents

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Executive Summary

CHEMICAL ENGINEERING occupies a special place among scientific and engineering disciplines. It is an engineering discipline with deep roots in the world of atoms, molecules, and molecular transformations. The principles and approaches that make up chemical engineering have a long and rich history of contributions to the nation's technological needs. Chemical engineers play a key role in industries as varied as petroleum, food, artificial fibers, petrochemicals, plastics, ceramics, primary metals, glass, and specialty chemicals. All these depend on chemical engineers to tailor manufacturing technology to the requirements of their products and to integrate product design with process design. Chemical engineering was the first engineering profession to recognize the integral relationship between design and manufacture, and this recognition has been one of the major reasons for its success.

This report demonstrates that chemical engineering research will continue to address the technological problems most important to the nation. In the chapters that focus on these problems, many of the discipline's core research areas (e.g., reaction engineering, separations, process design, and control) will appear again and again. The committee hopes that by discussing research frontiers in the context of applications, it will illustrate both the intellectual excitement and the practical importance of chemical engineering.

The research frontiers discussed in this report can be grouped under four overlapping themes: starting new technologies, maintaining leadership in established technologies, protecting and improving the environment, and developing systematic knowledge and generic tools. These frontiers are described in detail in Chapters 3 through 9. From among these, the committee has selected eight high-priority topics that merit the attention of researchers, decision makers in academia and industry, and organizations that fund or otherwise support chemical engineering. These high-priority areas are described below. Recommendations from the committee for initiatives that would permit chemical engineers to exploit these areas are briefly stated in Chapter 10 and detailed in Appendix A.

RESEARCH FRONTIERS IN CHEMICAL ENGINEERING

Starting New Technologies

Chemical engineers have an important role to play in bringing new technologies to commercial fruition. These technologies have their origin in scientific discoveries on the atomic and molecular level. Chemical engineers understand the molecular world and are skilled in integrating product design with process design, process control, and optimization. Their skills are needed to develop genetic engineering (biotechnology) as a manufacturing tool and to create new biomedical devices, and to design new products and manufacturing processes for advanced materials and devices for information storage and handling. In the fierce competition for world markets in these technologies, U.S. leadership in chemical engineering is a strong asset.

Biotechnology and Biomedicine (Chapter 3)

The United States occupies the preeminent scientific position in the "new" biology. If America is to derive the maximum benefit of its investment in basic biological research—whether in the form of better health, improved agriculture, a cleaner environment, or more efficient production of chemicals—it must also assume a preeminent position in biochemical and biomedical engineering. This can be accomplished by carrying out generic research in the following areas:

- Developing chemical engineering models for fundamental biological interactions.
- Studying phenomena at biological surfaces and interfaces that are important in the design of engineered systems.
- Advancing the field of process engineering. Important generic goals for research include the development of separation processes for complex and fragile bioproducts; the design of bioreactors for plant and mammalian tissue culture; and the development of detailed, continuous control of process parameters by rapid, accurate, and noninvasive sensors and instruments.
- Conducting engineering analyses of complex biological systems.

Electronic, Photonic, and Recording Materials and Devices (Chapter 4)

The character of American industry and society has changed dramatically over the past three decades as we have entered the "information age." New information technologies have been made possible by materials and devices whose structure and properties can be controlled with exquisite precision. This control is largely achieved by the use of chemical reactions during manufacturing. Future U.S. leadership in microelectronics, optical information technologies, magnetic data storage, and photovoltaics will depend on staying at the forefront of the chemical technology used in manufacturing processes. Chemical processing will also be a vital part of the likely manufacturing processes for high-temperature superconductors.

At the frontiers of chemical research in this area are a number of important challenges:

- Integrating individual chemical process steps used in the manufacture of electronic, photonic, and recording materials and devices. This is a key to boosting the yield, throughput, and reliability of overall manufacturing processes.
- Refining and applying chemical engineering principles to the design and control of the chemical reactors in which devices are fabricated.
- Pursuing research in separations applicable to the problem of ultrapurification. The materials used in device manufacture must be ultrapure, with levels of some impurities reduced to the parts-per-trillion level;
- Improving the chemical synthesis and processing of polymers and ceramics;
- Developing better processes for deposition and coating of thin films. An integrated circuit, in essence, is a series of electrically connected thin films. Thin films are the key structural feature of recording media and optical fibers, as well.
- Modeling the chemical reactions that are important to manufacturing processes and studying their dynamics.
- Emphasizing process design and control for environmental protection and process safety.

Microstructured Materials (Chapters 5 and 9)

Advanced materials depend on carefully designed structures at the molecular and microscopic levels to achieve specific performance in use. These materials—polymers, ceramics, and composites—are reshaping our society and are contributing to an improved standard of living. The process technology used in manufacturing these materials is crucial—in many instances more important than the composition of the materials themselves. Chemical engineers can make important contributions to materials design and manufacturing by exploring the following research frontiers:

- Understanding how microstructures are formed in materials and learning how to control the processes involved in their formation.

• Combining materials synthesis and materials processing. These areas have traditionally been considered separate research areas. Future advances in materials require a fusion of these topics in research and practice.

• Fabricating and repairing complex materials systems. Mechanical methods currently in use (e.g., riveting of metals) cannot be applied reliably to the composite materials of the future. Chemical methods (e.g., adhesion and molecular self-assembly) will come to the fore.

Maintaining Leadership in Established Technologies

The U.S. chemical processing industries are one of the largest industrial sectors of the U.S. economy. The myriad of industries listed at the beginning of this chapter are pervasive and absolutely essential to society. The U.S. chemical industry is one of the most successful U.S. industries on world markets. At a time of record trade deficits, the chemical industry has maintained both a positive balance of trade and a growing share of world markets (Figure 1.1). The future international competitiveness of these industries should not be taken for granted. Farsighted management in industry and continued support for basic research from both industry and government are required if this sector of the economy is to continue to contribute to the nation's prosperity.

In a report of this scope and size, it is not possible to spell out the research challenges faced by each part of the chemical processing industries. For example, the committee has reluctantly chosen to pass over food processing, a multibillion-dollar industry where chemical engineering finds a growing variety of applications. The committee has focused its discussion of challenges to the processing industries on energy and natural resources technologies. These

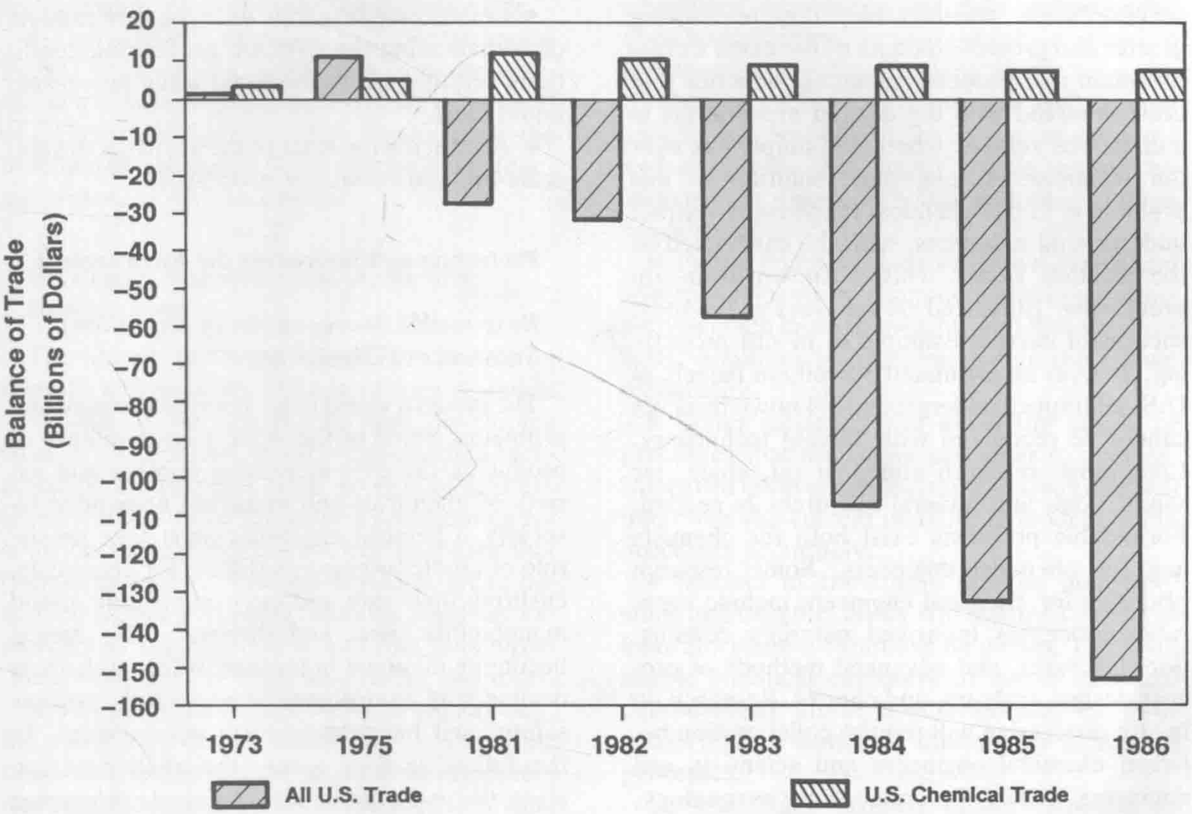

FIGURE 1.1 While the overall U.S. trade balance has plummeted to a deficit of more than $150 billion, the U.S. chemical industry has maintained a positive balance of trade. Courtesy, Department of Commerce.

technologies are key to supplying crucial national needs, keeping the United States competitive, and providing for national security. They are also the focus of substantial research and development in academia and government laboratories, in addition to industry. The committee has identified two high-priority initiatives to sustain the vitality and creativity of engineering research on energy and natural resources. These initiatives focus on in-situ processing of resources and on liquid fuels for the future.

In-Situ Processing of Energy and Mineral Resources (Chapter 6)

The United States has historically benefited from rich domestic resources of minerals and fuels located in readily accessible parts of the earth's crust. These easily reached resources are being rapidly depleted. Our remaining reserves, while considerable, require moving greater and greater amounts of the earth's crust to obtain and process resources, whether that crust is mixed with the desired material (as in a dilute ore vein) or whether it simply lies over the resource. A long-range solution to this problem is to use chemical reactions to extract underground resources, with the earth itself as the reaction vessel. This is known as in-situ processing. Enhanced oil recovery is the most successful current example of in-situ processing, and yet an estimated 300 billion barrels of U.S. oil trapped underground in known reserves cannot be recovered with current technology. Long-range research aimed at oil, shale, tar sands, coal, and mineral resources is needed. Formidable problems exist both for chemists and for chemical engineers. Some research priorities for chemical engineers include separation processes, improved materials, combustion processes, and advanced methods of process design, scale-up, and control. Research on in-situ processing will require collaboration between chemical engineers and scientists and engineers skilled in areas such as geology, geophysics, hydrology, environmental science, mechanical engineering, physics, mineralogy, materials science, metallurgy, surface and colloid science, and chemistry.

Liquid Fuels for the Future (Chapters 6 and 9)

Our current and foreseeable transportation technologies depend completely on a plentiful supply of liquid fossil fuels. Anticipatory research to ensure a future supply of these fuels is a wise investment. Research of this type subsumes a number of generic challenges in chemical engineering, including:

- Finding new chemical process pathways that can make large advances in the production of liquid fuels from solid and gaseous resources.
- Processing solids, since equipment design and scale-up are greatly limited by our lack of fundamental understanding of solids behavior.
- Developing better separation processes.
- Conducting research on materials capable of withstanding the extreme processing conditions that may be encountered when processing liquid fuels.
- Advancing the state of the art in the design, scale-up, and control of processes.

Protecting and Improving the Environment

Responsible Management of Hazardous Substances (Chapter 7)

The modern world faces many environmental problems. Some of these are a consequence of producing the ever-increasing number and variety of chemicals and materials demanded by society. Chemical engineers must take up the role of cradle-to-grave guardians for chemicals, ensuring their safe and environmentally sound manufacture, use, and disposal. This means becoming involved in a range of research areas dealing with environmental protection, process safety, and hazardous waste management. In the following four areas, the challenges are clear, the opportunities for chemical engineering research are abundant, and the potential benefits to society are great.

• Conducting long-term research on the generation, control, movement, fate, detection, and environmental and health effects of contaminants in the air, water, and land. Chemical engineering research should include the fundamental investigation of combustion processes, the application of biotechnology to waste degradation, the development of sensors and measurement techniques, and participation in interdisciplinary studies of the environment's capacity to assimilate the broad range of chemicals that are hazardous to humans and ecosystems.

• Developing new chemical engineering design tools to deal with the multiple objectives of minimum cost; process resilience to changes in inputs; minimization of toxic intermediates and products; and safe response to upset conditions, start-up, and shutdown.

• Directing research at cost-effective management of hazardous waste, as well as improved technologies (e.g., combustion) or new technologies for destroying hazardous waste.

• Carrying out research to facilitate multimedia, multispecies approaches to waste management. Acid rain and the leaching of hazardous chemicals from landfills demonstrate the mobility of chemicals from one medium (e.g., air, water, or soil) to another.

Developing Systematic Knowledge and Generic Tools

The success of chemical engineers in contributing to a diverse set of technologies is due to an emphasis on discovering and developing basic principles that transcend individual technologies. If, 20 years from now, chemical engineers are to have the same opportunities for contributing to important societal problems that they have today, then the research areas described in the preceding sections must be explored and supported in a way that maximizes the development of basic knowledge and tools.

In surveying the field of chemical engineering, the committee has identified two cross-cutting areas that are in a state of rapid development and that promise major contributions to a wide range of technologies. Accordingly, this report singles out for special attention the advances under way in applying modern computational methods and process control to chemical engineering and the promise of basic research in surface and interfacial engineering.

Advanced Computational Methods and Process Control (Chapter 8)

The speed and capability of the modern computer are revolutionizing the practice of chemical engineering. Advances in speed and memory size and improvements in complex problem-solving ability are more than doubling the effective speed of the computer each year. This unrelenting pace of advance has reached the stage where it profoundly alters the way in which chemical engineers can conceptualize problems and approach solutions. For example:

• It is now realistic to imagine mathematical models of fundamental phenomena beginning to replace laboratory and field experiments. Such computations increasingly allow chemical engineers to bypass the long (2 to 3 years), costly step of producing process and product prototypes, and permit the design of products and processes that better utilize scarce resources, are significantly less polluting, and are much safer.

• Future computer aids will allow design and control engineers to examine many more alternatives much more thoroughly and thus produce better solutions to problems within the known technology.

• Better modeling will allow the design of processes that are easier and safer to operate. Improved control methodology and sensors will overcome the current inability to model certain processes accurately.

• Sensors of the future will be incredibly small and capable. Many will feature a chemical laboratory and a computer on a chip. They will enable chemical engineers to detect chemical compositions inside hostile process environments and revolutionize their ability to control processes.

To realize the promise of the computer in chemical engineering, we need a much larger effort to develop methodologies for process design and control. In addition, state-of-the-art computational facilities and equipment must become more widely disseminated into chemical engineering departments in order to integrate methodological advances into the mainstream of research and education.

Surface and Interfacial Engineering (Chapter 9)

Surfaces, interfaces, and microstructures play an important role in many of the above-mentioned research frontiers. Chemical engineers explore structure-property relationships at the atomic and molecular level, investigate elementary chemical and physical transformations occurring at phase boundaries, apply modern theoretical methods for predicting chemical dynamics at surfaces, and integrate this knowledge into models that can be used in process design and evaluation. Fundamental advances in these areas will have a broad impact on many technologies. Examples include laying down thin films for microelectronic circuits, developing high-strength concrete for roadways and buildings, and inventing new membranes for artificial organs. Advances in surface and interfacial engineering can also move the field of heterogeneous catalysis forward significantly. New knowledge can help chemical engineers play a much bigger role in the synthesis and modification of novel catalysts with enhanced capabilities. This activity would complement their traditional strength in analytical reaction engineering of catalysts.

HIGHLIGHTS OF THE RECOMMENDATIONS

Education and Training of Chemical Engineers (Chapter 10)

The new research frontiers in chemical engineering, some of which represent new applications for the discipline, have important implications for education. A continued emphasis is needed on basic principles that cut across many applications, but a new way of teaching those principles is also needed. Students must be exposed to both traditional and novel applications of chemical engineering. The American Institute of Chemical Engineers (AIChE) has set in motion a project to incorporate into undergraduate chemical engineering courses examples and problems from emerging applications of the discipline. The committee applauds this work, as well as recent AIChE moves to allow more flexibility for students in accredited departments to take science electives.

A second important need in the curriculum is for a far greater emphasis on design and control for process safety, waste minimization, and minimal adverse environmental impact. These themes need to be woven into the curriculum wherever possible. The AIChE Center for Chemical Process Safety is attempting to provide curricular material in this area, but a larger effort than this project is needed. Several large chemical companies have significant expertise in this area. Closer interaction between academic researchers and educators and industry is required to disseminate this expertise.

The Future Size and Composition of Academic Departments (Chapter 10)

A bold step by universities is needed if their chemical engineering departments are (1) to help the United States achieve the preeminent position of leadership in new technologies and (2) to keep the highly successful U.S. chemical processing industries at the forefront of world markets for established technologies. The universities should conduct a one-time expansion of their chemical engineering departments over the next 5 years, exercising a preference for new faculty capable of research at interdisciplinary frontiers.

This expansion will require a major commitment of resources on the part of universities, government, and industry. How can such a preferential commitment to one discipline be justified, particularly at a time of budgetary austerity? One answer is that the worldwide contest for dominance in biotechnology, advanced materials technologies, and advanced information devices is in full swing, and the United States cannot afford to stand by until it gets its budgetary house in order. As the uniquely "molecular" engineers, chemical engineers have powerful tools that need to be refined and applied to the commercialization of these technologies. A second answer is that the alternative to expansion, a redistribution of existing resources for chemical engineering research, would cut into vital programs that support U.S. competitiveness in established chemical technologies. The recommendation for an expansion in chemical engineering departments is not a call for "more of the same." It is the most practical way to move chemical engineering aggressively into the new areas represented by this report's research priorities while maintaining the discipline's current strength and excellence.

Balanced Portfolios (Chapter 10)

The net result of an additional investment of resources in chemical engineering should be the creation of three balanced portfolios: one of priority research areas, one of sources of funding for research, one of mechanisms by which that funding can be provided.

The eight priority research areas described above constitute the committee's recommendation of a balanced portfolio of research areas on the frontiers of the discipline.

In terms of a balanced portfolio of funding sources, the committee proposes initiatives for industry and a number of federal agencies in Chapter 10 and Appendix A to ensure a healthy diversity of sponsors. Table 1.1 links specific research frontiers to funding initiatives for potential sponsors.

A third balanced portfolio, of funding mechanisms, is needed if the above-mentioned research frontiers are to be pursued in the most effective manner. Different frontiers will require different mixes of mechanisms, and the decision to use a particular mechanism should be determined by the nature of the research problem, by instrumentation and facilities requirements, and by the perceived need for trained personnel in particular areas for industry. This topic is discussed in more detail in Chapter 10.

The Need for Expanded Support of Research in Chemistry (Chapter 10)

Chemical engineering builds on research results from other disciplines, as well as those from its own practitioners. Not surprisingly, the most important of these other disciplines is chemistry. A vital base of chemical science is needed to stimulate future progress in chemical engineering, just as a vital base in chemical engineering is needed to capitalize on advances in chemistry. The committee endorses the recommendations contained in the NRC's 1985 report *Opportunities in Chemistry*, and urges their implementation in addition to the recommendations contained in this volume.

TABLE 1.1 High-Priority Research Frontiers and Initiatives[a]

	Relevant Audiences[b]							
Priority Research Area	NSF	DOE	NIH	DOD	EPA	NBS	BOM	CPI
Biotechnology and biomedicine	✔✔	✔	✔✔			✔		✔
Electronic, photonic, and recording materials and devices	✔✔	✔		✔✔				✔
Microstructured materials	✔✔	✔✔		✔✔		✔		✔
In-situ processing of resources	✔	✔✔					✔✔	
Liquid fuels for the future	✔	✔✔				✔		✔✔
Responsible management of hazardous substances	✔				✔✔			✔✔
Advanced computational methods and process control	✔✔	✔						✔✔
Surface and interfacial engineering	✔✔	✔✔						✔

[a] ✔✔ = major initiative recommended; ✔ = supporting initiative recommended.
[b] NSF = National Science Foundation; DOE = Department of Energy; NIH = National Institutes of Health; DOD = Department of Defense; EPA = Environmental Protection Agency; NBS = National Bureau of Standards; BOM = Bureau of Mines; CPI = U.S. chemical processing industries.