Vision 2020: 2000 Separations Roadmap

Published by the Center for Waste Reduction Technologies of the

AIChE

In cooperation with

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ISBN 0-8169-0832-X

Printed in the United States of America

CONTENTS

ACKNOWLEDGMENTS

We thank the organizations whose sponsorship made the preparation of this roadmap report possible:

American Chemical Society, American Institute of Chemical Engineers, Center for Waste Reduction Technologies, BF Goodrich, Council for Chemical Research, Dow Chemical Company, DuPont, Electric Power Research Institute, Koch-Glitsch, Inc., Monsanto Company, National Center for Clean Industrial & Treatment Technologies, Nofsinger, Inc., Rohm & Haas, Texas Tech Process Control and Optimization, Union Carbide, and U. S. Department of Energy/ Office of Industrial Technologies.

The programmatic support of the US Department of Energy's Office of Industrial Technologies' Chemical and Agricultural teams is greatly appreciated: Doug Faulkner, Henry Kenchington , Tom King, Charles Russomanno, and Paul Scheihing.

We also acknowledge the following individuals who assisted at the roadmapping breakout sessions, took notes, and helped prepare drafts of the roadmap activities: John Barton (ORNL), John Begovich (ORNL), Bill Brosey (ORNL), Brian Davison (ORNL), Susan DePaoli (ORNL), Kerry Irons (Dow), Bob Jubin (ORNL), Greg Keeports (Rohm & Haas), Thomas Klasson (ORNL), Mike Maskarinec (ORNL), Jim McLaren (Inverizon), George Muhlebach (CWRT), Erik Sall (Monsanto), Tom Schmidt (ORNL), William Scouten (Utah State University) and Bill Steele (ORNL).

Honorable mention goes to reviewers of the roadmap documents: ***Adsorbents***—Tony Flammino (Merck) and Kent Knaebel (Adsorption Research Inc.); ***Crystallization***—Ronald Bray (SRI Consulting) and Timothy C. Frank (Dow Chemical); ***Distillation***—Krish Krishnamurthy (BOC Gases R&D); ***Extraction—***Lanny Robbins (Dow Chemi-

cal) and Robin Rogers (University of Alabama); ***Membranes***—David Li (Air Liquide), Pushpinder Puri (Air Products), and Hans Wijmans (MTR); ***Separative Reactors***—Jeff Siirola (Eastman Chemical) and Tyler Thompson (Dow Chemical); ***Ion Exchange—***Paul F. Bryan (GE Plastics); ***Bio-Separations***—Timothy Frank (Dow Chemical); ***Dilute Solutions***—Timothy Oolman (Cargill)

FOREWORD

The 2000 Separations Roadmap is a part of an industry-wide effort to create a blueprint of the research and technology milestones that are necessary to achieve long-term industry goals. This report documents the results of four workshops on the technology barriers, research needs, and priorities of the chemical, agricultural, petroleum, and pharmaceutical industries as they relate to separation technologies utilizing adsorbents, crystallization, distillation, extraction, membranes, separative reactors, ion exchange, bioseparations, and dilute solutions. The workshops brought together about two hundred and thirty experts from industry, universities, and government research laboratories. The workshops were a part of the chemical industry's effort to develop its technology roadmap for the future.

This document must be viewed as evolutionary in nature. The 2000 Separations Roadmap report is an update of the *Vision 2020: 1998 Separations Roadmap* (also published by the Center for Waste Reduction Technologies). The 1998 report summarized the results of the first two workshops held in 1998, and the 2000 report covers all four workshops held in 1998 and 1999. While this document presents an impressive compilation of critical research needs, the workshops were necessarily limited in time, scope, and participation, and the emerging roadmap may not fully incorporate all viewpoints. Every effort was made to include a broad range of industry participants, but it is inevitable that valuable ideas may have been left out. Thus, this document is a snapshot in time of industry research needs. It will evolve as additional information becomes available.

I. SUMMARY

Background: The 2000 Separations Roadmap is based on the information gathered in four workshops held on seven separation technologies (adsorption, crystallization, distillation, extraction, membranes, separative reactors and ion exchange) and two cross-cutting areas (bioseparations and dilute solutions). These areas are utilized by other industries in addition to the chemical industry and are specifically identified as barriers and challenges in *Technology Vision 2020: The Chemical Industry*. *Technology Vision 2020* details the challenges faced by the US chemical industry as it strives to maintain its competitive position in the next millennium. Over two hundred and thirty individuals with appreciable expertise in each of the technical areas participated in the workshops. Technical presentations covering three of the technologies are available separately as a monograph.[1]

Workshops: Workshop participants defined the present challenges faced by industries producing and using chemicals, and they identified the technical barriers and the research needs required to overcome those barriers so the technologies would play important roles in improving future processing economics. The participants identified research that will be important in contributing to a 30% reduction in relative indicators for material usage, energy usage, water consumption, toxic dispersion, and pollutant dispersion by the year 2020 for the industries involved in the separations roadmapping. The relative indicators are those which were partially developed by the National Roundtable for the Environment and the Economy where material usage, for example, is indexed to the selling price of the product minus the cost of raw materials and energy.

Research Needs: Research needs for each technical area are discussed in Section III , while a comprehensive list of all research needs is given in Appendix C. The *highest priority* key research needs are:

Adsorbents: New materials with improved selectivity and stability and more favorable geometries, tools to predict adsorbent performance and aid in process design, and demonstration of commercial feasibility.

Crystallization: Physical property data and molecular modeling capability for solid/liquid equilibrium and crystal growth mechanisms, and instruments to measure degree of super-saturation.

Distillation: Improved understanding of physical phenomena, better *in situ* sampling, analytical and flow-visualization methods, and better predictive modeling tools.

Extraction: New solvents, a better understanding of the fundamental physical processes, and an enhanced physical property database.

Membranes: Economic evaluations to direct research efforts, membrane system development to enhance operability and robustness, new membrane materials, increasing surface area at lower cost, and predictive models.

Separative Reactors: New materials, economic evaluations to prioritize applications for separative reactors, and improved design capabilities.

Ion Exchange**:** New materials with greater selectivity, improved regeneration methods, lower cost materials, innovative ion exchange equipment, and hybrid systems.

Bioseparations: Development of robust biocatalysts; development of better separations technologies with emphasis on membranes, extractants, adsorbents, and hybrid systems; obtaining physical properties data; extending predictive models; pursuing *in vitro* synthesis; and development of closed-loop fermentation processes.

Dilute Solutions: Improved understanding of physical phenomena and intermolecular chemistry, enhanced physical properties databases, better predictive modeling tools, and improved separations technologies including hybrid systems.

Key R&D Linkages: Exhibits I.1-I.9 show the linkages between key research needs and the time-frame for

[1] Available from CWRT by calling (212) 591-7424.

obtaining the research results. The linkages indicate where the results from one or more research areas provide important support to other areas either in the same or another time frame. Additional details about the key research needs are provided in Section III.J.

Cross-Cutting Research Needs: Major research needs that cut across several or all of the technologies include: new materials, new physical property data, new predictive models, and demonstrations of technical feasibility in real world systems using dedicated pilot-plants. The development of new hybrid separations technologies is also a cross-cutting need, particularly for bioprocessing and dilute solutions. Additional information is found in Section III.J. The importance of process economic studies to guide research programs was cited for all but the most established technologies.

Research-Related Needs: Needs that are research-related include: improved means for sharing information in industry, such as publicly available or limited-access database sites by professional societies on the Internet, a greater emphasis on crystallization, distillation, and extraction in university chemical engineering curricula and improved communications within industry, and collaborative initiatives among industry, universities, and national laboratories to address major industrial issues in a more efficient and cost-effective way.

Table I.1 Key R+D Linkages for Adsorbents

(H= High Priority, M= Medium Priority)

	Ongoing	Near-Term (0-3 years)	Mid-Term (3-10 years)	Long-Term (10+ years)
Materials	Develop new adsorbents with high selectivity in complex mixtures (H)	Develop more and better adsorbent forms and geometries (M) Reduce manufacturing cost per unit of performance (M)	Develop switchable adsorbents (M) Develop improved high performance conductors (M)	Develop non-conventional adsorbents (M)
Process Systems	Integrate materials research and process development (M)		Non-conventional ways to desorb adsorbed molecules (e.g. microwave, sonic energy) (M)	
Predictive Modeling	Collect/correlate data on equilibrium and kinetics for a variety of adsorbents (M)			Develop molecular modeling tools to predict interaction of molecule with adsorbent surface (M)
Demonstrating Feasibility		Demonstrate adsorption technology on important process streams to promote use of technology (M)	Process design tool to allow technology comparisons on an equal basis (H)	
Education/ Information Transfer		Develop comprehensive information source to identify specific waste stream opportunities (M)	Create adsorbent handbook of physical properties (H)	

Table I.2 Key R+D Linkages for Crystallization

(H= High Priority, M= Medium Priority)

	Ongoing	Near-Term (0-3 years)	Mid-Term (3-10 years)	Long-Term (10+ years)
Fundamental Data		Develop methodology for estimating solid/liquid equilibrium (H)		
Predictive Modeling	Improve process modeling to permit for better scale-up capabilities (H)		Develop models of crystallization mechanism (H)	Develop molecular modeling methodology to determine solid/liquid equilibrium (H)
Process Systems		Develop spectroscopic monitors for measuring degree of saturation (M)	Design continuous equipment to replace batch equipment (M)	Automate crystallizer design based on fundamental material properties (H)
Education/ Information Transfer		Involve engineering early in product development cycle (M)		

Table I.3 Key R+D Linkages for Distillation

(H= High Priority, M= Medium Priority)

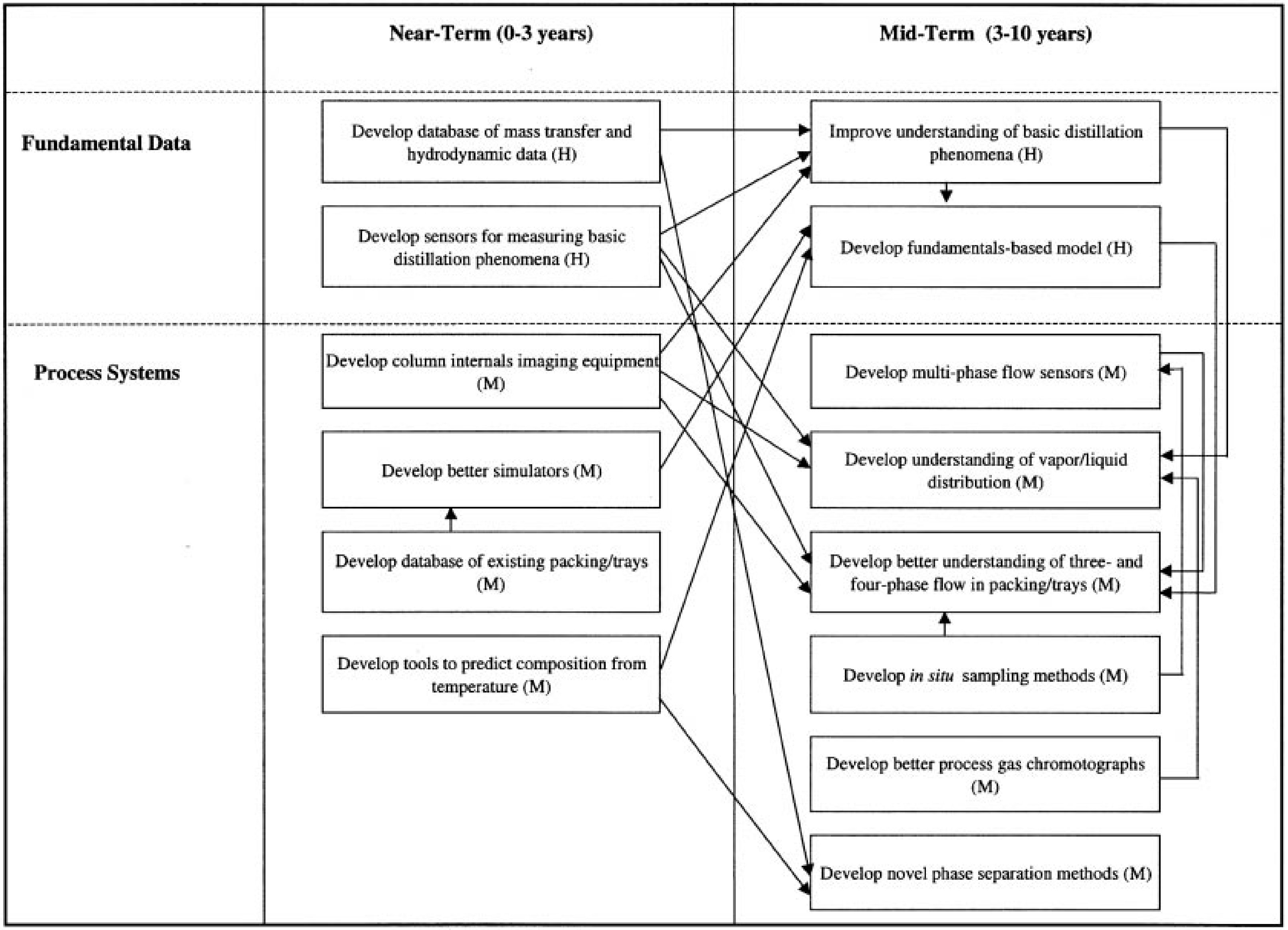


Table I.4 Key R+D Linkages for Extraction

(H= High Priority, M= Medium Priority)

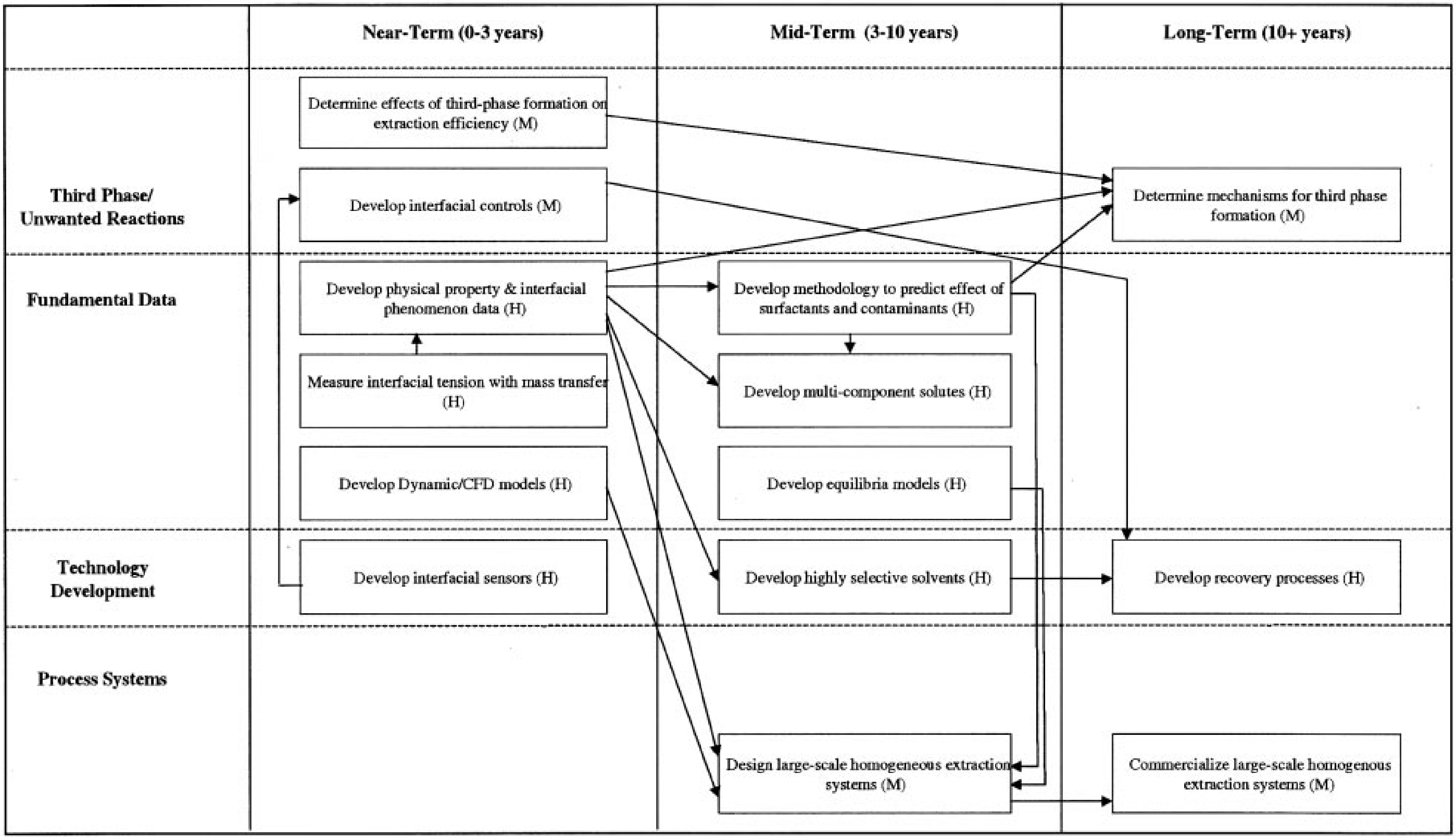


Table I.5 Key R+D Linkages for Membranes

(H= High Priority, M= Medium Priority)

	On-going	Near-Term (0-3 years)	Mid-Term (3-10 years)	Long-Term (10+ years)
Materials		Develop high-temperature membrane, time-frame dependent upon application, throughput & pore size (M)	Investigate novel material concepts (M) Conduct applications development of ionic membranes in aqueous systems (M)	Develop new materials for separating hydrophilic compounds from dilute streams (M)
Process Systems	Improve long-term performance (M) Integrate membrane technology with other processes (M) Prove robustness on real streams (H) Improve operating efficiency and lower maintenance costs of membrane systems (M)	Overcome scale-up difficulties for industrial streams (M) Cost effective increase in surface area per unit volume (H) Develop better sealing strategies for high temperature & pH balance (M) Design automated module assembly (M)	Develop scaleable low cost manufacturing techniques (M) Step-change in ability to create surface area (M)	
Predictive Modeling		Develop process simulation packages for membranes (e.g., hybrid models) (M)		
Other	More thoroughly examine membranes & tailor to the future chemical industry (M)	Find high potential applications in specialty chemicals and the top 100 chemicals and conduct R&D (H)		

Table I.6 Key R+D Linkages for Separative Reactors

(H= High Priority, M= Medium Priority)

	On-going	Near-Term (0-3 years)	Mid-Term (3-10 years)
Materials	Perform basic research on new pathways with separative reactors (M) Develop new adsorbents, membranes, & high performance catalysts (M)		"Green" technology initiative for pharmaceuticals to deal with solvent use/impact (M)
Process Systems	Conduct pilot and industrial scale demonstrations (M)	Develop methods to convert existing equipment to separative reactor systems (M)	Develop separation devices with wider operating ranges (M)
Demonstrate Value		Develop early stage full cost economic evaluation tools (M) Broadly analyze combinations of reactors and separators (H) Define the potential applications map (H)	
Fundamental Data	Develop reactive 3-D modeling (M)		

Table I.7 Key R+D Linkages for Ion Exchange
(H = High Priority, M = Medium Priority)

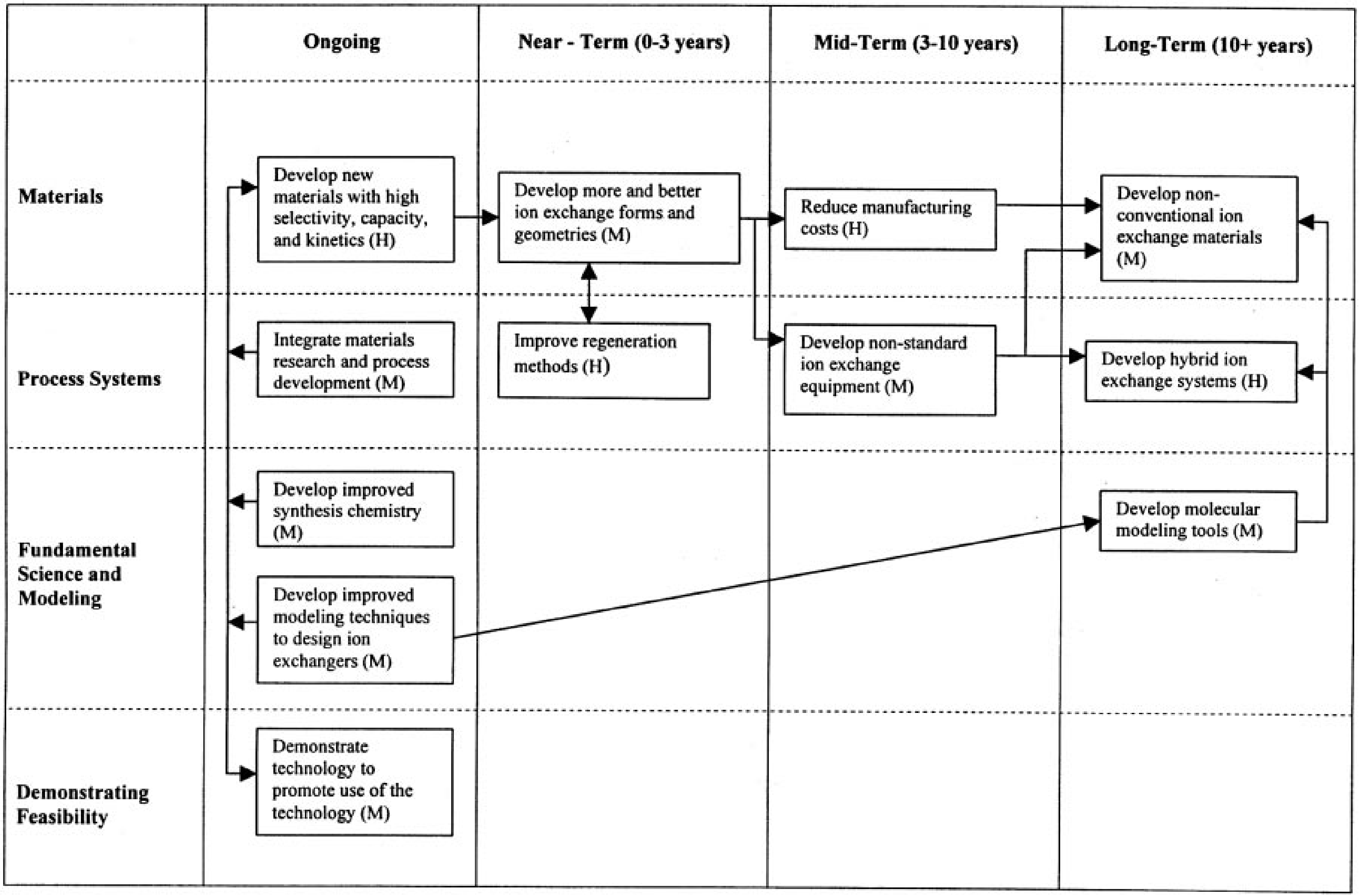
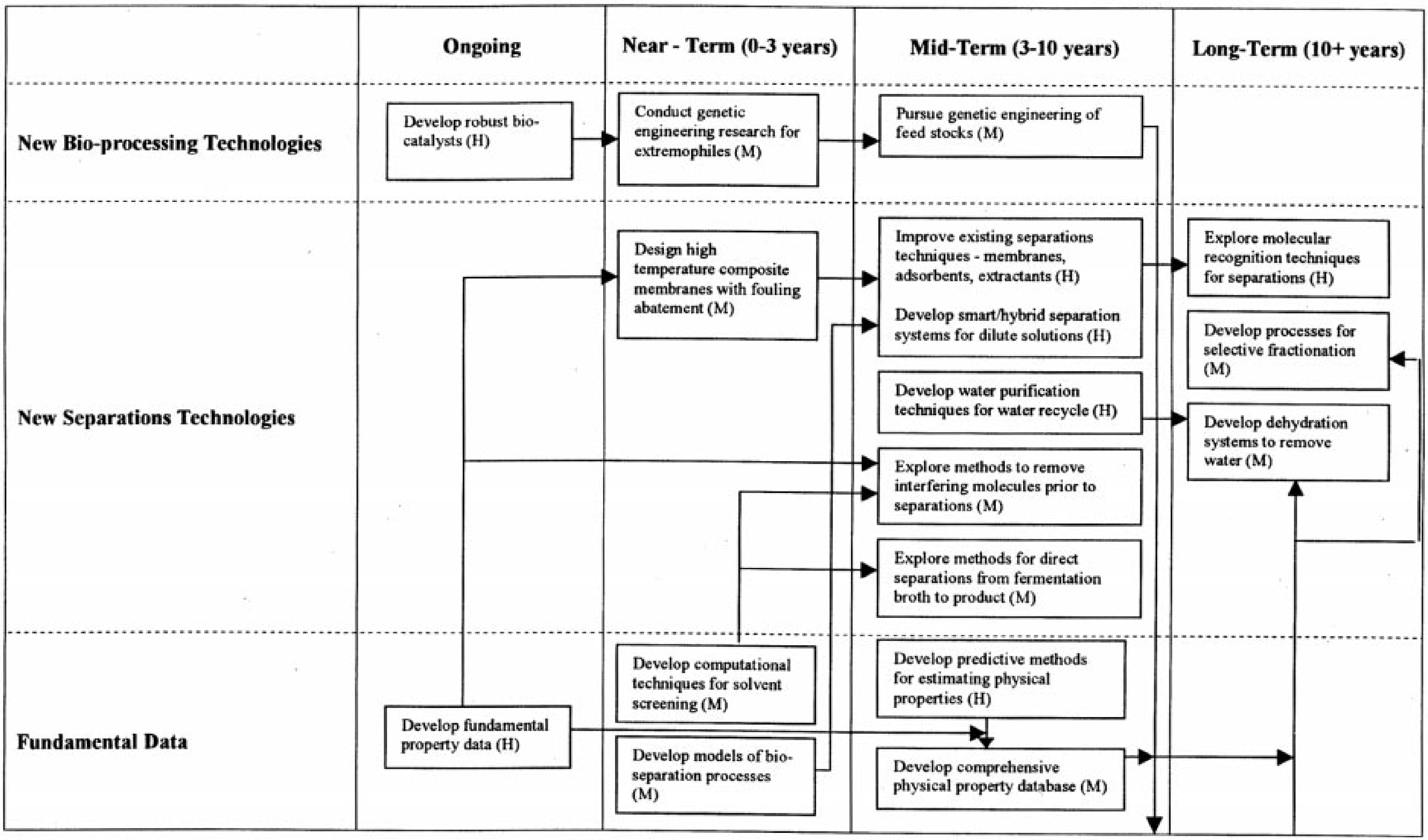


Table I.8 Key R+D Linkages for Bio-separations
(H = High Priority, M = Medium Priority)



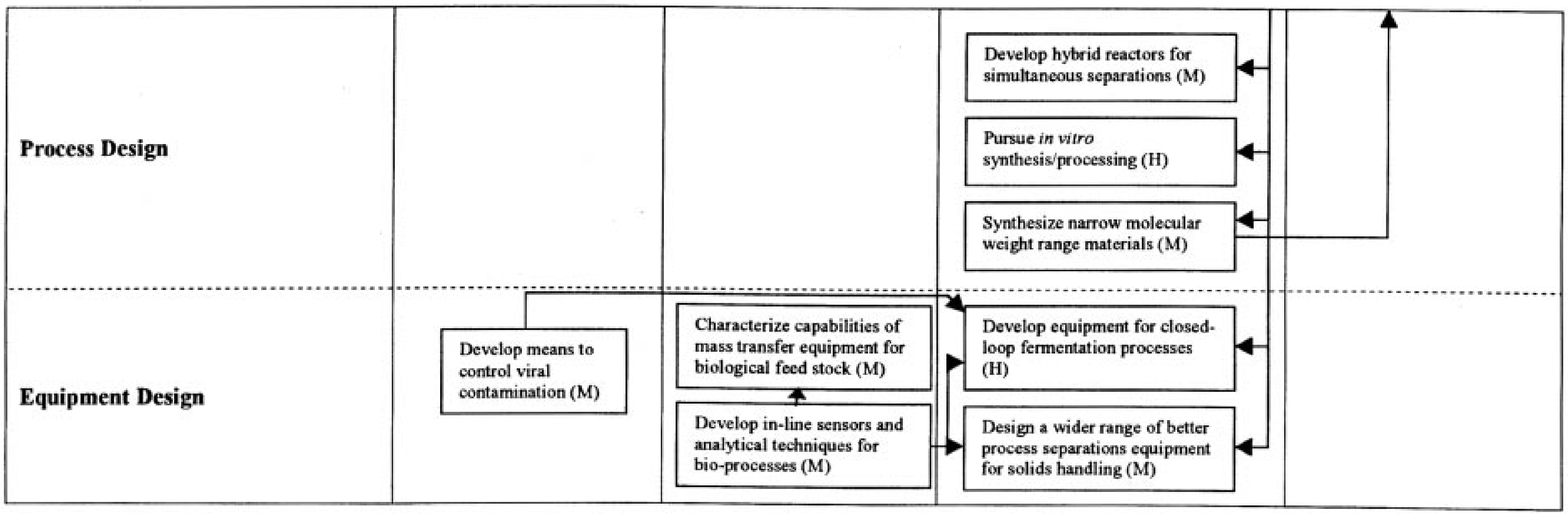

Process Design
Equipment Design
Develop hybrid reactors for simultaneous separations (M)
Pursue in vitro synthesis/processing (H)
Synthesize narrow molecular weight range materials (M)
Develop means to control viral contamination (M)
Characterize capabilities of mass transfer equipment for biological feed stock (M)
Develop in-line sensors and analytical techniques for bio-processes (M)
Develop equipment for closed-loop fermentation processes (H)
Design a wider range of better process separations equipment for solids handling (M)

Table I.9 Key R+D Linkages for Separations From Dilute Solutions
(H = High Priority, M = Medium Priority)

	Near - Term (0-3 years)	Mid-Term (3-10 years)	Long-Term (10+ years)
Fundamental Data	Compile physical phenomena and property data in databases (H) Develop understanding of molecular level interactions (H) Understand interaction of physics of separations and equipment (H)	Develop complexation chemistry (H) Develop better understanding of intermolecular interactions (H) Develop fast ion/phase transfer chemistry (M)	Understand interfacial phenomena for hybrid systems (M)
Predictive Modeling	Develop improved computer models for scale up and design (H)	Develop clear design evaluation methods (M) Develop improved computational models (H)	
Materials and Equipment	Immobilize separating agents (H)	Improve separations materials (H) Develop on-line, real-time sensors (M) Establish dedicated pilot-plant facilities (H)	
Process Systems	Develop hybrid systems for treatment of dilute solutions (H)	Improve hybrid systems for dilute solutions treatment (H) Increase testing of non-traditional processes in plants (M) Develop thermodynamically efficient energy transfer (M)	Develop improved hybrid systems for dilute solutions treatment (H)

II. INTRODUCTION

Background: In 1994, the US Department of Energy/ Office of Industrial Technologies (DOE/OIT) identified several industries, among them the chemical industry, which have major roles in raw materials production and/ or consumption, energy usage, and waste generation. DOE/OIT has worked with these industries to develop vision documents defining goals for the Year 2020 related to reduced raw material and energy usage, and lowered waste generation. Goals have been developed for the chemical industry in a cooperative effort among DOE/ OIT, the American Chemical Society, the American Institute of Chemical Engineers, the Specialty Organic Chemical Manufacturers Association, and the Council for Chemical Research. These goals and action proposals are detailed in the publication entitled *Technology Vision 2020: The Chemical Industry*.

Also, DOE/OIT has encouraged the individual industries to prepare technology roadmaps that will lead to meeting their respective Vision 2020 targets. A technology roadmap is analogous to an automobile roadmap employed in traveling from Point A to Point B. In the case of driving, the driver knows where he is (Point A), where he is going (Point B), and he has some knowledge of the terrain between points (A) and (B). In the case of a technology roadmap, the current state of the technology (A) and the desired future state (B) are defined. Then, the barriers to the journey and related research needs required to complete the journey are identified and prioritized.

The complexity of the chemical industry, with tens of thousands of different products, suggests that a chemical industry needs an atlas of roadmaps covering various technical areas, rather than a single roadmap, to define the path to implementation for *Vision 2020*. The creation of an atlas can be approached in a number of ways and, with this in mind, the Council for Chemical Research and the American Institute of Chemical Engineers created a task force to coordinate roadmap development activities. Several approaches were considered: (a) types or classes of chemicals (e.g., acids, bases, solvents, monomers), (b) broad attainment targets (e.g., reduction of water use, reduction of energy use, increased sustainability), and (c) various processing operations (e.g., distillation, separation, reaction, adsorption, extraction). The task force opted for a combination of alternatives (a) and (c) as the preferred approach. This choice was made because of the significant potential for: (a) the reduction in the use of both energy and raw materials by improving and optimizing various separations processes, and (b) the importance of new separation technologies which are expected to become increasingly more prevalent in the next century. Six separations technologies (adsorption, crystallization, distillation, extraction, membranes, and separative reactors) were selected for brainstorming assuming primarily petroleum-based feed streams because of their importance to the chemical and related industries. These and other separations technologies were then evaluated for two specific feed streams which are expected to increase in the future: bioprocessing and dilute solutions.

Trends and Drivers: Factors that will influence industry in 2020 include: fossil fuel prices and taxes; environmental regulations; growth in alternative processing technologies, such as biotechnology; recycling; use of total life-cycle evaluations in decision-making processes; information technology; international competition; and the industrial growth rates in Asia, Europe, and North America. Various scenarios can be developed based on different rates of change in each of these variables. The process streams generated and the major chemicals produced in the United States are likely to vary significantly among the scenarios.

Although no single scenario is likely to be correct, several key factors will drive the need to change industrial practices. In all cases, the public is expected to demand increases in pollution prevention/reduction and public safety, the value of fresh water will increase significantly, the cost for raw materials will increase and improved access to and availability of information will change the industry. To remain competitive in the future, the industry will need to tighten product specifications, reduce investment and operating costs, and increase the flexibility of plant operations.

Separations processes account for 40–70% of both the capital and operating costs in industry (*Separation Process Technology*, McGraw Hill 1997). Their application can significantly impact costs, energy use, and waste generation in the future. The maturity of separations processes is shown in Figure II.1. Although some technologies have been in use longer than other, no separations process has reached its full maturity, i.e. not everything is

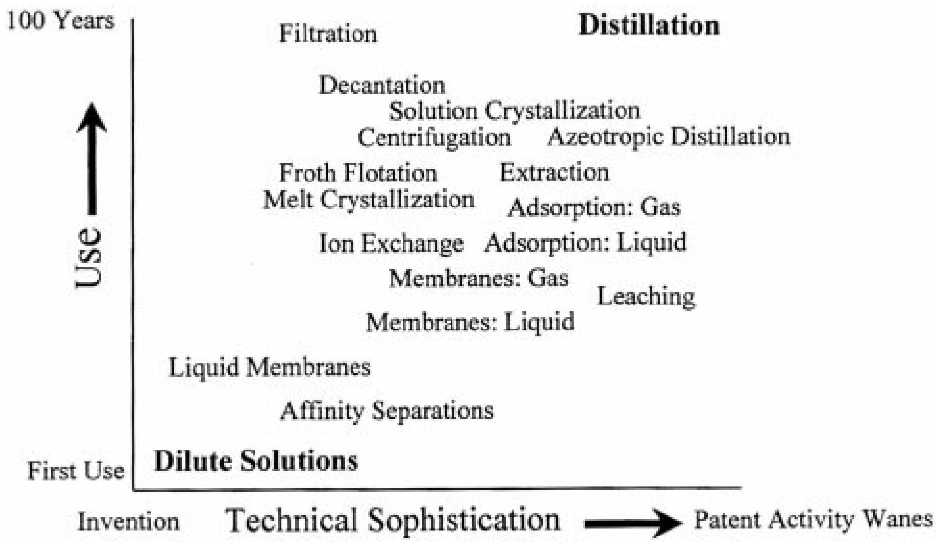


Figure II.1. Maturity of separations processes.

known about the process and further improvements are possible. In addition, combining individual separations processes in hybrid systems has the potential to revitalize the separations industry. These trends are reinforced by an internal study performed by DuPont that concluded:

- Water separations are everywhere,
- Water separations are likely to be more prevalent in the future,
- New methods are needed to make rapid and accurate flowsheet predictions for separations technologies, and
- Nondistillation separations technologies need to be made as predictable as distillation.

Goals: The general goal for the separations roadmap is to identify research needed to meet the chemical industry's vision. Elements of that vision include: maintaining or achieving positions of a leader in technology development; enhancing the quality of life; providing excellence in environment, safety, and health; good community relationships; seamless partnerships with academe and government; and promoting sustainable development.

A visioning process and its related roadmaps are incomplete if there are no commonly understood and communicated goals. Goals require some sort of indicator or yardstick. The simplest indicators are absolute numerical targets for energy use, material use, and pollutant release. However, this approach has major shortcomings since it can stifle growth and fail to deal with expected changes in product-mix. The approach also breaks down if applied to different geographical regions and individual companies.

Relative indicators that are based on the mass of product or the amount of revenue, while better than absolute indicators, also have shortcomings. They fail, by and large, to consider the impact created by the role of the supply chain in a company's production. An example is a company that is back-integrated into the supply chain compared to one that buys all ingredients in their final form and only performs the packaging, distribution, and marketing functions. The former company would have far higher energy and raw material consumption than the latter, but might actually be more efficient than the latter when all production steps are considered.

A group of companies, working with the National Roundtable for the Environment and the Economy (NRTEE), developed a number of alternative indicators and is testing them in their respective operations. One of the possible sets of indicators utilizes either material, energy, mass of pollutants, or water usage in the numerator while the denominator, in each case, is the difference between the selling price of the companies' products and the cost of raw materials. This approach allows for growth, and it rewards innovation in products that perform the same function while consuming less material and energy and emitting fewer pollutants.

This approach also obviates the problem of the supply chain segment described earlier. Some may question the use of a denominator that relates to profit, but this reflects, albeit imperfectly, the value that the manufacturer brings to society as judged by what consumers are willing to pay for the goods and services. The data required to generate the indicators are relatively easy to obtain by product, by location, or by company. The proposed NRTEE indicators are shown in Table II.1. For roadmapping purposes, a target of 30% reduction in all five of the indicators shown in Table II.1 by the year 2020 has been proposed as a reasonable stretch goal.

TABLE II.1
National Roundtable for the Environment and the Economy Indicators

Material Indicator	**MI=**	$\frac{\text{Mass of material purchased (mt)} - \text{Mass of product (mt)}}{\text{Revenue (US\$) - Cost of purchased materials (US\$)}}$
Water Consumption Indicator	**WCI=**	$\frac{\text{Volume of fresh water used}^1\ (m^3)}{\text{Revenue (US\$) - Cost of purchased materials (US\$)}}$ [1] Definitions are required (e.g., non-contact cooling water, etc.)
Energy Indicator	**EI=**	$\frac{\text{Net energy used (fence line) (mega-joules)}}{\text{Revenue (US\$) - Cost of purchased materials (US\$)}}$
Toxic Dispersion Indicator	**TDI=**	$\frac{\text{Total mass of recognized toxic materials released}^1\ \text{(mt)}}{\text{Revenue (US\$) - Cost of purchased materials (US\$)}}$ [1] Using a nation's most recognized list (e.g., excludes the Toxic Release Inventory in USA, National Pollutant Release Inventory in Canada, etc.)
Pollutant Dispersion Indicator	**PDI=**	$\frac{\text{Total mass of recognized pollutants released}^1}{\text{Revenue (US\$) - Cost of purchased materials (US\$)}}$ [1] The Pollutant Dispersion Indicator would include greenhouse gases, acid rain gases, eutrophication materials, ozone depleting chemicals, etc.

Separation Technologies Workshops: The groundwork for the roadmap was laid at a CWRT General Meeting in Richland, WA, in July 1997 and at a special topics session at the Twentieth Symposium on Biotechnology for Fuels and Chemicals held in Gatlinburg, TN, on May 6, 1998. Full details of these meetings and the subsequent workshops are provided in Appendix A. The participants are shown in Appendix B.

The first workshop (Separations I) was held in New Orleans on February 4-6, 1998, and was attended by about one hundred persons from industry, academia, and the government. This workshop was held in conjunction with a symposium that consisted of technical presentations summarizing the current state of adsorbents, membranes, and separative reactors. A monograph (see Appendix D) that documents the technical presentations made at the workshop and a number of process streams that would be good candidates for future research purposes is available from CWRT.[2]

The second workshop (Separations II) was held in Oak Ridge, TN, on May 11–13, 1998, and focused on crystallization, distillation, and extraction. Approximately fifty people attended Separations II. Attendees were experts in their respective fields and came mainly from industry, with smaller numbers from universities and government. The third workshop (Separations III) was held in St. Louis, MO, on March 9–11, 1999, and focused on bioseparations. The fourth workshop (Separations IV) was held in Gatlinburg, TN in conjunction with the *11th Symposium on Separation Science & Technology*. The theme for the fourth workshop was dilute solutions, but an effort was made to include separations technologies that were not specifically covered in previous workshops, including hybrid systems, field-enhanced systems, ion exchange, leaching, and filtration. Since ion exchange came up repeatedly in the workshops, the information on ion exchange was consolidated in a separate section of this report.

Breakout sessions were used in each workshop to allow participants to focus on their technical area of expertise. The task of each breakout group was to assess the current and future state of the technical area, predict typical feed streams for the technology in the next century, scope out the technical challenges facing separations technologies in order for it to be used to meet the workshop indicator goals, identify technical barriers to meeting those challenges, and to list and prioritize the research needed to address the barriers. Participants also had the assignment of sorting the prioritized research needs into four broad timeframes in which they should be conducted, 0–3 years, 3–10 years, and 10+ years, and ongoing.

Roadmapping: Smaller working groups of people who attended the workshops used the output of the workshops

[2] Available from CWRT by calling (212) 591-7424.

to develop the roadmap given in this document and refine the linkages between the research needs. Linkages are important to identify because they indicate instances in which the results of one research activity are the input to another research activity, typically occurring between research needs in different time frames. The results were reviewed by several industrial workshop participants to assure accuracy of the final product.

III. SEPARATION TECHNOLOGIES

III.A. Adsorbents

Summary: The most pressing research need was in the area of new materials. New adsorbent materials are needed that have either greater or more selective adsorbency, have better stability under extreme process conditions, have more favorable geometries, are available at lower cost than current materials, and/or are able to operate more readily on adsorption/desorption cycles. Process improvements will also be needed to take full advantage of improved adsorbent materials. Other research needs related to adsorbent performance are tools to predict performance and to aid in process design. Demonstration of commercial feasibility is essential to overcome the natural reluctance of industrial users to adopt this new technology.

Current State: Adsorption is typically considered as a process option when a high degree of purity is required and where the adsorbent can be regenerated easily and is not susceptible to fouling or degradation by the feed components. Adsorption applications are used in gas bulk separations (alcohol drying, air separations, hydrogen purification), gas purification (gas drying and VOC, sulfur and odor removal), and liquid separations and purifications (glucose–fructose separation, color and odor body removal, and recovery of fermentation products from fermentation broth). Most improvements in adsorption over the last decade have been process- and not materials-related. More details on the current state of adsorbents and adsorption technology are provided in the monograph (see Appendix D).

Future State: Increasing energy costs and life cycle cost considerations should act as catalysts for the increased use of adsorbents, although it will be important to find ways to regenerate and reuse adsorbents efficiently. Under these conditions adsorbents might displace energy intensive cryogenic distillation and liquefaction systems and displace distillation as a separation technology in applications where reflux ratios greater than 10:1 are required. Other areas where the technology might make inroads are in minimizing net in-process air and water use and in reducing waste generation and improving material reclamation. Additional possibilities exist in complex separations of high-boiling or thermally-unstable compounds.

Barriers: Barriers to achieving the desired future state were identified and prioritized according to perceived importance. Table III.A.1 details the key barriers identified. Table C.A. I in Appendix C includes all the barriers cited. The two most critical technical barriers based on participants voting were (a) *the difficulty in tailoring adsorbents to handle complex streams,* and (b) *the lack of predictive methods for mass transfer, adsorption equilibrium, and other physical data.* These two barriers captured the essence of the most pressing technical issues: (a) the need to be able to make adsorbents with improved and more selective adsorbent properties, and (b) the need to be able to model, and thereby predict, adsorbent behavior under various conditions and with various adsorbate molecules. Additional key technical barriers that were cited included the paucity of physical property data applying to

Table III.A.1 Key Technical Barriers for Adsorbents
(H= High Priority, M= Medium Priority)

Process Systems	Materials	Fundamental Data	Institutional Issues	Risk	Cost Issues
Disposal of metals and other environmentally unacceptable materials from adsorption systems (M)	*Difficulty in tailoring adsorbents to handle complex streams (H)*	*Lack of predictive methods for mass transfer, adsorption equilibria, and other physical data (H)* *Scarcity of physical property data applying to different geometries and process conditions (M)*	*Technology underutilized due to users' lack of understanding (H)* *Inability to integrate technical solutions and cost information across institutional and organizational lines (M)* *Lack of life cycle perspective by users (M)*	*Perceived high technical risk connected to investing in this technology (M)*	*Capital costs too high (M)*

different adsorbent geometries and process conditions, the high capital costs for adsorbent-based systems, and difficulties associated with the disposal of environmentally unacceptable material from adsorption systems.

Some categories—institutional issues, risk, and cost issues—touched on matters with less of a technical content but raised issues based on the state of the technology. The highest rated among these was the general lack of understanding of the technology in industry. Other barriers in this category related to (a) the high economic hurdle that technology needed to overcome relative to more traditional separation processes, and (b) the lack of a life cycle perspective in evaluating this technology versus others.

Research Needs: The key research needs, based on priority and time-frame, are summarized in Table III.A.2. Lower priority research needs and other action items that were cited are summarized in Table C.A.2 in Appendix C.

Materials: This category was judged to be the highest priority research need. New adsorbent materials are needed that (a) possess either greater or more selective adsorbency, (b) have better stability under extreme process conditions, (c) have more favorable geometries, (d) are available at lower cost than current materials and/or are able to operate on adsorption/desorption cycles more readily (i.e., readily switched between adsorption and desorption by some means other than thermal cycling such as, for example, microwave energy). Success in these areas would allow adsorbents to be used for difficult separations and/or on important process streams where alternative technologies are presently employed. In addition, new adsorbent materials might permit the recovery of valuable moieties from waste streams where their recovery is not presently feasible. Although not explicitly stated, workshop participants seemed to feel several of the materials improvement areas need to be addressed simultaneously.

Process Systems: Process improvements will also be needed to take full advantage of improved adsorbent materials. For example, the development of a new adsorbent designed to make desorption possible with non-thermal energy would require a process that provides both the new energy source and all the requisite process equipment to integrate desorption and adsorption cycles.

Predictive Modeling: Tools are required to predict adsorbent performance and to aid in adsorbent process design improvements. The value of a predictive tool would be twofold: (a) as an aid in the development of new materials using structure-activity correlations and combinatorial chemistry techniques, and (b) as an aid to optimum design of adsorbent units to achieve reduced size, capital, and operating costs. Because of the fairly long time needed to generate such predictive models, these tools would be available only in the medium- to long-term. Breakout session members expressed the view that the lack of adequate predictive models was based on two subsidiary needs, namely: (a) comprehensive data on which to base predictive models, and (b) a model with the power to allow the user to predict not only which molecule(s) will adsorb on an adsorbent but also which adsorbent is going to be the most effective material for any given adsorbate molecule.

Demonstrating Feasibility: It is a reality that large producers and users of chemicals generally prefer to use processes and technologies that are robust and well understood over those that are newer, even when those newer technologies offer better economics and/or are more environmentally friendly. Therefore, the demonstration of commercial feasibility is essential to overcome a natural reluctance to use that new technology.

Education/Information Transfer: This category of need attracted significant votes and included broad subareas of information gathering related to the eventual compilation of databases, either for their own sake or to facilitate the construction of predictive modeling tools. The compilation of a database on adsorption and adsorbents is important for the ready identification of waste streams that are ideal targets for adsorption. The use of adsorption to deal with wastes presently being handled by more traditional technologies would allow adsorption technologies to establish a track record of accomplishment and help reduce the perception that there are risks associated with this technology that are too great to accept. This is connected to the broader issue of demonstrating commercial viability.

R&D Linkages: The key linkages of R&D needs for adsorbents are shown in Table I.1. The needs are sorted according to the following categories: *materials, process systems, predictive modeling, demonstrating feasibility,* and *education/information transfer.* Only those needs that garnered a significant number of votes are shown.

Research-Related Needs: A number of non-research needs were cited that will have an influence on adsorption research if they are addressed. The group members expressed the view that adsorption should be better integrated into the chemical engineering curriculum so that graduating Ch.E.s will enter the workplace with a sound background in this technology. Attendees believed that chemical engineers in industry generally use unit operations they are comfortable with to solve the

Table III.A.2 Key Research Needs for Adsorbents

(H= High priority, M= Medium priority)

Time - Frame	Materials	Process Systems	Predictive Modeling	Demonstrating Feasibility	Education/ Information Transfer
All (Ongoing Processes)	*Develop new adsorbents for high selectivity in complex mixtures (e.g., using combinatorial chemistry approach) (H)*	*Integrate materials research and process development (M)*	*Collect/correlate data on equilibrium and kinetics for a variety of adsorbents (M)*		
Near-Term (0-3 Years)	*Develop more and better adsorbent forms and geometries (M)* *Reduce manufacturing cost per unit of adsorbent performance (M)*			*Demonstrate adsorption technology on important process streams to promote use of the technology (M)*	*Develop comprehensive information source to identify specific waste stream opportunities (M)*
Mid-Term (3-10 Years)	*Develop switchable adsorbents using non-thermal desorption energy (M)* *Develop improved high performance conductors (M)*	*Non-conventional ways to desorb adsorbed molecules (e.g., microwave, sonic energy) (M)*		*Process design tool to allow technology comparisons on an equal basis (H)*	*Create adsorbent handbook of physical properties (H)*
Long-Term (10+ Years)	*Develop non-conventional adsorbents (e.g., micelles, liquid crystals, enzymes, colloids) (M)*		*Develop molecular modeling tools to predict interaction of molecules with adsorbent surfaces (M)*		

problems they confront. Thus, there is a built-in barrier to their utilizing the newer technologies if those technologies are not a part of the Ch.E. curriculum.

Another need cited related to the creation of a national institute capable of funding or carrying out fundamental research on adsorbents and adsorption. Such an institute would provide the means for both collecting data and evaluating new concepts that will be needed to advance the field of adsorbents to a point where the 2020 goals can be met.

III.B. Crystallization

Summary: A better understanding of physical properties, in particular solid/liquid equilibria, is by far the most important research need facing crystallization. Developing molecular modeling methodologies to determine both solid/liquid equilibrium and the mechanisms that control crystal growth was considered to be the top long-term goal. Using fundamental properties data to develop models to design crystallizer systems was also a high-priority long-term goal; this modeling would enable designers to make the transition from batch to continuous processes. Instruments are required to measure the degree of super-saturation.

Current State: Crystallization processes are presently used to isolate and purify a wide range of inorganic and organic chemicals and food products. Applications range from high-volume, continuous processing of inorganic salts to low-volume, batch processing of high-value, specialty chemicals such as pharmaceuticals. Crystallization is most often used to produce high-purity materials; for example, melt crystallization can provide a purity of 99.99%. Crystallization is also used in the treatment of waste streams, the separations of close boiling mixtures (e.g., mixed xylene separation), and for mixtures that have a tendency to polymerize and/or thermally degrade at distillation temperatures. Crystallization from solution is complicated by the need to handle solids, but crystallization from a melt (a solventless process) can sometimes avoid this drawback by producing a pumpable, liquid product.

Future State: Crystallization is expected to remain a critical separation technology for the foreseeable future. Increasing energy costs may make crystallization attractive in the applications where it is not now considered economical. However, energy recovery will be an important factor in future applications. The importance of crystallization will also likely increase as biotechnology-based processes become more prevalent. A key consideration in the greater use of crystallization, however, is that industry must make a transition from batch to continuous processes.

Barriers: The brainstorming group developed a long list of technical barriers for each major industrial application of the technology—specialty chemicals and pharmaceuticals, large-volume organic and inorganic chemical production, food processing, and waste treatment. The barriers were then organized into categories and ranked by perceived importance. The key technical barriers that were identified are shown in Table III.B.1 and summarized below in order of priority.

Additional barriers that were cited are included in Table C.B.1 in Appendix C.

Physical Properties: The major physical property barriers identified were the lack of understanding of the mechanisms of crystal growth and the handling of crystal systems (dewatering, filtering), the lack of adequate phys-

Table III.B.1 Key Technical Barriers for Crystallization
(H= High priority, M= Medium priority)

Process Control	Analytical	Process Systems	Education/ Information Transfer	Physical Properties	Predictive Modeling
Particle size control capability is inadequate (M) *Lack of control systems to handle feedstock complexity and variability* (M)	*Lack of means to measure super-saturation* (H)	*Need for more continuous crystallizers* (M) *Lack of adequate deliquoring & filterability capabilities* (M)	*Lack of crystallization knowledge by chemical engineering graduates* (H) *Lack of knowledge of solids and solids handling* (M)	*Lack of understanding of polymorphs* (H) - *mechanism for crystal growth* - *dewatering* - *filterability* *Lack of physical property databases* (H) *Lack of molecular modeling* (M)	*Lack of data for simulation* (M)

ical property databases, and a lack of molecular models for crystallization processes. A need for better methods of estimating solubility in a wider variety of solvents and as a function of temperature was identified as a major barrier to a broader use of crystallization. Improved capabilities in this area would allow faster identification of suitable solvent systems and faster evaluation of processing alternatives. This would help to reduce the time and expense involved in developing and implementing a new process. It would also enhance the quality of the final process design by providing process designers with a powerful, easy-to-use tool that could help them identify better, more optimal solvent systems and operating conditions. A high priority should be placed on improving our ability to estimate the solubility of nonionic organic solids dissolved in organic solvents, since there are a large number of potential new applications for crystallization for these mixtures. Another top priority is for systems in which ionizable organics are dissolved in organic/water mixed solvents.

Education/Information Transfer and Process Control: Educational issues and a need for improved process control were ranked equally. Chemical engineers and chemists graduating from universities do not have strong backgrounds in crystallization and solids handling. Few mentors are available to provide on-the-job training for new employees in the practical aspects of crystallization. One result is that crystallization may not be as readily chosen by the engineering community when various other processing options are considered. An example is a lack of awareness of the merits of melt crystallization. Improved process monitoring and control technology are needed to let the user better manage crystal particle size and cope with feedstock variability.

Predictive Modeling, Analytical and Process Systems: The lack of analytical and predictive modeling capabilities were ranked equally. On-line microscopy methods and probes utilizing light-reflection techniques to measure properties related to particle-size distribution are the type of analytical methods presently being used for crystallization monitoring. Although these probes are quite useful, they are limited in the type of information they can provide. For example, there are no on-line monitors capable of measuring particle-size distribution, particle shape, and suspension density for crystals with a high aspect ratio. Most importantly, there are presently no adequate means for directly measuring the degree of supersaturation, the driving force for crystallization.

The data needed to construct process models are either inadequate or do not exist. Generating this type of information is time-consuming and expensive. Existing models are not adequate to allow confident scale-up from batch data or to develop designs of continuous crystallizers. There is a lack of adequate deliquoring and filterability capability and a need for more continuous crystallizers.

Other: Barriers associated with process economics and equipment/system design were identified (see Table C.B.2), but were considered to be far less significant than the areas described above.

Research Needs: Research activities needed to overcome the barriers described above were identified and organized into a number of technical categories of which four were most important: *fundamental data, predictive modeling, process systems,* and *education/information* transfer. The research needs were also ranked by importance to the industries that primarily use crystallization. The results are shown in Table III.B.2 (next page) and summarized below in order of priority. Lower priority research needs and other action items identified are provided in Table C.B.2 in Appendix C.

Fundamental Data: Crystallization experts concluded that a better understanding of solid/liquid equilibrium is by far the most important research need facing their field today. Available solubility data should be collected and incorporated into a central database over the next three years. Information on inorganic solutes in aqueous solvents and organic solutes in organic solvents are most plentiful. More data are needed for organic solutes in aqueous solutions, organic solutes in mixed aqueous/organic solutions, and organic melt mixtures. Having a greatly expanded database on nonionic organics dissolved in organic solvents would be valuable, for example, in determining values of UNIFAC interaction parameters. Presently, use of UNIFAC to estimate solubility is hampered by a lack of interaction parameters for many of the functional groups in complex organics such as pharmaceuticals and agricultural chemicals. Most of this work should be done over the next three years, but organic solute research may extend into the 3- to 10-year time-frame. Developing molecular modeling methodologies for calculating solid/liquid equilibrium was considered to be a long-term goal.

The group suggested having a center, such as Design Institute for Physical Properties Research (DIPPR), to direct the collection of physical property data and the maintenance of a database. Participants estimated that a database for existing data would contain approximately 1000–1500 entries. If ten companies were to contribute some of their in-house data, it would likely take a staff of two professionals and three support personnel to develop a database in a reasonable time-frame. Molecular modeling was identified as a long-term development need. Improvements in well-known correlations and activity-

Table III.B.2 Key Research Needs for Crystallization
(H= High priority, M= Medium priority)

Time-Frame	Process Systems	Education/ Information Transfer	Fundamental Data	Predictive Modeling
All (Ongoing processes)				*Improve process modeling to permit for better scale-up capabilities* (H)
Near-Term (0-3 years)	*Develop spectroscopic monitors for measuring degree of super-saturation* (M)	*Involve engineering early in the product development cycle* (M)	*Develop methodology for estimating solid/liquid equilibrium* (H)	
Mid-Term (3-10 years)	*Design continuous equipment to replace batch equipment* (M)		*Develop models of crystallization mechanism* (H) - *polymorph* - *size* - *shape*	
Long-Term (10+ years)	*Automate crystallizer design based on fundamental material properties* (H)		*Develop molecular modeling methodology to determine solid/liquid equilibrium* (H)	

coefficient models for solid/liquid equilibrium are needed in the interim.

Predictive Modeling: The group identified the need to better understand and quantify crystallization mechanisms as a mid-term need. The payoff to understanding such phenomena at the mechanistic level is better control over parameters such as crystallization rate and crystal morphology, shorter development times for new processes, and waste minimization.

Predictive modeling and equipment/system design research needs were the next highest priority area after fundamental data. The highest priority need in process modeling is developing a predictive capability for scale-up of crystallization processes. These should take into account the impact of scale and equipment geometry on crystal size and shape. Scale-up methods must be validated with field data from complex multiphase systems in crystallizers with complicated geometries. Lower priority research needs in this area include improved computational fluid dynamics (CFD) modeling and better kinetic models for multiphase systems. Simple systems are easily handled by present-day modeling methods, but existing methods are inadequate for handling real world systems that combine multiple components and phases.

The crystallization experts indicated that kinetics, nucleation rate, crystal growth rate (as a function of degree of saturation), and particle attrition data would be needed for incorporation into predictive models.

Process Systems: The highest priority needs in process systems include development of micro-mixing models and crystallizer design strategies (both manual and automated) based on fundamental material properties. Important scale-up parameters include transport phenomena, hydrodynamics, micro-mixing, mass transfer, and heat transfer. The desired output of models would be identification of the best equipment configuration for a given crystallization application. Thermodynamic and kinetic data will be required to develop such models. An industrial consortium should develop the model in two parts: CFD and crystallization. Established vendors should develop the software. It is expected that such an effort could cost about $500K per year and may take up to five years to develop. Instruments to directly measure the degree of supersaturation are needed to help control the crystallization process.

Education/information Transfer: An important need is to involve engineering personnel earlier in the life of a product and process. By so doing, the chemical engineer can help bring the advantages and strengths inherent in crystallization to the development of the process.

Other: Although research needs in process control, analytical techniques, and economics were identified, they were considered to have lower potential impact on the future of crystallization with the exception of spectroscopic monitors for measuring the degree of supersaturation mentioned earlier. New instruments are needed which have higher resolution (better discrimination for non-uniform particle-size, shape, and clusters), have more sophisticated image analysis algorithms, and are more robust and nonfouling; the last two requirements are for continuous systems applications and for use at high temperatures and in harsh environments. The group suggested approaches to developing better analytical equipment. Vibrational spectroscopy methods such as FTIR or Raman spectroscopy should be adapted for on-line analysis of crystallization.

Infrared and fluorescence techniques have been shown in university research to allow direct measurement of the degree of saturation for specific chemistries. Technical experts doing research in this area, crystallization users, users of robust monitoring equipment from other industries, and equipment vendors could participate in a separate workshop to develop a more detailed plan.

R&D Linkages: The key research linkages for crystallization are shown in Table I.2. The needs are sorted according to the following categories: process systems, education/information transfer, fundamental data, and predictive modeling.

Research-Related Needs: As discussed earlier, the lack of formal academic courses on crystallization in the chemical engineering curriculum was cited as a barrier to increased future use of this technology.

III.C. Distillation

Summary: The most important research need was judged to be a better understanding of physical fundamentals. The experts cited transport phenomena such as fluid flow, heat and mass transfer, and multi-phase flow processes occurring within trayed or packed distillation columns as insufficiently understood subjects. Better *in situ* sampling, analytical, and imaging techniques are needed to determine phase mixing and flow distributions on trays and in packed beds. Better distillation simulators and computer models are needed for column design. A larger quantity and higher quality of fundamental research, especially in academia, are needed to support all of these areas as well as areas not rated as highly.

Current State: Distillation is one of the best developed chemical processing technologies with a long and successful industrial history. It is considered to be a "mature technology" and is often the separation technology of choice because of its well-understood nature.

Future State: Distillation is expected to continue as an important process for the foreseeable future even in the face of increasing energy costs because of its preeminent position in the separation field. Factors which could influence the use of distillation in the future include: advances in ways to enhance relative volatilities, progress in equipment design to improve vapor-liquid disengagement, close coupling of unit operations (heat integration, hybrid processes, etc.), changes in feed stocks, and increased energy costs.

Barriers: The brainstorming group developed an extensive list of technical barriers that could, when overcome, influence the future of the technology. The barriers were organized into major categories and ranked by importance to the industry. The key barriers that were identified are shown in Table III.C.1 and are summarized below in order of importance. Table C.C.1 in Appendix C provides details on all the barriers identified.

Fundamental Data: Of the dozens of issues raised by the distillation group, among the most important was judged to be an inadequate understanding of physical fundamentals. A lack of in-depth understanding of the processes occurring within a distillation column was believed to be a significant barrier to the further improvement of equipment performance. The experts cited transport phenomena such as fluid flow, heat and mass transfer, and multi-phase flow as subjects that are insufficiently understood. They also listed foaming, frothing, and other processes occurring within distillation towers among the topics requiring more study and a better understanding. Most applications-related data and methods are proprietary within various companies, and there are no effective mechanisms to promote sharing of the data among potential users with a common goal of achieving important improvements in distillation.

Equipment Performance and Education/Research Management: Equipment performance and education/research management were ranked equally as the next highest priority barriers after lack of fundamental data. The inability to see inside distillation columns during operation, lack of effective sensors for large columns, and lack of modeling capabilities to predict column performance make it difficult to design and operate equipment in a reliable and predictable manner. The inability of the researcher to adequately image liquid and vapor in an operating distillation column impedes advances in this field. It remains largely unknown just how the gas and liquid phases mix and how fluids are distributed in packed beds. There is a need for better scale-up methods and a need to be able to extrapolate data from one distillation system to another. Corrosion degradation of trays and packing is also a problem for specific applications.

Table III.C.1 Key Technical Barriers for Distillation[1]
(H= High Priority, M= Medium Priority)

Physical Fundamentals (H)	Equipment Performance (M)	Education/Information Transfer (M)
Lack of accurate real stage efficiency calculation *Lack of adequate mixing characterization* *Lack of adequate understanding of distillation phenomena* *Lack of adequate vapor liquid imaging techniques* *"Bad actor" (foam) separation is inaadequate* *Lack of ability to measure multi-phase traffic* *A better understanding of mass transfer and multi-phase flow is required* *A better understanding of the processes of phase formation, mixing, interface area formation, and mass transfer, etc. is required* *Lack of adequate data on bubble formation*	*Flow control on trays is inadequate* *Liquid distribution in packed beds is inadequate* *Scanning methods for tower operation troubleshooting are inadequate* *Lack of non-fouling distributors* *Lack of active devices for phase disengagement* *Lack of adequate means to prevent fouling in the towers* *Lack of methods to handle multi-phase feeds* *Equipment size-determining rate processes need to be re-evaluated* *Hybrid column internals are required* *Means of reducing stage spacing to less than 2 inches are required*	*Companies and vendors will not share information* *Industrial R&D funds are being reduced* *Universities and national labs are not emphasizing distillation research* *Universities are reducing courses in distillation*

[1] Participants prioritized categories and not individual needs within each category.

Support for distillation research is declining in industry, universities, and the national laboratories. There is a general lack of both sponsors and mentors in this field. It has been recognized for at least five years that the number of distillation experts with an international reputation is sharply declining. Graduating students are not well-trained in distillation. This will ultimately result in a work force that is inadequately trained in the fundamentals and the practical aspects of distillation for the chemical and petrochemical industries. Many advances and much know-how are proprietary to individual companies or consortia, and this inhibits public domain research and cross-fertilization of new ideas, models, and theories.

Other: Of the several other lower priority technical barriers identified (Table C.C.1) the group felt the following were the most important. Distillation systems are not understood well enough to allow engineers to operate columns at maximum efficiency for some separations or to design flexible units that can accommodate changes in users' needs. Existing computer models adequately predict performance of around 80% of industrial systems. The remaining systems are considered to be problematic and cannot be adequately modeled by existing software. Highly reactive or corrosive chemicals are examples of systems that are least well served by existing distillation models. Mixtures of aqueous and organic materials are also troublesome. Another barrier identified by the participants is the dearth of publicly available data. Models that relate one distillation system to another are available, participants noted, but most of the data needed to create the models are proprietary.

Research Needs: The research needs for distillation were organized into major categories and prioritized by timeframe. The most important of these categories are shown in Table III.C.2. The breakout group also stressed the importance of improving the "image" and level of financial support for R&D in distillation, particularly in academia, with the overall goal of producing more fundamental work *in the public domain.*

Fundamental Data: A better understanding of physical fundamentals was judged to be the most important research need because of its potential impact on improved equipment performance. Research needs fell into three major categories: development of sensors, obtaining basic fundamental data, and developing better computer models. Sensors for measuring basic distillation phenomena should account for packing/tray type, multi-phase flow (void fraction and density), bubble-size distribution, local concentration gradients, liquid flow on packing surfaces, surface tension gradients, and temperature gradients. Experimental studies aimed at understanding basic distillation phenomena should account for mixing, interfacial area, mass transfer, multi-phase flow, non–air/water systems, and packing/trays. Comprehensive computer models based on fundamental phenomena are needed to predict mass transfer

Table III.C.2 Key Research Needs for Distillation
(H= High Priority, M= Medium Priority)

Time-Frame	Fundamental Data	Process Systems
All (Ongoing Processes)	*N/A*	*N/A*
Near-Term (0-3 years)	*Develop sensors for measuring basic distillation phenomena* (H) *Develop database of mass transfer and hydrodynamic data* (H)	*Develop column internals imaging equipment* (M) *Develop better simulators* (M) *Develop database of existing packing/trays* (M) *Develop tools to predict composition from column temperature* (M)
Mid-Term (3-10 years)	*Improve understanding of basic distillation phenomena* (H) *- mixing* *- interfacial area* *- mass transfer* *- multi-phase flow* *Develop fundamentals-based model for predicting mass transfer and hydrodynamics in complex "difficult" systems* (H)	*Develop sensors for multi-phase flow* (M) *Develop understanding of factors affecting vapor/liquid distribution* (M) *Develop better understanding of three- and four-phase flow in packing/trays* (M) *Develop in situ sampling methods* (M) *Develop better process gas chromatographs* (M) *Develop novel phase separation methods* (M)
Long-Term (10+ years)	*N/A*	*N/A*

and hydrodynamics in distillation columns. Databases for fundamental physical properties and bubble-formation mechanisms will need to be developed for "difficult, complex" distillation systems before computer models for these systems can be developed. Data from equipment performance research, such as internal imaging data, will also need to be fed into these models. Models will most likely require a computational fluid dynamics-type of approach as significant advances have been made within recent CFD-based modeling tools on multi-phase flow analysis.

Process Systems: Better imaging techniques are required to determine phase mixing and flow distribution in packed beds. These methods must have high resolution and minimal interference. The equipment must be economical and potentially portable for use on multiple operating columns.

Better distillation simulators are needed for column design. Results from fundamental data research will need to be fed into these models. Computer-aided process design tools should be considered for predicting column internals design. Several group members suggested that the field would be well-served by learning how to adapt tools for modeling fluid flow to distillation-specific problems. Other areas of engineering benefit from advances in newly developed computational methods such as computational fluid dynamics.

Better *in situ* sampling and analytical methods are needed. Novel phase separation methods should be developed to reduce column height requirements. A database of existing packing and trays using a knowledge-based system should also be developed.

Existing systems are not well enough understood to optimize operations. More reliable instrumentation and better simulators must be developed prior to optimization. Operations optimization should be implemented in a phased approach, initially optimizing single columns or trains. This should be expanded to include plant-wide and refinery-wide optimization.

R&D Linkages: The key research linkages identified for distillation are shown in Table I.3.

Research-Related Needs: A major concern of the group was a work force that is, increasingly, inadequately schooled and trained in the area of distillation. This could have a major impact on the future of industries using or considering the use of distillation. Management of research and development activities is as important as the research that is performed. Position papers need to be developed on the best approach to improve the image of distillation in the research community and more effectively utilize the shrinking funding available to do research and development. This should include industrial/university/government collaborations and the creation of incentives to support distillation research. Universities should be encouraged to emphasize distillation in their chemical engineering curricula.

III.D. Extraction

Summary: Key research needs were identified to address the top four technical barriers—new solvents/equipment/processes, improved understanding of fundamentals, retrofitting existing equipment, and elimination of third phase/unwanted reactions. The two greatest research needs were for new solvent extraction technologies and a better understanding of the fundamental science of extraction. New solvent extraction processes should emphasize use of highly selective solvents, recovery of solvents, and more effective interfacial sensors. Fundamental data relating to physical properties and interfacial phenomena are needed for computational models that account for drop dynamics, hydrodynamics, and multi-phase flow. A second priority group includes research to predict performance of retrofitted equipment and to eliminate third phases and unwanted reactions.

Workshop Scope: For the purposes of the workshop "extraction," when used as a separations technology was deemed to apply to liquid–liquid systems. Participants chose to exclude leaching as part of liquid/liquid extractive processing; this should be considered as a separate topic area for a future workshop. Participants also chose to include supercritical extractions that do not involve solid materials in the scope of extraction. Resins and membranes were excluded from discussion with the exception of liquid/liquid membranes (resins and membranes were deemed to be sufficiently different to warrant a separate workshop). The terms "solvent" and "extractant" are used interchangeably in this discussion. The stream to be separated is referred to as the feed stream.

Current State: Extractive separation technologies are not nearly as well developed as distillation—the ratio of the number of distillation units to extractors in industry is estimated to be 20:1. Extraction is only slightly more developed than crystallization. Participants agreed that this lack of development stems from many causes, primarily: (a) predictive methods are difficult to implement in extraction processes because impurities can be present that greatly affect extraction efficiency, (b) many variables/parameters play a role in determining extraction efficiency.

Current large-scale extraction processes include separations such as (a) aliphatic/aromatic splits, and (b) C_4 separations (where solids formation is a serious issue). Extraction is also used in acrylonitrile production.

Future State: Extraction will continue to be a major separations unit operation in the future. The increasing use of bioprocessing will open the way to a much larger role for extractive separations. As major technical improvements are made in bioprocessing, new and/or more economical process options will become viable alternatives to extant processes. An illustrative example of the use of extraction in a bioprocess that might be viable in the future is the production of protein from kudzu. Kudzu, a rapidly growing vine of eastern Asian origin, produces certain proteins that are valuable but cannot be extracted efficiently with current technology. A typical kudzu feed stream (after pretreatment) contains 10% generic protein. Only 1% of this protein is potentially valuable material. Current extraction techniques are too expensive to achieve narrow-band molecular weight separations to permit the isolation of the valuable protein component. New solvents or processes using new solvents to extract these proteins could make kudzu processing viable in the future.

Participants in this workshop attempted to envision which extraction processes are likely to be important in the Year 2020. A list of these processes follows:

- Selective extraction of proteins based on molecular weight; functionally (ligand) specific extractions.
- Fractional extraction (in which two immiscible solvent streams run counter-currently to each other with the feed stream added to the middle of the extraction column) and other underutilized technologies must be developed (cross-platform technologies). Bottlenecks for these processes will have to be overcome, and simulation data and tools must be generated. Fundamental research will most likely be generated at universities or in national laboratories.
- Development of new, compatible, pretreatment technologies to make extraction processes more efficient and cost-effective.
- Use of computational chemistry for solvent (diluent, extractant(s), and modifier) selection and also to develop new solvents/extractants based on desired characteristics.
- Use of combinatorial chemistry for solvent (diluent, extractant(s), and modifier) selection. This

process involves intelligent screening of solvents and development of large databases.

- Combined unit operations of reaction with extractive separation for enhanced production, while presently underdeveloped, will likely play an important role in a number of processes by 2020.

Barriers: The workshop participants identified eleven key barriers that must be overcome for extraction to meet the Vision 2020 objectives. The participants then analyzed, grouped, and prioritized these barriers. The top four barriers are given in Table III.D. I (high and medium priority barriers) and discussed below. All the technical barriers cited are provided in Table C.D.1 Lack of new solvent extraction technologies and the level of understanding of the fundamental science involved in this technology were the two highest priority barriers. The ability to retrofit existing equipment and elimination of third phases and unwanted reactions were considered low priorities.

Solvent Extraction Technologies: Existing solvents and extraction technologies are inadequate with respect to selectivity for target metals and other selected compounds. Methodologies for selection of the optimal solvents for a given process are also inadequate.

Existing designs for contactors and coalescers or decanters do not lead to the required processing efficiencies or to low environmental impacts. Particular emphasis should be given to back-end processing. Interfacial sensors are needed. New analytical methods and/or instruments (e.g., drop size determination) are needed for on-line process control and monitoring and for off-line characterization.

Present processes lead to phase changes of major unwanted components and result in poor extraction efficiencies for very dilute but significant components in extraction streams. Downstream processes needed to recover extractants in pure form are not available. Capabilities are needed to facilitate the design of efficient, inexpensive recovery processes. New aqueous/aqueous two-phase extraction processes are needed using, for example, cyclodextrin, PEG, micellar, and bioenhanced solvents.

Understanding of Fundamentals: The highest priority need is to understand surface/interfacial chemistry, particularly for "rag" layer (or third-phase emulsion phase) formation, which is the plague of extraction processes. There is a need for a better understanding of the fundamental science involved in extraction such as solvent properties, solvent performance, mass transfer, interfacial tension, equilibrium, and hydrodynamics (e.g., back-mixing). Improvements in the state of knowledge in these areas would lead to better predictive mathematical models and better *a priori* decision making.

Retrofitting Existing Systems: Engineers need the ability to predict and design retrofits for both existing equipment and existing solvents. This includes altering

Table III.D.1 Key Technical Barriers for Extraction[1]

(H= High Priority, M= Medium Priority)

New Technologies Development (H)	Understanding Fundamentals (M)	Retrofitting Existing Equipment/Solvents (M)	Third Phase/ Unwanted Reactions (M)
Materials: *- better solvents* *- more selectivity for target metals* *- more selectivity for other compounds* *- better understanding of existing solvents* *- better methodology for selecting new or existing solvents* *Equipment:* *- better design capabilities* *- better interfacial sensors* *- better drop size determinations* *Processes:* *- improve efficiency to reduce dilute streams* *- improve downstream recovery of pure extractant* *- better coalescence* *- better process control* *- improve aqueous/aqueous two-phase extraction*	*Improve understanding of surface/interfacial chemistry to prevent rag layer formation* *Need dynamic modeling for controlling processes* *Need better equilibrium models* *Inadequate ability to predict coupled processes* *Better interfaces are required for computational fluid dynamic type codes to produce a visualization tool*	*Need better capabilities to design retrofits for existing equipment and solvents for:* *- altered conditions* *- altered streams* *- altered capacities* *Need better capabilities to predict performance of existing equipment and solvent to allow de-bottlenecking of process*	*Need methods for eliminating rag layer formation* *Need better methods for dealing with solids in extraction streams* *- existing solids* *- solids that form during processing* *- cell biomass* *- fermentation broth* *- rust* *- catalyst* *- larger particulate contaminants* *Eliminate unwanted reactivity* *Treatment of extreme waste streams (due to chemical reaction)*

[1] Participants prioritized categories and not individual needs within each category.

operating conditions, stream compositions, and equipment capacities to de-bottleneck existing processes.

Elimination of Third Phase/Unwanted Reactions: Rag layer formation is a major plague of liquid/liquid extraction processes. Significant needs that were identified included: (a) an understanding of the fundamental science and interfacial chemistry involved in rag layers so that their formation can be managed, (b) methods for more effectively handling solids in extraction processes, (c) improved understanding and control of unwanted reactions which occur during extraction processes, such as "popcorn" and polymerization, and (d) an ability to treat extreme waste streams.

Other: Several other barriers were identified, but they were ranked low in priority (see Appendix Q). These included: (a) a fundamental understanding of extraction processes in order to predict the environmental cost/benefit of extraction streams/processes, (b) the capability to extrapolate data from one contactor type to other contactor types, and (c) data for total life cycle cost-estimating, safety decisions, and hybrid processes.

There is a lack of data on extraction unit operations needed for total life cycle costs and flow sheet optimization evaluations. Impacts on flow must be considered when the extractant changes. Solvent recovery is also important. Product life cycle analysis should be considered as well. The capability to incorporate cost, health rating, flammability rating, effectiveness, and environmental aspects in a balanced decision-making process is needed. Toxicity needs to be included in industrial hygiene decisions.

Research Needs: Participants in the workshop identified research needs to address the high and medium priority technical barriers. The results are presented in Table III.D.2 (Table C.D.2 summarizes all research needs identified) sorted according to priority and time frame, and are discussed below.

New solvent extraction technologies and an increased level of understanding of the fundamental science involved in this technology were the two top priority research needs. Enhancing the ability to predict performance of retrofitted equipment, and eliminating third phases and unwanted reactions were the medium priority research areas.

New Technologies Development: Research should focus on development of highly selective solvents and recovery processes. Development of liquid/liquid interface sensors and subsequent demonstration of performance of these sensors under real world conditions should be promoted. A center for collecting critical data for thermodynamic properties and other operating parameter is needed.

Fundamental Data: There is a major need for a better understanding of the fundamental science associated with equilibrium models. Specifically, there is a need to account for electrodynamic, quantum-mechanical, and diluent effects in extraction processes. Research needs fall into six categories: physical properties, equilibrium models, multi-component solutes, hydrodynamics, dynamic models, and process/equipment simulation.

Research needs for physical property data, particuarly interfacial phenomena, include emulsion phenomena, coalescence phenomena, and Marangoni phenomena. Data are also needed to predict the effect of surfactants and contaminants on extraction efficiency, measure interfacial tension with mass transfer (methods such as cup and capillary inside an extraction column), and for diffusion coefficients, density, and viscosity.

Research on multi-component solutes must include reaching a better understanding of the science governing fractional extraction. Predictive multi-component extraction models could be developed that reduce the amount of data required.

Hydrodynamics research should focus on predictive mathematical modeling (e.g., computational fluid dynamics), tray efficiency, and drop dynamics. CFD modeling should include drop breakage and coalescence frequency, large-scale homogeneous systems, and interfacial and drop convection. Models should predict and quantify the effect of surfactants and contaminants. Two-phase flow models with breakage and coalescence are needed for highly dispersed-phase holdup. Tray efficiency studies should focus on reducing poor coalescence and/or mixing. Drop dynamics and hydrodynamics studies should focus on developing a phenomenological understanding of flooding in various extraction columns as well as on axial mixing of either the continuous or dispersed phases.

Process simulators are needed that will permit an engineer to make heuristic equipment selection and achieve more efficient process operations. Ultimately, methodologies for liquid/liquid extraction processes should be addressed.

Retrofitting Existing Technologies: Research in this field should be directed at: (a) understanding how to change the chemistry of existing processes, (b) incorporating a mixer-settler stage as a pre-extractor on the feed and extract end for the process (e.g., packed tower), (c) increasing the feed rate for the same solvent rate (lower extraction factor), and (d) changing internals in the existing shell and phase separation fundamentals and enhancement. There is a need for side-by-side economic comparisons of existing and new processes.

Unwanted Reactivity, Third-phase Formation, and Decantation: Traditional solutions to unwanted reactivity

Table III.D.2 Key Research Needs for Extraction
(H = High Priority, M = Medium Priority)

Time-Frame	New Technologies Development (H)	Fundamental Data (H)	Process Systems (M)	Third Phase/ Unwanted Reactions (M)
Near-term (0-3 years)	*Develop interfacial sensors*	*Develop physical property & interfacial phenomena data* *- emulsion phenomena* *- coalescence phenomena* *- Marangoni phenomena* *Measure interfacial tension with mass transfer* *- diffusion coefficients* *- density* *- viscosity* *Develop dynamic CFD models* *- drop breakage and coalescence frequency* *- large-scale homogeneous* *- interfacial and drop convection* *- effect of surfactants and contaminants* *- two-phase flow with breakage and coalescence* *- tray efficiency* *- drop dynamics and hydrodynamics*	*Develop models of existing systems* *Perform side-by-side comparison of existing and new processes; use to evaluate models*	*Determine effects of third-phase formation on extraction efficiency* *Develop interfacial controls to minimize third-phase formation*
Mid-term (3-10 years)	*Develop highly selective solvents*	*Develop methodology to predict effect of surfactants and contaminants* *Develop equilibria models* *- electrodynamic effects* *- quantum-mechanical effects* *- diluent effect* *Develop multi-component solutes* *- fractional extraction* *- multi-component* *- extraction*	*Design large-scale homogenous extraction systems*	*Develop additives, etc., to eliminate unwanted reactions* *Determine effect of rag layers on drop coalescence at interface* *Develop structured packing with understanding of time-dependent wetting of materials* *Develop chemical coalescence aids* *Develop new devices for decantation* *Develop external field-enhanced decantation* *Quantify solids that each extract type could handle*
Long-term (10+ years)	*Develop recovery processes*		*Commercialize large-scale homogenous extraction systems*	*Determine mechanisms for third-phase formation*

[1] Participants prioritized categories and not individual needs within each category.

include: adding a modifier, salt, pH modifier, or an inhibitor to prevent polymerization; pulling a slip stream to remove the unwanted compound; using alumina to adsorb surface-active agents; reducing the residence time; operating at a different temperature; and reducing the number of components (the more components present, the better the chance of an unwanted reaction). These areas need continuing work and other innovative approaches need to be encouraged.

Third-phase, or rag layer, formation is a widespread problem for extraction processes. Research to address this problem should include: interface control and the effects of third-phase formation on extraction processes, the effect of rag layer on drop coalescence at the liquid–liquid interface, and mechanisms of third-phase formation. A fundamental problem that needs to be resolved is the dependence of "rag" formation on the type of extractor versus the type of chemical system.

Decantation research needs that were identified included: (a) a structured packing that could be used internally or externally to handle the time-dependent wetting characteristic of materials, (b) chemical coalescence aids, (c) new devices for decantation both internal and external to the extractor, (d) development of a validated method for decanter design, and (e) investigation of external-field enhanced (acoustic, thermal, electric, ultrasonic, magnetic, microwave, e-beam, gravitational, or other external fields) decantation.

Solids handling other than the rag layer should also be studied. Focus is needed on quantifying the types and concentration of solids that each type of column could handle and the effects of the surface of the extractor. There is a need to quantify the characteristics of solids, to determine how they change with time, and to characterize the effect of materials of construction. Research should also address the presence of bacteria on processing, a generic problem in extraction.

R&D Linkages: The key research linkages for extraction are shown in Exhibit I.4. The needs are sorted into categories: fundamental data, predictive modeling, materials, and process systems.

III.E. Membranes

Summary: Participants thought that a high priority should be placed on undertaking a critical review of the processes used to manufacture high tonnage chemicals and larger volume specialty chemicals in order to determine where membrane technology, as currently practiced, could have a significant impact on process economics and help focus research efforts. Improving the robustness of membrane systems on "real-world" streams was also ranked as a high priority as was the need to develop ways of increasing surface area per unit volume at lower cost. Other important needs that were identified were the continued development of high temperature membranes (ceramic, metal), overcoming scale-up difficulties for industrial streams (fouling, oil mists, etc.), and developing better process simulation packages for design, process evaluation, and training. Longer term investigations of novel membrane materials, nano-composites, and chemically inert materials were also given a high priority. Lower priority needs included the development of scalable low-cost manufacturing techniques, a step-change in the creation of membrane surface area, application of ionic membranes to aqueous systems, and the development of mixed organic/inorganic composites as membrane materials.

Current State: Membranes processes are considered when bulk rather than precise separations are sufficient and when processing rates are modest and the membrane is resistant to fouling by system components. Membranes are being successfully used in a number of applications such as: gaseous separations (O_2/N_2, H_2/CH_4, olefin/N_2), reverse osmosis and ultra-filtration (desalination and various applications in the paint and beverage industries) and recovery of PFC's and HFC's in the semiconductor industry. Further details on the current state of membrane technology is covered in the monograph (see Appendix D). A synopsis of additional comments from breakout session participants about present-day membrane R&D is provided below.

A number of attendees felt that membrane R&D as practiced today possibly places too strong an emphasis on materials science research as opposed to process system development. Development work is important in order to demonstrate how membrane systems can operate robustly in real world applications rather than on clean model streams. For example, feed pretreatment, cited as an important aspect of any successful membrane system design, needs research attention. Some participants believed that the present focus on materials science stems from the relative ease of obtaining funding for new membrane research (interesting science and relatively cheap), and the dearth of critical peer review of the output. The lack of process development and engineering design work stems from weak economic driving forces arising from low energy prices. There was a perception that decision-making management was reluctant to focus efforts on developing breakthrough systems in critical services with a technology that was less understood than conventional approaches. Such concerns with the technology tend to make engineers overdesign systems, further increasing the capital cost of membrane systems versus competing technologies.

Future State: De-bottlenecking and azeotrope breaking were considered fruitful fields for the use of membrane or hybrid membrane systems. New membranes are usable for alkane/olefin separations (e.g. propylene from propane). However, for membrane systems to be used in major processing streams and in critical services (rather than on vent streams or minor process streams) to meet Vision 2020 goals, long term reliability and durability in application specific services will be key considerations. This will be particularly true for systems in service in commodity chemical plants where high on-stream factors are important, and the robustness of extant processing steps is well documented. In addition, membrane systems will have to demonstrate substantial economic benefits in the form of reduced operating and capital costs (capital cost is still a significant determinant in the selection of process options) over competing technologies. In this regard, a life cycle assessment approach for evaluating membrane systems versus other technologies might be a more rigorous approach in determining the best available technology. However, absent dramatically increased energy costs it will be very difficult for membranes to make much of an inroad versus distillation in many applications. The hurdle for introducing new technology is likely to be lower for grass-roots plants (now mostly being built outside the United States) rather than in retrofitting existing plants, suggesting the preferred route to commercializing membranes in the United States might be via experience gained in overseas operations. This has already happened with other chemical process technologies. Finally, there was a strong view that more emphasis has to be put on applications for existing membranes and systems rather than on new membrane materials if the technical challenges in Vision 2020 are to be met. A significant number of participants felt the future focus of membrane systems should be on the manufacture of those chemicals likely to be manufactured in the United States in 2020, rather than on improving the processes used to produce today's commodity chemicals in the United States. Commodity chemical production is moving offshore and the processes used in the United States today may not be relevant by 2020.

Barriers: Various barriers hindering the broader application of membranes in the process industry were identified and prioritized according to perceived importance. The key barriers identified are summarized in Table III.E.I. Table C.E.1 in Appendix C includes all barriers cited. The highest priority barriers were: (a) the need for membranes to work in real world situations (robustness in the face of *dirty* process streams); (b) the prohibitive scale-up economics for large process flow applications; (c) the lack of cross-cutting fertilization among technologies and companies; (d) the lack of funds to take the technology from bench to commercial use; and (e) the low energy cost.

Research Needs: The key R&D needs in the membrane area are shown in Table III.E.2. They are described below as topics within the following technical categories: *materials, process systems, predictive modeling.* Participants agreed that there was an urgent need for a critical review of extant chemical processes (both high volume and specialty chemical) as well as potential processes likely to be of importance in the future in order to identify the most fruitful areas of research.

Materials: High priority needs related to developing lower cost membrane materials with higher surface area per unit volume. Other important but lower priority needs included continued development of high temperature (e.g., ceramic, metal) membranes, nanocomposites and chemically inert membrane materials, materials suitable for hydrophilic compounds in dilute streams, and mixed organic/inorganic composite membranes. Focusing efforts away from generalized research on membrane materials and towards more highly focused research on specific materials targeted at carefully defined commercial applications was considered important. Integrating process evaluation and economic analysis with the R&D effort would greatly aid this effort

Process Systems: There was a strong view that efforts should also be aimed at the development and commercialization of membrane process systems using extant membranes. Attention should be focused on the development of integrated membrane systems that can be shown to be robust in "real-world" situations. Other needs that were identified in this area included: overcoming scale-up problems related to contaminants in industrial streams (fouling, oil misting, etc.), the development of scalable low-cost membrane manufacturing techniques, and the development of manufacturing technologies that could reduce the cost of inorganic modules by a factor of ten. Lower tier needs that were cited included (a) improvement of the long-term operability of membrane systems

Table III.E.1 Key Technical Barriers for Membranes
(H= High Priority, M= Medium Priority)

Materials	Process Systems	R&D Climate/ Practices	Government Policy	Other
Inadequate selectivity for hydrogen sulfide and carbon dioxide (M) *High capital cost of robust bi-polar membranes (M)* *Inadequate chemical specificity of membrane (M)* *Lack of in situ healing of membrane defects (M)*	*Membrane systems must fit real world (dirty) conditions (H)* *Existing membranes do not have cost-effective capacity (prohibitive scale-up economics) (H)* *Pervaporation systems/modules are too expensive (M)* *High manufacturing costs for membranes/membrane systems (M)*	*Lack of cross-cutting fertilization among technologies and companies (H)* *Too much focus on materials versus manufacturing technology (M)*	*Cost of energy is too low (H)* *Not enough positive incentives to drive improvements (e.g., investment tax policy not conducive to new technology commercialization) (M)*	*Insufficient funds to take technology from bench to demonstration to commercial scale (H)* *Too much focus on present commodity chemicals versus chemicals likely to be produced in the US in 2020 (H)* *Large risk-aversion to using membranes (M)*

Table III.E.2 Key Research Needs for Membranes
(H= High Priority, M= Medium Priority)

Time-Frame	Materials	Process Systems	Predictive Modeling	Other
All (Ongoing Processes)		*Prove robustness on real streams (H)* *Integrate membrane technology with other processes (M)* *- systems approach tied to another technology* *- target augmenting existing system* *Improve long-term performance (interim products here feed other activities) (M)* *- anti-deterioration* *- schemes for regenerating activity* *- anti-fouling* *- anti-flux decline* *Improve operating efficiency and lower maintenance of existing membrane systems (increase efficiency via maintenance procedures) (M)*		*More thoroughly examine the future chemical industry to tailor membranes to it (M)* *Find high potential applications in specialty chemicals (e.g., pharmaceuticals) and conduct R&D. Apply to "Top 100 Chemicals" (H)*
Near-Term (0-3 Years)	*Cost-effectively increase surface area per unit volume of membrane (H)* *Develop high-temperature membranes (time-frame depends on application) (M)* *- selectivity and throughput* *- pore-size distribution*	*Overcome scale-up difficulties for industrial streams (M)* *- fouling, oil mists, etc.* *Develop better sealing strategies for high temperature & pH balance (M)* *Design automated module assembly (M)*	*Develop process simulation packages for membranes (e.g., hybrid modules) (M)* *- more specific modes* *- generic modules/training modules*	
Mid-Term (3-10 Years)	*Investigate novel material concepts (M)* *- nano-composites* *- chemically resistant properties/ characterizations* *Conduct applications development of ionic membranes in aqueous systems (bipolar) (M)*	*Develop scaleable, low-cost manufacturing techniques (M)* *Step-change in ability to create surface area (M)*		
Long-Term (10+ years)	*Develop new materials for separating hydrophilic compounds from dilute streams (M)* *- covers the entire R&D spectrum*			

with anti-fouling and antiflux-declining schemes, (b) ways to regenerate membrane performance, and (c) lowering membrane maintenance costs. Integrating membrane systems with other technologies to address specific process issues should also be considered.

Predictive Modeling: Participants felt that the development of design and information tools useful for evaluating and optimizing membrane system designs would be valuable in accelerating the development of membrane-based systems; simulation models might also have value as training aids.

R&D Linkages: The key linkages of R&D needs for membranes are shown in Exhibit 1.5. The needs are sorted according to the following categories: *materials, process systems,* and *predictive modeling.* Only those needs that garnered a significant number of votes are shown.

Research Related Needs: Some discussion took place concerning various incentives that might be necessary to encourage more widespread use of membrane systems, recognizing that avoiding the "corporate welfare" label was important. Such incentives would be particularly useful for promoting membranes system use in the production of commodity chemicals where producers are notoriously risk-averse and where production goals may often conflict with environmental stewardship. Thoughts on this issue included: (a) revising the investment tax policy to be more conducive to technologies that have long development cycles and that require substantial and sustained financial support through the commercialization process, (b) developing government incentives that are more "carrot" and less "stick," and (c) finding ways to cross-link the innovation process with other disciplines rather than narrowly targeting and compartmentalizing research activities.

III.F. Separative Reactors

Summary: Separative reactors have elicited much academic interest because of their potential for improving the economics of a number of potentially important processes. However, there are few commercial applications despite the fact that separative reactors offer an elegant technical solution. As such, the technology faces considerable commercialization challenges and must have economics that are far superior to conventional processes.

Principal technology gaps identified were inadequacies in scale-up and simulation capability, lack of validated thermodynamic and kinetic data, and the lack of materials, such as catalysts, with the requisite activity, selectivity, permeability, stability, and other characteristics. The lack of an acceptable methodology for carrying out high-level process syntheses was cited as a somewhat lower priority.

A high priority need is for economic evaluations that will help prioritize R&D efforts and show the potential value of the technology to encourage investment in the long run. New materials—adsorbents, membranes (including molecular sieves) that are stable in harsh environments and high-activity, low-temperature catalysts or catalysts that allow better matching of operating conditions—were also considered to be important research needs. In addition, a number of needs relating to improving design capability were cited as being of high priority.

Current State: A separative reactor is any device that allows a chemical reaction and a separation to occur *simultaneously.* Examples include adsorption and membrane reactors, reactive distillations, and biological reactor systems. Separative reactors are not neatly definable as a specific technology and do not fit into the traditional field of unit operations. Thus, separative reactors are not part of the chemical engineering curriculum. The absence of formal coursework means that their application in industry requires a smoothly working multi-disciplinary team. The simultaneous functioning of two technologies, as in a separative reactor, reduces the degrees of freedom available for successfully developing the application. However, when this is achieved the results are technically elegant, often providing high yields and throughputs, improved economics, and low waste generation.

Although there is significant academic interest in separative reactors because of their potential to have a significant impact on the process economics of a number of important syntheses, the technology is viewed as new and largely unproved. One notable exception is the Eastman Chemicals process for producing methyl acetate.

The main opportunities for separative reactors lie in reducing both capital investment and energy costs. The latter is a longer-term opportunity since, given present US energy costs, energy reduction projects often do not meet the payback criteria that are used by most chemical producers. In addition, separative reactors provide an opportunity for decreasing waste generation as a consequence of increased product yield.

The current state-of-the-art of separative reactor technology is summarized in the monograph (see Appendix D).

Future State: To be competitive with existing technologies and to overcome understandable concerns of corporate management with unproved technology, separative reactors will have to show outstanding economics (probably close to "shut-down" economics) relative to extant technology. Reduced material and energy intensity and a lowered level of pollutant dispersion, as looked at from a full life-cycle perspective, will need to be considered when assessing separative reactors relative to alternative and in-place technologies. Such superior economics probably will not be achieved by simply applying separative reactor technology to improving existing processes. Rather, it will be necessary to: (a) exploit new and more efficient chemical pathways made possible by the use of separative reactors, (b) find uses for separative reactors to improve the subsequent separation steps, and (c) reduce fixed and working capital requirements via a reduction in the number of processing steps to achieve a given transformation.

Targets that were identified for the use of separative reactors were: (a) reduction of waste generation and pollutant dispersion (i.e., reduced net CO_2 production, solvent use, and the release of persistent, bioaccumulating, and toxic materials into the environment, and more efficient waste treatment), and (b) improved process control.

Barriers: Two workshop breakout groups, including representatives from industry, national laboratories, universities, and government, helped identify and prioritize barriers to the use of separative reactors. The prioritized barriers were grouped into three categories *technology gaps, technology transfer, and general.* The key barriers identified are shown in Table III.F. 1, while the complete list of prioritized barriers is provided in Table C.F. 1 in Appendix C.

Technical Gaps: Principal technology gaps identified were (a) inadequacies in scale-up and simulation capability, (b) lack of validated thermodynamic and kinetic data, and (c) the lack of materials, such as catalysts, with the requisite activity, selectivity, permeability, stability, and other characteristics. The lack of an acceptable methodology for carrying out high-level process syntheses was cited as a somewhat lower priority.

Technology Transfer: The group identified the lack of a multi-disciplinary team approach as one of the more significant barriers to commercializing separative reactors. Other technology transfer issues that were considered important were: (a) the application-specific nature of the processes that can be addressed using separative reactors which makes it difficult to transfer the lessons learned from one application to another, and (b) scale-up difficulties stemming from a lack of prior experience and mathematical models to predict performance.

Other: The fact that separative reactors, as a new technology, are likely to be judged by a higher standard than existing technologies was considered to be the most significant barrier in this category. Other lower priority barriers cited included the lack of industrial R&D funding and the physical limitations in matching chemical reactions and the associated separation technology

Research Needs: Research needs were prioritized and grouped into the following categories: *materials, process systems, fundamental data,* and *demonstrate value.* The key R&D needs identified are shown in Table III.F.2 (Table C.F.2 in Appendix C provides a summary of all needs cited) and discussed below.

Demonstrate Value: Economic evaluations are needed to help prioritize R&D efforts and show the potential value of the technology to encourage investment in the long run. Developing several case studies on model reaction systems for important chemical pathways to show the advantages of a separative reactor was believed to be an important undertaking, as was a broadly based systematic evaluation of the interaction between reaction classes and separation technologies.

Materials: New materials—adsorbents, membranes (including molecular sieves) that are stable in harsh environments, and high-activity, low-temperature catalysts or

Table III.F.1 Key Technical Barriers for Separative Reactors
(H= High Priority, M= Medium Priority)

Technical Gaps	Technology Transfer	General
Lack of simulation and scale-up capability (experience, lack of models) (H) *Lack of validated thermodynamic and kinetic data (H)* *Lack of materials (e.g., integrated catalysts) with activity, selectivity, permeability, stability, and manufacturability (H)* *Lack of high-level process synthesis methodology (H)*	*Lack of multi-disciplinary team approaches to process integration (H)* *Lack of commonality of problem because technology is application-specific (M)* *Separative reactors still a science rather than a technology. Lack of demonstration on a reasonable scale (prototype) (M)*	*Must overcome the financial hurdles associated with new technology competing against depreciated in-place equipment ("shut-down economics") (H)* *Lack of R&D resources from industrial community (M)* *Physical limitations to matching chemical reaction and separation technologies (M)*

Table III.F.2 Key Research Needs for Separative Reactors

(H= High priority, M= Medium priority)

Time-Frame	Materials	Process Systems	Demonstrate Value	Fundamental Data
All (Ongoing Processes)	*Perform basic research for new chemical pathways using separative reactors (M)* *Develop new materials; new adsorbents; new membranes; high- activity, low- temperature catalysts (M)* *- more selective* *- able to operate in harsh environments*	*Conduct pilot and industrial scale demonstrations (M)*		*Develop reactive 3-D modeling (M)* *- couple computational fluid dynamics with kinetics* *- user-friendly systems needed*
Near-Term (0-3 Years)		*Develop methods to convert existing equipment to separative reactors (M)*	*Perform broad analysis of possible combinations of reactor types and separation technologies (H)* *- go beyond combinations presently known* *- include separator types, reactor types, chemistry* *Define the potential applications map (H)* *- prioritize key chemical reaction chains* *- define common model reactions* *Develop early stage economic evaluation tools (incorporating full cost accounting) (M)*	
Mid-Term (3-10 Years)	*"Green" technology initiative for pharmaceuticals to deal with solvent use / impact (M)*	*Develop separation devices with wider operating ranges (M)*		
Long-Term (10+ years)	*N/A*	*N/A*	*N/A*	*N/A*

catalysts that allow better matching of operating conditions—were considered to be important research needs.

Fundamental Data: A number of needs relating to improving design capability were cited as being high priority. These are: (a) a well-funded and coordinated program to develop better thermodynamic and kinetic data for key chemical reaction chains, (b) a user-friendly 3-D model that couples computational fluid dynamics with kinetic models, and (c) a better understanding of the interactions between chemical and physical rate processes.

Process Systems: The development of equipment that has improved operating flexibility (wider operating range) was considered a medium-level priority, as was the need for developing methods to convert existing equipment to separative reactors and the need for pilot and industrial scale demonstrations

R&D Linkages: The key linkages of R&D needs for separative reactors are shown in Table I.6, grouped according to the categories used for the research needs. Only those needs that garnered a significant number of votes are shown.

III.G. Ion Exchange

Summary: The most pressing research need in ion exchange is development of new materials. The capacity, selectivity, and specificity of existing ion exchange materials are limitations to increased separations efficiencies for treatment of dilute solutions and bioprocessing. Robust ion exchange resins are needed that can perform well in aqueous and organic media. Improved methods of regeneration are needed. The cost of producing materials must be lower. Innovative ion exchange equipment should be designed for hybrid systems where reactions and separations can occur combined with other separations steps and/or electrically enhanced. Demonstration of commercial feasibility is essential to overcome the natural reluctance of industry to adopt new technology.

The key barriers and major research needs are listed in Tables III.G.1 and III.G.2, while the complete list of prioritized barriers and research needs for each breakout group are provided in Tables C.G.1 and C.G.2 in Appendix C.

Current State: Ion exchange is presently used in several chemical processes to separate ionized molecules, both inorganic and organic, from aqueous solution as well as contaminants from organic streams. They are used in biologically derived processes, such as high fructose corn syrup. Ion exchange has been used industrially for many years, but the use of modern synthetic ion exchange materials has developed during the last half century. During this period, standard cationic and anionic resins with strong acid, weak acid, strong base, and weak base groups achieved success in water softening and other operations that require removal/exchange of ions in dilute solutions. In more recent years, important advances have been made in several directions, especially in the development of new resins that are more selective for specific ions and in the development of new resin materials with shorter diffusion paths and, thus, better exchange rates (mass transfer coefficients). Ion exchange remains a separations technology best suited for use with dilute systems where regeneration is required less frequently.

Future State: The need to remove/recover materials from dilute solutions is expected to increase in the future. Regulations are likely to require removal of more contaminants to lower levels in the future. Growth of biotechnology and pharmaceuticals is likely to drive production of higher purity chemicals. Clean water will likely become a scarcer resource, requiring improved treatment of wastewater. Separations processes are expected to move from mainly physical processes to chemical processes. More processes will be continuous rather than batch operations. Smaller, more flexible separations processes will be needed, and the use of hybrid systems will become standard.

These industrial needs will require more robust, highly selective ion exchangers with higher capacities in the future. Therefore, there will continue to be an effort to develop more selective ion exchange materials. Selectivity allows the resins to be used for longer periods between regeneration cycles, since smaller quantities of other ions are exchanged. It can also result in lower volumes of regeneration solutions and higher concentrations of the target ions in the regeneration solutions, provided efficient regeneration methods can be developed. The concentration of a specific ion on the loaded resin can be greater when more selective resins are used. Highly selective resins will make ion exchange more attractive for environmental applications where there is/are one or few contaminants that can be removed by ion exchange. Recent work on inorganic ion exchange materials with pore size and charge distributions particularly well suited for selective exchange of key ions is one example of the kind of improvements that could be possible. Other examples are the use of imprinted pores in polymers that are particularly suited for specific ions. Another idea that has been explored in recent years is the use of carefully sized pores in silica that can be used as a substrate for ion exchange. The pores can be formed by micelles of surfactants as the silica is produced. With uniform sized pores, the ion exchange groups can be attached to the pore sur-

Table III.G.1 Technical Barriers to Ion Exchange
(H = High Priority, M = Medium Priority, L = Low Priority)

Fundamental Science and Data	Materials	Risk	Cost Issues
Lack of fundamental property data for modeling (M) *Kinetics, thermodynamics (including thermodynamic limits), solubilities, organic/inorganic species* *Mechanical properties*	*Material limitations (H)* *Loading capacity, stability* *Selectivity and specificity, such as separating metals in presence of organics and chelating agents* *Mechanical stability* *Lack of good regeneration methods (M)*	*Perceived high technical risk connected to investing in this technology (M)*	*Capital costs too high (H)*

Table III.G.2 Research Needs for Ion Exchange
(H = High Priority, M = Medium Priority, L = Low Priority)

Time-Frame	Materials	Process Systems	Fundamental Science and Modeling	Demonstrating Feasibility
All (On-going Processes)	*Develop new materials with high selectivity, capacity, and kinetics (H)*	*Integrate materials research and process development (M)*	*Develop improved synthesis chemistry (M)* *Develop improved modeling techniques to design ion exchangers (M)*	
Near-term (0–3 years)	*Develop more and better ion exchange forms and geometries (M)*	*Improve regeneration methods (H)*		*Demonstrate technology on important process streams to promote use of the technology (M)*
Mid-Term (3–10 years)	*Reduce manufacturing cost of ion exchangers (H)*	*Develop nonstandard ion exchange equipment (M)*		
Long-term (10+ years)	*Develop nonconventional ion exchange materials (M)*	*Develop hybrid ion exchange systems (H)*	*Develop advanced molecular modeling tools (M)*	

face on polymers of selected lengths to give the effective pore size desired for removing an ion selectively.

Improvements also involve production of high efficiency (high mass transfer rate) ion exchange materials at nominal or lower costs. There have been developments during the past decade that resulted in more efficient ion exchange materials for use in small-scale chromatography applications. However, these materials are far too costly for use in large-scale operations. In the future, these costs are likely to decline, and ion exchange resin use will begin to penetrate into larger and larger scale operations, but the applications of these materials may remain limited to smaller preparative operations, such as biotech operations, for some time.

A related trend that is likely to occur is the development of very cheap ion exchange materials that can be used for solving environmental problems, perhaps even cheap enough to be used *in situ*. Such materials could be used only once and discarded as a waste material. Unfortunately, to be effective in removing trace contaminants, such materials may have to be quite selective, and only a few such applications may find materials with both sufficiently low cost and selectivity.

Barriers: The principal barrier to further development of ion exchange operations is the fact that the capital costs of ion exchange (like adsorption) scales with a relatively high power of the column size (and, thus, throughput). The cost of the ion exchange material used is almost linearly related to the size of the column. If major reductions are to occur in the cost of ion exchange materials, the scale-factor could be decreased. The cost and difficulty of regeneration of ion exchange materials is another of the most significant problems that discourages use of ion exchange. Normal regeneration could become even more difficult, as more selective ion exchange materials are developed, because the more favourable the loading is, the more difficult it is to induce unloading. The capacity, selectivity, and specificity of existing ion exchange materials are limitations to increased separations efficiencies for treatment of dilute solutions and bioprocessing. Robust ion exchange resins are needed that can perform well, particularly for organic streams.

Research Needs: The future state of ion exchange describes many of the opportunities for advancing ion exchange technology, and research should address those opportunities. Research should address the barriers described above to accelerate beneficial use of ion exchange. The high priority research needs are summarized below.

Materials Development. Development of more selective, higher capacity ion exchange materials that can remove target ions from more concentrated solutions with higher concentrations of other competing ions. Ion exchange will remain more attractive for dilute solutions, but with sufficiently selective ion exchange materials, the term "dilute" may only apply to the concentration of the target ion, not to the total solution concentration. Improved ion exchange kinetics could also result in reduced capital costs on processing equipment.

Development of ion exchange materials with sufficient selectivity for specific contaminants in wastewater and groundwater is needed so that the materials can be used for only a single cycle and in large quantities. Sufficiently cheap ion exchange materials also reduce the problems with scale-up of ion exchange operations since the cost of resin, the cost of which scales linearly with ion exchange column size (and throughput) is often a major contribution to capital costs.

The cost of producing new ion exchange materials, particularly those with extremely high mass transfer rates must be lowered. The costs of these materials need not reach the cost of traditional ion exchange materials for new applications to appear. As the costs come down, the chances of their being used for small-scale preparative operations increases. Further reductions in the costs should result in greater expansion in the use of these innovative materials.

Improved synthesis chemistry and modeling will be required to support development of materials with these capabilities in a timely and cost-effective manner.

The majority of ion exchange operations are carried out in traditional packed columns containing spherical or granular ion exchange materials. Future innovation could involve the use of different shapes of the ion exchange materials but still retain the standard column shape. The new ion exchange materials could even be formed in monoliths somewhat like those being tested for adsorption operations. The shapes of ion exchange materials and the equipment that contain them may often follow innovations in adsorption operations.

Regeneration Methods. More innovative regeneration methods would help the economics of many ion exchange operations. When the ion exchange loading operations are highly selective and, thus, involve a "favorable" loading (effective) isotherm, it is difficult to achieve "favorable" conditions for regeneration using conventional techniques. Alternate regeneration methods should be specific to each application, such as the removal of cations as anion complexes and regeneration with complexant-free water. The improved regeneration method could be specific to the ion exchange material, as with the use of some inorganic materials whose ion exchange capability can be altered by a redox change in the ion exchange material itself. The improvements could come from innovations in the equipment used for ion exchange operations such as the examples of electrically regenerated beds.

New Equipment. Significant improvements in ion exchange operations can also be achieved by the use of innovative equipment. The shapes of ion exchange materials and the equipment that contain them may follow innovations in the more widely studied adsorption operations. Modifications in the equipment could include changes such as the incorporation of electrodes for electrical regeneration and the subsequent preference for flat or annular vessels for ion exchange operations. Ion exchange systems should be designed for use in hybrid systems where reactions and separations occur in one process step and/or where combining technologies could improve resin efficiency (e.g., the capacity of resin could be improved by adding a modulated electric field).

Test Facilities. Demonstration of commercial feasibility is essential to overcome the natural reluctance of industry to adopt new technology.

R&D Linkages: The key linkages of research needs for ion exchange are shown in Table I.7, grouped according to the categories used for the research needs.

III.H. Bioseparations

Summary: Forty-seven chemical processing and separations experts from industry, academia, and government participated in brainstorming sessions to identify future research needed to expand the use of bioprocessing in the chemical and related fields. The brainstorming sessions focused on three feed streams: agricultural crops, forestry products, and all other biomass. There are many examples of cross-cutting themes

among the high priority research areas identified by the three groups. These include development of robust biocatalysts; development of better separations technologies with emphasis on membranes, extractants, adsorbents and hybrid systems; obtaining physical property data; predictive models; pursuing in vitro synthesis; and development of closed-loop fermentation processes. The most important research need in the bioprocessing separations for agricultural crops is the development of new separations techniques for dilute products in the raw crop or fermentation broth. The type of solids and the large volumes of water make it difficult to design effective separations techniques. There is a need to develop facilitated-transport membranes and highly selective adsorbents. The two greatest specific needs for all other biomass are for development of new membrane technologies and closed-loop fermentation processes. The top forestry product needs are obtaining measurements data and predictive methods for physical properties, and developing new separations techniques for dilute streams. Among the most important challenges are lack of specificity in current separations technologies, reducing the overall number of required separation steps, emissions recovery/elimination, and inability to utilize closed-loop processing. The key barriers and major research needs are listed in Tables III.H.1 and III.H.2, while the complete list of prioritized barriers and research needs for each breakout group are provided in Tables C.H.1 through C.H.6 in Appendix C.

In addition to improving separations, enhancing biocatalysts or developing crops to produce higher levels of desired product would decrease energy use, reduce carbon dioxide emissions, and make separations easier.

Current State: Transitional bioprocessing industries are using unit operations developed for non-biological systems to a large extent—distillation, adsorption, extraction, crystallization, and chromatography. These processes have been adapted for use in industry, but there has been no major effort to develop separations processes unique to biochemicals. This has resulted in separations processes, associated with a wide variety of bioprocessing streams, that make product recovery/purification expensive. New separations processes specifically designed for bioseparations will be needed for the future.

The agricultural crops that are prevalent now or are likely to be prevalent in the next twenty years were divided into eight categories. Some of the feed streams were raw feed streams and others were streams collected from an earlier processing step or as a waste from processing. Each of these feed streams has its set of separation challenges. The categories are:

- Low concentrations of high-value products in a large volume: crops, engineered or natural, with trace elements (e.g., 1–10% of bulk, or <0.1% for really high value) of high-value chemical, e.g., a drug or antibody chemicals in an engineered crop. The solubility of the compound in water or other solvent is going to be an important factor in the separations. The temperature at which separations take place will be near ambient. The remainder of the unused feedstock may (or must) be used for other processing. The volume of this high-value stream may be small, due to the many alternative ways that these compounds can be created.
- High concentrations of lower-value products. Plant-derived, hydrophobic (C_{10}–C_{100}) compounds present in plants. These may be liquids or solids for fuels, lubricants, and additives to paint and varnishes. Sources of feed stock may be soybeans, oil seeds, or other crops. These compounds are generally stable at high pH and moderately high temperature and the crop itself will not contain much salt. The volume of these products may in the future demand production in the range of 100 billion lb/year.
- Crops, engineered or natural, that produce a structural component (e.g., fiber, protein, natural rubber, or polymer). The concentrations in the crop may be as high as 10–50% of the target plant component. Temperature stability of these products is likely to be good. It was anticipated that a large volume of these materials might be needed in the future.
- Biomass as a carbohydrate source for further processing, e.g., fermentation and gasification. The stream may be a starch (or cellulose) -based solid or be a slurry in water. The streams were anticipated to be at ambient temperature, be near neutral pH, have some salt content, and be processed at a very high volume. Some activities can result in the fermentation broth being the major stream that will need enhanced separations. Lignin is usually a waste and is high in phenolics. This is a stream that may be useful for gasification or power generation. Other biomass streams include silage and water-based plants.
- Ash from inorganic components in plants. Depending on the processing of plants, ash may accumulate as an undesirable byproduct or waste stream. Potentially 2–10% of some crops contain ash. An example of this is silica in rice.
- Processing residuals (fiber) further that result from grain processing was listed as a separate category, and a lot of this type of product is used for animal feed, but may potentially have additional value.

Table III.H.1 Key Technical Barriers for Bioseparations
(H = High Priority, M = Medium Priority)

Process Design/ Control	Separations	Economic/ Institutional/ Regulatory	Fundamental Understanding	Feedstock
Inability to have closed-loop systems (M) *Lack of on-line, real-time sensors and controls (M)*	*Difficulty separating desired products from others with similar composition and achieving high purity. (H)* *Difficulty separating components from dilute fermentation broth. (H)* *Reaching high purity without conventional methods (e.g., distillation, crystallization). (H)* *Difficulty removing water from the feed and in the process (high water use requirement). (H)* *High costs of solids handling compared to liquid handling (most bio-separations involve a solid-liquid separations). (H)* *Lack of specificity for current separation technologies. (H)* *Product inhibition and low fermentation productivity. (H)* *Too many purification steps for current processes. (M)* *Difficult product removal from water. (M)* *Separation of commodity chemicals from green plants is not well developed. (M)* *Lack of technologies to separate salt from the component you are interested in. (M)*	*Cost and risk of process research is high and uncertain (i.e., Who will do the research?). (H)* *Lack of effective CO_2 recovery/emissions technologies. (M)*	*Lack of accessibility of physical properties for biologically derived chemicals (e.g., critical tables, solubility, distribution coefficients, mathematical models). (H)* *Lack of understanding of how to design efficient biocatalysts. (H)* *Lack of ability to make adequate membranes. (H)* *Lack of process modeling capabilities. (M)*	*Difficulty fractionating multi-component feeds. (M)* *Variability of feed stocks. (M)* *Rapid characterization of feedstocks (M)*

The biomass streams which are prevalent now and are likely to be prevalent in the next twenty years include, among others, fermentations (microbial, plant, and mammalian), pre-digested biomass, biosolids/sludge, food processing waste, plant streams for chemical production, municipal solid waste, and food animal wastes. Bioprocessing streams that were analyzed included fermentation streams, predigested biomass, food processing wastes, food animal wastes, and others likely to be relevant in the future (these are listed in Table A.1).

Several forestry streams were considered for bioseparations that range between 1 million lb/year to about 1 billion lb/year (see Table A.2). Most of the streams listed are liquids that contain salts, lignin or other dissolved solids. These liquids must be processed to make them acceptable as waste streams for disposal or treated to isolate fractions that are either difficult to handle as waste or that have a high value. Taxol, an anticancer chemical, is a good example of the latter situation. A major exception to the notion of liquid waste streams is "hogfuel." Hogfuel is the sum of all the scrap material produced when a tree is prepared for pulping or timber production. This includes side-branches, leaves, needles and cones, and bark that is pressurized or scraped off the trunk. Hogfuel is presently burned simply for its BTU value.

Future State: The market for new products replacing or augmenting current products of the petroleum industry is uncertain but there was a general agreement that the bioprocessing industry will become an important factor in the future as oil reserves are depleted. Bioprocessing is an expanding area and many new types of streams are likely to be more common by the Year 2020. As major technical advances are made, new and/or more economical process options will become viable alternatives to existing processes. Tighter regulations will also strongly impact the types of unit operations used for product recovery. Future streams, which are likely to be even more common in Year 2020, include:

- Fermentation processes. Included in this category would be streams resulting from the use of microbial, plant, and mammalian cells. Genetically engineered organisms will make this an expanding area as new and existing commodity chemicals are produced in this manner. Recent advances with extremophilic organisms (e.g., thermophiles,

Table III.H.2 Key Research Needs for Bioseparations

(H = High Priority, M = Medium Priority)

Time - Frame	New Bioprocessing Technologies	New Separations Technologies	Fundamental Data	Process Design	Equipment Design
All (Ongoing)	*Develop robust biocatalysts not inhibited by by-products or pH.*		*Develop fundamental property data. (H)*		*Develop means to control viral contamination. (M)*
Near Term (0-3 Years)	*Genetically engineer extremophiles (M)*	*Develop high temperature composite membranes. (M)* *Design better molecule configuration in membranes for fouling abatement. (M)*	*Develop computational techniques for predicting candidates for solvent screening. (M)* *Develop simple models for bioseparation processes, including economic models. (M)*		*Carefully characterize capabilities of mass transfer equipment for biological feed stock. (M)* *Develop new line of sensors and analytical techniques that are robust for bioprocesses. (M)*
Mid-Term (3-10 Years)	*Pursue genetic engineering of feed stocks to optimize bio-processing. (M)*	*Develop facilitated transport membranes to separate "like" molecules. (H)* *Develop membrane adsorbent materials (H)* *- Ionic liquids* *- Solid polymeric* *Develop smart membranes and separations systems for low concentration / high value products. (H)* *Develop better membranes for selective chemical separations. (M)* *Develop highly selective adsorbents/ desorbents. (H)* *Develop methods for better water purification and reuse, with emphasis on zero discharge. (H)* *Develop new extractants. (M)* *Remove interfering molecules prior to using traditional chemical separation. (M)* *Combine membranes and ion exchange chromatography for processing under extreme conditions. (M)* *Develop direct separations methods from fermentation broth to product (M)*	*Develop predictive methods for physical properties. (H)* *Develop comprehensive physical property database. (M)*	*Develop hybrid reactors for simultaneous separations. (M)* *Pursue in vitro synthesis/ processing (H)* *Develop process to recover narrow molecular weight ranges (M)*	*Develop equipment for closed-loop fermentation processes (H)* *Design a wider range of better process separations equipment for solids handling. (M)*
Long-Term (10+ Years)		*Develop new molecular recognition techniques for separations of dilute streams, including high efficiency separations. (H)* *Develop processes for selective fractionation. (M)* *Develop low-energy dehydration systems to remove water. (M)*			

halophiles, and acidophiles) promise radically different production techniques. These changes are likely to impact downstream processing significantly by Year 2020.

- Closed-loop systems. Industry can and should move toward closed-loop systems to reduce emissions and conserve potential resources where possible. The constraints placed upon separation of bioprocessing streams are likely to change as this goal is pursued.
- Predigested biomass (e.g., manure)
- Sludge (biosolids)
- Food processing waste (green-plant wastes)
- Food animal wastes
- Plant streams for chemical production and phytoremediation
- Municipal solid waste
- Marine Biomass
- Natural Fibers

Possible future separations processes targeted to bioprocessing chemicals are:

- Absorption
- Adsorption
- Chemi-osmotic
- Chromatography
- Completely new separations technology
- Crystallization
- Distillation (mature)
- Electrochemical processes
- Electrodialysis
- Extraction
- Facilitated transport
- Membranes

Two future paths were recognized for the industry: (a) continue to produce the traditional products (lumber, pulp, paper, etc.) with some genetic engineering to improve these products, and (b) modify the feedstock genetically to make the processing of pulp easier. In the first case, the result could be with waste from lumber, for example, that the handling of that waste might be more difficult. The second path of genetic modification of feedstock (i.e., the trees) is the more technologically challenging of the two paths.

Barriers: The top five barriers are: difficulty in separating product from similar components, difficulty in separating product from dilute solutions, lack of needed physical properties for biologically derived chemicals, lack of ability to make adequate membranes, and product inhibition and low fermentation productivity. The key barriers identified for each feed stream are given in Appendix C and are summarized below.

Agricultural Crops

Separations. The greatest challenge is the low concentrations of some products in the crop itself or in fermentation broth. In many cases, the separations process should yield a high purity product. High purity might be difficult to achieve without the use of conventional methods such as distillation and crystallization. The difficulty of separating the large amount of water present in the crop or fermentation broth is a barrier. Drying crops is common to reduce transportation cost to processing plants. However, processing requires the addition of water that later must be separated or efficiently and economically recycled. Another barrier to effective separations is that the bioprocessing area involves solids processing and solid/liquid separation steps, which are traditionally costly.

Chemical and Biological. Product inhibition could be overcome and fermentation productivity greatly increased, the product concentration would be much higher. This, in turn, would ease downstream product separation. Large cost savings are likely to be realized if these barriers can be overcome.

Economics. Cost and technical risks for research in the processing (e.g., separations) are high. Even if the energy requirement for separations is high, the current cost for energy is low. It is hard for the bioprocessing industry to compete with the petroleum industry with identical products, since the true cost for the petroleum industry to produce that product is not known.

Fundamental Research. There is a lack of fundamental data such as critical tables, solubility data, phase distribution coefficient data, etc. for biologically derived products such as carbohydrates and proteins. It is difficult to do theoretical evaluations of separations techniques and to develop reliable designs. Much of the work is trial and error. Instrumentation to monitor many biological products is lacking.

Feedstock. The most significant barrier to effective separations of desired multi-products directly from the feedstock is the ability to fractionate. Many of the products are present in the entire plant and initial fractionation is difficult.

All Other Biomass

Product Extraction and Recovery. Lack of specificity is the key barrier facing modern fermentation bioprocessing—product removal from aqueous solutions is often difficult and may require several successive stages or multiple unit operations to achieve the desired purity and/or concentration. Separation of chemical products from plant sources is not well developed; co-product separation is likewise poor. Physical separation of materials in green-plant processing has not been optimized, and there are few examples of efficient small-scale green-plant separations. For predigested biomass streams, lack of technologies for efficient product removal from solid-phase fermentation is a key barrier.

Process Design and Control. The lack of economical closed-loop systems is a major barrier, particularly for fermentation streams. Lack of continuous fermentation processes (versus batch and fed-batch operations) in current operations is a barrier; these have the potential for increasing yields significantly if they can be implemented successfully. The lack of thermo-physical property data is a cross-cutting barrier affecting the development of separations processes for a variety of stream types.

Emissions. Recovery of carbon dioxide, a greenhouse gas, is a barrier, along with nitrogen, phosphorus, and potassium separation from certain process streams. Industries that generate noxious odors during bioprocessing will also have to develop new methods or improve existing ones for cleaning polluted air streams as air quality restrictions tighten.

Forestry Products

Feedstock. Feedstock variability for bioprocesses leads to decreased yields and significantly more complex waste streams; downstream processing can be simplified considerably by better substrate selection or feed stream purification. Non-localization of desired products in plant tissues is a barrier (one unique to green plants)—if a given product were expressed in only one plant part (e.g. leaves, roots, bark), separation could be simplified considerably.

Trees are an inherently wasteful raw material. They represent 50% wasted raw material because of their shape, bark mass, side-branches, etc. Waste material, trimmed from trees before they can be processed, is routinely used for low-quality fuel value. If a tree can be genetically modified to have a lower percentage of bark or grown with squarer cross-section than is true for trees today, the yield of pulp or lumber per unit mass of tree would be higher. Such modifications have implications for the inherent mechanical stability of the tree but the ability to produce such altered shapes and structures would lead to a dramatic reconfiguration of the mass and energy utilization of the industry.

Fundamental Knowledge. Barriers relate to inadequacies in knowledge, processing materials or systems, data for key properties, and new ways to run reactions and processes. The most critical barriers are inadequate knowledge to allow development of membranes with desirable qualities, inefficient biocatalysts, and lack of physical properties data.

Processing. Processing barriers relate to the design of processing schemes including the handling of difficult separations, dilute solutions, high salts, etc. The primary barrier is difficulty of achieving separations from dilute solutions.

Cross-cutting. Cross-cutting barriers include lack of on-line real-time sensors and controls, and lack of the capability to model processes.

Research Needs: High priority research needs include robust biocatalysts; better separations technologies with emphasis on membranes, extractants, adsorbents and hybrid systems; physical properties data; predictive models; *in vitro* synthesis; and development of closed-loop fermentation processes. High priority research needs for each feed stream are given in Appendix C and are discussed below.

Agricultural Crops

Improvements in Existing Separations Techniques. There is a need to characterize and study the performance of traditional mass and heat transfer equipment not specifically designed for processing of biological feedstock. There is a need for heat and mass transfer data to be determined for equipment. Another important area is equipment design for separations of liquids from solids. Improvements needed are sorbents with higher selectivity and capability, easier regeneration procedures, and membranes with improved flux and decreased fouling.

New Separations Techniques. The most pressing research needs are new separations techniques: membranes, sorbents, and dehydration processes. Future membrane should be directed toward facilitated membranes and the fundamental understanding of natural membrane to create such membranes. The development of new adsorbents/sorbents for bioprocessing applications is needed. Techniques for low-energy-consumption dehydration methods are also needed.

Fundamental Knowledge Base. Research is needed to construct computational models for prediction of physical and chemical properties of biological chemicals; experimental property data were also rated as important research goals. The data can be used for predicting the performance of candidate solvents for extraction and to build a property database. Fundamental research in the area of how to make carbohydrates into useful chemical building blocks is a need.

Process Design. Research is needed to address separations difficulties in fermentation and to develop hybrid reactors for simultaneous separations.

There is a need to develop robust biocatalysts that are not inhibited by by-products, concentration, or pH, and to develop new catalysts (biological or conventional) to achieve higher yields. Achieving these goals aids separations cost-reduction efforts that are now dealing with higher product concentrations. More robust industrially viable microorganisms (other than *E. coli*) are needed. These microorganisms should have properties that would make them easy to process, that is, to separate. This must be a multi-disciplinary effort to develop and characterize the organism on the most fundamental level.

Research in Waste Management. The importance of water in bioprocessing is high, e.g., the need for better water reuse and purification and moving toward zero discharge. Research is also needed in the area of by-product utilization for energy generation on small scales.

All Other Biomass

Materials Development. Development of high selectivity, high capacity separations materials, particularly for adsorbent membranes, is a key research area. Tailored molecular design of adsorbents should be emphasized.

Fundamental Data. Several types of basic work in the biological and biochemical sciences will lead to more efficient separations processes. *In vitro* chemical synthesis (using enzymes or multi-enzyme processes to replace whole cell fermentations) is the highest priority research need in this category. This technology would obviate complex feed streams and make downstream separations much simpler. Synthesis of narrow molecular weight ranges (through genetic engineering or adaptation), localization of products in specific plant tissues, and modifying cells to package new products/chemicals is also a priority research area.

Equipment Design. There is a need for closed-loop fermentation process equipment, as well as equipment to eliminate multiple separations steps in going from the stream to the isolated compound. Separative reactors are precursors for this process goal, particularly in non-membrane areas that are poorly developed. Technologies for detecting and controlling viral contamination (e.g. prions) are needed, being virtually absent from modern day processing.

Closed-loop systems need to be in place by 2020. Research and development needs associated with closed loop bioprocessing include water reclamation and reuse, as well as recycling of nitrogen, phosphorous, and solid biomass. Product recovery during fermentation and biocatalyst immobilization are research areas for further exploration.

Development of an accessible physical property database that includes a variety of thermo-physical data is needed. In particular, data are needed for enzymes and enzyme/substrate interactions. Better understanding of mass transfer characteristics can be realized through advances in computational fluid dynamics.

Novel Separations Needs. In many cases, traditional chemical separations techniques can be used to separate a product if one or two interfering co-products could first be removed. Methods are needed for accomplishing this type of removal, as well as those for fractionating components more selectively. By 2020, engineered/modified materials may require new separations technologies to handle them, particularly as applied to plant tissues. Better methods for separating chiral molecules from racemic mixtures and techniques for large-scale separation of enzymes/macromolecules are also required.

Forestry Products

Feedstock. Genetic modification of trees can produce a more desirable result. These ideas include tree modification to have a squarer cross-section, to utilize the sap instead of destroying the whole tree, to make the tree into a metabolic factory for the desired chemicals, to understand and take advantage of the natural variation of lignin among different tree varieties, to understand the effect of tree growth on the crystallinity of cellulose, and to achieve better separation of sugars from the tree. A high priority is genetic engineering of trees and a better understanding of the factors determining cellulose crystallinity.

Fundamental Knowledge. Forestry products is deficient in both critical property data and models that will serve to predict processing and reaction behavior based on physical property measurements. There are numerous databases and modeling needs that, if met, would aid the researcher in predicting the composition of various streams, screen for high value components, and deal with the inherent variability of the feedstock. Of these various needs, measurements of and predictive methods for physical properties is the highest priority.

Better Membranes. Better membranes are needed for selective separations of certain components, handling dilute solutions, dealing with extreme conditions of temperature, and coping with fouling. Of these ideas, improved membranes for selective separation of dilute solutions and/or those containing high value components is the most important.

Molecular Recognition for Separations. There are needs related to the ability of an adsorbent or adsorption system to recognize molecular structure especially from dilute solutions. This is a key to achieving greater selectivity and probably capacity as well. This need, when met, will result in large savings in energy usage.

Better Biocatalysts. Enzymes are needed that are more efficient, selective, longer lasting, and more stable. Other biocatalyst ideas concern better cellulase expression, directed evolution, genetic engineering of extremophiles, and better degradation of lignin. Genetic engineering of extremophiles is the highest priority**.**

Processing. There are many research needs concerned with improved processing. These range from processes using membranes, ion exchange materials, sensors and controls, fermenters, enzyme recovery, "smart" bioreactors, and dilute solutions to avoid mixing problems. Process needs related to combination of membranes and ion exchange chromatography under extreme conditions is a top priority.

R&D Linkages: The key linkages of research needs for bioseparations are shown in Table I.8, grouped according to the categories used for the research needs.

III.I. Separations from Dilute Solutions

Summary: Twenty-eight chemical processing and separations experts from industry, academia, and government participated in brainstorming sessions to identify future research needed to improve separations from dilute solutions. The brainstorming sessions focused on three types of feed streams: ionic species from aqueous streams, organics from aqueous streams, and contaminants from organic streams. For the purpose of this roadmap, a dilute solution is defined as a liquid containing species present in concentrations of one weight percent or less. For ionic species in aqueous streams this involves only dissolved species in the aqueous phase. Complicating factors such as the presence of minute quantities of organics, chelated species, and phase changes are also included.

There are many examples of cross-cutting themes among the high priority research areas identified by the three groups. These include improved understanding of physical phenomena and intermolecular chemistry, enhanced physical property databases, better predictive modeling tools, and improved separations technologies including hybrid systems. The high priority research needs for ion species from aqueous streams include the development of new computer models, compilation of improved databases, development of improved separations materials, and development of complexation chemistry for better selectivity and to reduce neutralization requirements. The research needs identified for organics from aqueous streams include a better understanding of computational chemistry, developing engineered forms of new separating agents, and developing hybrid processes, such as complexation filtration, magnetic filtration, field-induced filtration, and reactive extraction. The research needs for removing contaminants from organic streams include fundamental understanding of molecular interactions, particularly for non-covalent structures; better understanding of how the physics of separations interact with the physics of separations equipment; and development of properties and performance databases.

The key barriers and major research needs are listed in Tables III.I.1 and III.I.2, while the complete list of prioritized barriers and research needs for each breakout group are in Tables C.I.1 through C.I.6 in Appendix C.

Current State: Separations processes are widely used to remove small quantities of high-value materials or contaminants from dilute aqueous and organic streams. Separations from dilute solutions are unique in several respects. Very small volumes of materials are generally being recovered or removed from very large volumes of liquids. The value of the recovered materials is often very low, making the requirement to find economic separations processes uniquely challenging.

Ion Species from Aqueous Streams

Many processes currently wash materials, products, other streams, equipment, etc. with water. Washing generates the typical streams discussed here. Other processes that generate dilute, ionic species that must be separated from the aqueous medium for various reasons include: neutralization, batch processing, synthesis, reactions, catalyst neutralization, gas scrubbing, metals processing, and corrosion. Besides the generation of these streams that need to be "purified" for regulatory reasons, there are streams that need to be purified prior to being used in an operation. Examples beyond the chemical industry include the semiconductor industry, the pharmaceutical industry, and the biotech/medical industry. These industries must purify streams on-site, because the transfer/transport of highly purified aqueous streams is fraught with complications. Examples of these streams include:

- Oily wastewaters that contain dilute dissolved metals. These are aqueous streams, with organic traces and dissolved ionic species. Often the metals are bound up or chelated.
- Spent wash water.
- Byproducts from reactions.
- Caustic scrubber blow-down.
- Streams with dilute metal species.
- Circuit manufacturing waste.
- Purified feed streams for semiconductor, biotech, pharmaceutical, and medical industries.

The separative treatment options currently used to reduce/remove dilute, ionic species from an aqueous medium include: reverse osmosis, electrodialysis, solvent extraction, adsorption, ion exchange, precipitation, chromatography, and ultra-, nano-, and microfiltration. These processes are all currently used in industry. Some, such as

Table III.I.1 Key Technical Barriers to Separations from Dilute Solutions
(H = High priority, M = Medium priority)

Fundamental Science and Data	Constraints on Current Processes	Implementation and Evolution	Institutional/Educational
Materials limitations (H) *Temperature range, corrosion resistance, other mechanical properties* *Loading capacity, stability* *Selectivity and specificity, such as separating metals in presence of organics and chelating agents* *Management of interfacial phenomena (H)* *Lack of fundamental data properties for modeling (M)* *Kinetics, thermodynamics (including thermodynamic limits), solubilities, organic/ inorganic species* *Mechanical properties* *Lack of molecular level prediction and control of material synthesis for new separations technologies (M)* *Lack of an integrated "basics" approach to treatment of dilute solutions (M)* *Molecular* *Engineering* *Ecosystem*	*Low value per gallon, high cost to handle dilute streams (M)* *Lack of processing capabilities for treatment of multiple components in dilute streams (M)* *Inadequate sensing technologies for on-line, real-time monitoring/control (M)* *Lack of accurate predictive tools (M)* *Lack of economic methods to recover solutes from dilute solutions (M)*	*Cost and time of going to pilot scale testing (H)*	*Lack of funding for frontier R&D (M)* *Short-term results mentality* *Public perception (M)*

reverse osmosis and electrodialysis, are not limited to use on dilute streams, while others, such as ultra-, nano-, and micro-filtration, are used exclusively to separate dilute species from solution.

Organics from Aqueous Streams

Organics in aqueous streams are separated into two sub-groups:

- high activity hydrophobic streams, and
- low activity hydrophilic streams.

Examples of hydrophobic organic streams include hexane (paraffins), benzene (aromatics), trichloroethane, naphthalene, gasoline, and lube oil. Examples of hydrophilic organic streams include formaldehyde, ethylene glycol, low molecular weight alcohols, sugars, low molecular weight organic acids, and acetone.

Current separations processes used to remove organics from aqueous streams include activated carbon adsorption, crystallization, steam stripping, air or gas stripping, evaporation, membranes, biotreatment, solvent extraction, ion exchange for organic acids, distillation, incineration, supercritical extraction, precipitation, catalysis, chromatography, decantation, filtration, centrifugation, flotation, and absorption.

Contaminants from Organic Streams

Typical organic streams containing contaminants needing removal include:

- Petroleum streams contaminated with sulfur. Current sulfur limits vary from state to state, but are typically between 100 and 200 parts per million.
- Pharmaceutical streams containing one percent contaminants in various organic solvents (e.g., raw materials, reaction byproducts, poly-aromatics in methanol).
- Organic separations. High purity requirements of certain organic products, such as ethylene at 99.99 percent purity, make separations costs higher.
- Water removal from organic media.
- Solvent recycle. Examples include engine oil, acetone-based cleansers, and pharmaceutical streams.

Table III.I.2 Key Research Needs for Separations from Dilute Solutions
(H = High Priority, M = Medium Priority)

Time-Frame	Chemistry and Data	Design and Modeling	Materials and Equipment	Processing
Near-term (0–3 years)	*Compile improved property and performance databases (H)* *Speciation* *Near-critical fluids* *Alternative solvents and solutes* *Kinetics* *Thermodynamics* *Solubilities* *Mechanical properties* *Multi-component mixtures* *New ways to gather experimental data* *Understand molecular interactions (H)* *Understand interaction of physics of separations and equipment (H)* *Understand what happens at the surface of membranes to reduce fouling (M)*	*Develop improved computer models (H)* *Predictive solution behavior* *Speciation* *Fluid mechanics (transport phenomena)* *Design of extractants* *Precipitation* *Kinetics* *Design of systems, specifically hybrid systems* *Measure of confidence* *Computational chemistry for strong interactions*	*Immobilization of separating agents (H)*	*Develop hybrid systems for dilute solutions treatment (H)* *Complexation filtration* *Magnetic filtration* *Field-induced filtration* *Magnetic* *Electric* *Microwave* *Reactive extraction* *Sonic* *Switchable ligands*
Mid-Term (3–10 years)	*Develop complexation chemistry (H)* *For selectivity* *To reduce neutralization requirements* *Develop better understanding of intermolecular interactions (H)* *Develop fast ion phase transfer chemistry (M)*	*Develop clear design evaluation methodology (M)* *Reliable control strategy for reversible reactions* *Hybrid systems*	*Develop improved materials (H)* *Selectivity* *Operational conditions* *Robust catalysts* *Robust ion exchange resins for organics* *Tailored adsorbents for multi-component systems* *Increased lifetime* *Materials that stay in one phase* *Establish dedicated pilot-plant facilities (H)* *Develop robust instrumentation(M)* *Real-time, on-line control systems* *Analytical tools, including organic phases*	*Develop thermodynamically efficient energy transfer (M)* *Increase testing of non-traditional processes in plants (M)*
Long-term (10+ years)	*Understand interfacial phenomena for membrane absorbents (M)*			

- Biologically derived organic streams, such as high fructose corn syrup. Separations processes for these streams typically include removal of odors, flavors, and colors in the range of parts per billion or lower.

Several separations processes are used to remove contaminants from organic streams. These include: ion exchange (e.g., high fructose corn syrup), catalytic reaction, absorption (e.g., solid fixed bed), leaching, melt crystallization (e.g., separating isomers of materials from an organic-based medium), solution crystallization (e.g., precipitation processes), and filtration.

Future State: The need to remove/recover materials from dilute solutions is expected to be as big or bigger problem in the future as the one we face today. Regulations are likely to require removal of more contaminants to lower levels in the future. Growth of biotechnology and pharmaceuticals is likely to drive production of higher purity chemicals. Clean water will likely become a scarcer resource, requiring improved treatment of wastewater. Separations processes are expected to move from mainly physical processes to chemical processes. Smaller, more flexible separations processes will be needed, and the use of hybrid systems will become standard. More processes will be continuous rather than batch operations. The economics of recovery remains a major barrier for implementation of new separations processes because the value of many of the materials being recovered is expected to remain important.

By 2020, the feed and waste streams for separations processes are not expected to change significantly. What will change are the needs to (a) purify to a greater degree, (b) purify faster, (c) separate a greater variety of species, (d) reduce the volumes of secondary waste, (e) increase capacity/selectivity, and (f) reduce costs. Drivers for these requirements/goals will be tighter regulations, more complicated products and more complicated processes to produce these products, and increased site capacities.

Barriers: The top three barriers are materials limitations, management of interfacial phenomena, and cost and time required for pilot-plant testing of new processes. Materials limitations include lack of mechanical properties, such as temperature range, corrosion resistance, and stability; low loading capacities; and low selectivity and specificity, such as separating metals in the presence of organics and chelating agents. The key barriers identified for each feed stream are given in Appendix C and are summarized below in priority order.

Ion Species from Aqueous Streams

Fundamental Science and Data. The lack of fundamental materials data (kinetic, thermodynamic, physical, and mechanical properties) is a high priority barrier to implementing new separations technologies. These data are the basis of all computerized modeling; and while the modeling itself is important, the data that feed the models are also extremely important. Extension of these properties to multi-component solutions is also in need of development. Physical limitations of materials (used in equipment and processing) such as temperature sensitivity, corrosion resistance, and material strength/flexibility are barriers in that they cause the generation of more dilute waste and/or limit processing abilities. The capacity, selectivity, and specificity of separations materials used in adsorption, ion exchange, precipitation, and solvent extraction processes (among others) are limitations to increased separations efficiency. We have a limited molecular understanding of and ability to remove chelated/organically bound ions from solution; these limitations need to be "pushed." Computer methods for quantitatively screening process alternatives are in need of improvement. There is a need for advanced analytical equipment to more accurately and quickly identify and measure the concentration of species in solution. Highly hydrated ions require faster separations techniques to complete the separations more efficiently.

Constraints on Current Processes. The highest priority barrier or constraint on current processing is the large volumes (thus high cost) of handling dilute streams. An efficient technique for concentrating these streams, or using less volume initially, is needed. Generally, there are more treatment options available when treating a more concentrated stream; and while those options may not reduce the ionic species to the desired concentration, a more refined separations technique on the end of the process would then be handling significantly reduced volumes. Other current process barriers include: (a) residence times in contactors are too long, and (b) lack of options to replace neutralization. A lack of ways to deal with counter ions is a significant barrier. Many current processes use huge amounts of water and thus generate huge dilute aqueous waste streams. Economically viable ways of removing water and incentives for reducing water usage are needed. Blinding of separation media by hydrophobic organics is a problem for some processes. Phase changes occur sometimes when using various separations techniques; foaming, gels, and precipitates are formed during some separation processes and are particularly difficult to deal with.

Implementation and Evolution. The most significant barrier is the lack of effort/time/funding going to the development of new technologies for separations. Included is the extreme cost and time associated with going from bench to pilot scale testing, and the higher cost of going from an existing process to a new and improved process. Technology development that does not have an immediate benefit or cost recovery is a stumbling block.

Organics from Aqueous Streams

Fundamental Science and Data. The top barrier for removing organics from aqueous streams is the lack of understanding and ability to manage interfacial phenomena. This is a high priority for extraction and is discussed in more detail in Section III.D. "Inaccurate predictive tools" is a top priority barrier for removal of organics as well as ionic species from aqueous streams.

Constraints on Current Processes. The inability to design mass separating agents quickly is a high priority barrier. The areas requiring improvements are discussed in more detail above under "Ionic Species from Aqueous Solutions."

Implementation and Evolution. The highest priority barrier for implementation and evolution of new separations processes is the present lack of scale-up methods. Included in this barrier is the extreme cost and time associated with going from bench to pilot scale testing, and the higher cost of going from an existing process to a new and improved process.

Contaminants from Organic Streams

Fundamental Science and Data. The top barrier for removing contaminants from organic solutions is lack of understanding of the basic fundamental processes involved in the processes at the molecular, engineering, and ecosystem levels. A medium priority barrier is lack of better understanding at the molecular level how to control material synthesis.

Constraints on Current Processes. A top barrier for removing contaminants from organic solutions is the limitations of existing materials used in separations processes. Materials with better stability and separations performance are needed. Better methods of characterizing these materials are also needed. A medium priority barrier is the lack of capability to predict the performance of new separations technologies based on molecular-level data.

Implementation and Evolution. Lack of understanding and being able to predict scale-up of separations processes is one of the largest barriers to implementation of new separations processes. The ability to obtain or predict the important engineering principles for equipment design for new feed streams is very limited. Sensors are needed for on-line monitoring and control. An institutional barrier that prohibits use of new, improved processes is the industrial focus on short-term goals over long-term needs.

Research Needs: High priority research needs include understanding of physical phenomena and intermolecular chemistry, enhanced physical property databases, better predictive modeling tools, and improved technologies including hybrid systems. High priority research needs for each feed stream are given in Appendix C and are discussed below in priority order.

Ion Species from Aqueous Streams

Chemistry and Data. A high priority need is the development of complexation chemistry to increase the selectivity and specificity of separation materials. Development and compilation of materials' data and incorporation into freely accessible databases are also top priorities. This data should include speciation data and multi-component properties data. The development of fast ion phase transfer chemistry is of medium priority.

Design and Modeling. The highest priority need is to develop improved computer models for predictive solution behavior; speciation, transport phenomena, kinetics, phase change, and confidence measure predictions; and the design of extractants and various process systems. The development of clearer design evaluation technology is of medium priority.

Materials and Equipment. Development of improved materials for separations applications is a high priority. Examples of improvements include increased selectivity and capacity; increased resistance to attrition and therefore longer-lived, more robust materials; and materials able to be used in a wider variety of conditions. Funding and operation of pilot-plant facilities is a high priority need. Non-traditional facilities should be mobile and available to various institutions as user facilities.

Processing. Development of new non-traditional processes is a high priority need. These included development of field-based separations (electric-, sonic-, magnetic-, etc.). Development of these nontraditional systems include testing under field conditions.

Organics from Aqueous Streams

Chemistry and Data. A high priority need in this group is the development of computational chemistry. Molecular interaction studies are needed to support this technical area. Tying flow phenomena to diffusion and surface phenomena at the molecular level will be important.

Design and Modeling. The highest priority need is development of improved computer models for integrating fluid flow, chemical interactions, diffusion, and structure and shape of surfaces. Computational chemistry models also need to be developed, and existing models need to be extended to cover strong interactions. Linking models that describe phenomena on the molecular, surface, and bulk levels is important.

Materials and Equipment. The development of improved materials for separations applications is a high priority. Engineered forms of new, highly selective separating agents (e.g., on the surface of an adsorbent, in a membrane, soluble in a solvent) are needed.

Processing. Development of new non-traditional processes is a high-priority need. These include development of hybrid systems such as complexation filtration, magnetic filtration, field-induced filtration (e.g., electrodialysis), and reactive extraction (e.g., phase transfer catalysis). Simulation studies will be useful in the development of these systems since they will be solute specific.

Contaminants from Organic Streams

Chemistry and Data. Three research needs tied for highest priority: (1) to improve the understanding of intermolecular interactions (particularly for noncovalent structures),

(2) to develop validated, accessible property and performance databases (particularly for near-critical fluids, alternative solvents, and new solutes), and (3) to increase the understanding of how the physics of the separations process interacts with the physics of separating equipment. Improving understanding of interfacial phenomena for membrane absorbents is a medium priority need.

Materials and Equipment. Development of improved materials for separations applications is a medium priority. Robust ion exchange resins are needed that can perform well in organic streams are needed. Multi-functional materials that can perform separations and reactions (e.g., for adsorption and catalysts membranes) also need development.

Processing. Development of hybrid systems for separations from dilute solutions is a medium priority need.

R&D Linkages: The key linkages of research needs for dilute solutions are shown in Table I.9, grouped according to the categories used for the research needs.

III.J. Cross-Cutting Research Needs

Various research needs cross-cut all or most of the technical areas.

Adsorbents, membranes, and separative reactors are alike in that they are all relatively new or under-utilized technologies and they are all dependent on one or more new materials. The cross-cutting research needs are reflective of these characteristics of the three technologies. Major cross-cutting needs are for:

- new materials,
- comprehensive performance data,
- closer coupling of process economic evaluation and research to target processes that can benefit from the technologies,
- demonstration of utility in dirty "real world" systems in dedicated pilot facilities, as opposed to clean model systems, and
- consideration of the three separation technologies in the context of the larger process system in order to address all the operational issues and provide a robust and beneficial operating system.

Crystallization, distillation, and extraction are also alike in that they are established technologies and they are mostly dependent on process understanding and improvements. Cross-cutting research needs for these technologies are for:

- better understanding of the physical phenomena,
- additional scientific data about interfacial processes, and
- robust, real-time, in-line monitoring and control instrumentation.

These cross-cutting needs were reiterated when separations needs for bioprocessing and dilute solutions were evaluated. In addition, the need for new hybrid separations systems was identified as a cross-cutting need.

Research needs that apply to most or all of the technical areas are for: more relevant data relating to physical properties, kinetics, and thermodynamics, compilations of these data into handbooks that link the data with performance, and computerized models that permit the prediction of performance.

In addition to these common research needs, the entire area of separations technology would be well served by other changes. These are:

- strengthening the chemical engineering curriculum to include more coursework on separation technologies, and
- creating an institute to carry out or to fund research needed to develop the separations technologies.

APPENDIX A. SEPARATION TECHNOLOGIES WORKSHOPS

Separations I

In 1995, CWRT began planning for a two-day workshop/conference to explore the status, capabilities, and limitations of various technologies related to the generic unit operation of separation. The workshop was co-sponsored by CWRT, US DOE/OIT, the Council for Chemical Research, American Chemical Society, the Separations Division of the American Institute of Chemical Engineers, and the National Center for Clean Industrial and Treatment Technologies. The workshop plan required presentations detailing the current state of knowledge about three emerging areas of separation: adsorbents, membranes, and separative reactors. US DOE/OIT requested that the two-day workshop be followed by a third day devoted to roadmapping breakout sessions focusing on research needs for the three technologies.

The groundwork for Separations I was laid at a CWRT General Meeting in Richland, WA, in July 1997. The broad challenge of reducing energy waste and raw materials loss by thirty percent and reducing the generation of all wastes by the same amount by 2020 for the production of the "*Top 50 Chemicals*" was adopted for the Richland roadmapping exercise. This challenge was useful for providing a focus for the attendees in this early roadmap construction effort. The Richland meeting resulted in four rudimentary roadmaps on (1) sustainability, (2) novel reactor technology, (3) recovery of organic compounds from high salt aqueous streams, and (4) reduced water reuse. It also became clear during this exercise that the challenge adopted at Richland could not serve as a general chemical industry objective because of, among other things, the changing nature of the "*Top 50 Chemicals*" as newer off-shore capacity displaces older U.S.-based plants and the increasing importance of biotechnology-based processes. However, setting a "stretch goal" of this nature had value in stimulating "out-of-the-box" thinking.

This planning and the results from Richland led to the Separations I workshop, which was held February 4–6, 1998, in New Orleans, LA. The workshop brought together about one hundred experts from the chemical industry, its customer industries, universities, and government research programs. The meeting was used to begin the process of construction of roadmapping areas of general interest to the CWRT sponsors, and to set performance challenges for the industry.

The meeting agenda is included in this appendix. A monograph covering the two days of technical presentations from the Separations I workshop is available from CWRT (see Appendix D for an outline of the monograph).

Energetics, Inc., of Columbia, MD, facilitated the three workshop breakout sessions (see Appendix B for participants), which focused on adsorbents, membranes, and separative reactors in a brainstorming exercise that mirrored the roadmapping workshop previously held for the aluminum industry by Energetics, Inc. Each breakout group was given the broad goal of determining how the separation technology they were discussing could help in reducing energy and raw materials usage and the generation of wastes by thirty percent in the production of the top fifty chemicals by 2020. Using these goals, the groups developed performance targets, identified technical barriers to reaching those targets, and developed lists of research needs to address the barriers. Details on the guidelines provided to participants for each of these areas are provided below.

Performance Targets

Each breakout team was assigned the task of identifying the performance targets that were appropriate for its technology area by 2020. Those targets could be related to activity, selectivity, energy usage, raw material efficiency, waste generation, or any other factors associated with the achievement of the objectives. The targets could be stated somewhat broadly but preference was given to as quantitative a statement as possible.

Key Technical Barriers

Considering the performance targets, the teams were then asked to define, as completely as possible, the technical barriers that would prevent the attainment of those targets. Those barriers were grouped into categories of related items and team members were asked to vote on which of the barriers they believed were the most critical. Each member was limited to four votes (one high priority vote and three medium priority votes) on the barriers in order to force some prioritization. Those barriers receiving the largest numbers of "vote*s*" were considered to be the key barriers.

Research Needs

Next, the teams were asked to identify research needs that addressed the technical barriers. These needs were grouped in two ways, within various categories and according to the time frame in which the research needed to be undertaken. Time frames were expressed as near-term (0–3 years), mid-term (3–10 years), long-term (10+ years), and ongoing, respectively. Thus, the results were presented in a matrix of category versus time. As in the case of technical barriers, the team members were asked to identify the four most important needs and to indicate which one of these four should be given top priority. This voting allowed teams to focus attention on the research needs deemed most critical.

Research-Related Needs

The focus of the breakout sessions was on research needs that, when met, would allow the industry to meet its Vision 2020 goals. The breakout session participants also identified other needs that could impact these research needs significantly. These other needs include, for example, modifications in the chemical engineering curriculum that would strengthen the familiarity of the engineering student with the six technologies discussed here. This and other research-related needs are discussed in the sections on the individual technologies.

Key R&D Linkages

The last step in the roadmapping process was to establish a connection among the various key research needs. Arranging the needs in a diagram showing with arrows the way in which the results from some research areas feed into other needs areas did this. This part of the mapping process begins to show where and at what time critical research must be carried out if the larger performance targets stated at the outset are to be met in a timely way.

The results of the roadmap exercise from the February 1998 workshop were presented to the CWRT sponsors attending the CWRT General Meeting in New Orleans on March 4, 1998, for additional input. The intent was to get additional industry input to validate or modify the conclusions reached earlier. Attendees from each breakout group from Separations I were present to explain the results from that meeting. In the CWRT meeting of March 1998, the attendees were presented with the performance targets identified by the earlier group, and they were invited to add to or adjust the targets as they saw fit.

The attendees reviewed and modified the technical barriers. No deletions were permitted, but additions were encouraged. Attendees added their ideas for research needs that they believed might have been left out of the New Orleans exercise and then cast votes for research needs. The resulting modified performance targets, barriers, and prioritized research needs for adsorbents, membranes, and separative reactors formed the basis for this report.

Separations II

A meeting was held in Gatlinburg, TN, in early 1998 to look at bioprocessing opportunities that help to define a future state for separation technologies. A variety of drivers that will strongly affect the future of bioprocessing were discussed at Gatlinburg, TN. They include: (a) regulatory concerns (governmental restrictions), (b) feedstock changes, cost, and availability (alternative processes will become too expensive), (c) the desire for "greener" technology, particularly in foreign markets, and (d) availability of new bio-based products which cannot be chemically synthesized. Factors causing significant changes were discussed including ease of use and ability to integrate with other processes and biocatalyst development (both enzymatic and whole cell).

Many of today's unique or unusual process streams will be commonplace in industry in 2020. Examples include: cellular streams, mixed aqueous and organic streams, and streams from organic phase extraction. In the future, such streams will likely: (a) have higher carbon content and oxygen demand, (b) have higher organic and inorganic salt composition, (c) have extremes of pH, (d) contain dilute acids, (e) contain volatile organics and other volatile compounds (ammonia, CO_2, etc.), (f) require significant process water clean-up (regulations are likely to be based on ecological aspects of streams), and (g) have solids as waste products (e.g., biomass, metals).Streams from different products will become increasingly common. These include: (a) residues from paper/pulp, (b) non-ethanol fuel from biomass, (c) ethanol from biomass, (d) biological weapons from both production and destruction aspects, (e) "green" biological solvents, (f) solar collection devices—"photo biocell," (g) high energy and carbon yield products, (h) new polymers, (i) bio-based agricultural chemicals (e.g., fertilizer), (j) "nutriceuticals", (k) bio-refined fossil fuels, (l) more plant-based products, and (m) fiber polymer blend/bioinorganic blend construction road residues.Large fermentation-based streams will likely have the following characteristics: (a) pH = 5–9, (b) temperature = 35–60ºC, (c) flow rates ~1 billion lb/year aqueous broth, (d) salts < 3 wt %, and (e) toxins will be unacceptable when actually commercialized.Many process streams will be derived from plant-based chemical materials for which typical characteristics will be: (a) 10% total protein, (b) pH of 6-8, (c) temperature of 20–60ºC, (d) 0.1% valuable proteins if separated in molecular weight ranges, and (e) shear-sensitive.

Some processes will require development of more refined techniques such as: (a) gas separations (e.g., O_2/H_2), (b) biomass separation, (c) removing "viruses," (d) organic separation, (e) purification, and (f) product separation.

The information developed at the Gatlinburg meeting provides a strong foundation to the Separations Technologies Workshop II held on May 11–13, 1998, in Oak Ridge, Tennessee. It brought together approximately forty experts from the chemical industry, its customer industries, universities, and government to brainstorm the research needs in crystallization, distillation, and extraction. The workshop was co-sponsored by CWRT, US DOE/OIT, Dow Chemical Company, Electric Power Research Institute, Koch-Glitsch, Inc., Monsanto Company, Nofsinger, Oak Ridge National Laboratory (ORNL), Texas Tech Process Control and Optimization Consortium, and Union Carbide. The workshop was organized by Earl Beaver of Practical Sustainability and formerly of Monsanto, Paul Bryan of the Massachusetts Institute of Technology and formerly of Union Carbide, Sharon Robinson of ORNL, and Charles Russomanno of US DOE/OIT, and it was hosted by ORNL. The workshop agenda is part of this Appendix, and the participants are also included in Appendix B.

The goal of the workshop was to identify research required to meet the chemical industry's vision of maintaining or achieving: (a) leadership in technology development, (b) enhanced quality of life, (c) excellence in environment, safety, and health, (d) positive rapport with communities, and (e) seamless partnerships with academia and government, and sustainable development.

The first half-day of the workshop was spent setting the stage and ground rules for two days of brainstorming breakout sessions. Earl Beaver and Denise Swink, Deputy Assistant Secretary of US DOE/OIT Office of Industrial Technologies, gave presentations summarizing Technology Vision 2020: The Chemical Industry, the US DOE "Industries of the Future" partnership program, and a situational analysis of the chemical industry in 2020 based on information provided by DuPont, Shell, Arthur D. Little, the New York Times, Harvard Business Journal, Union Carbide, and the 20th Symposium on Biotechnology for Fuels and Chemicals.

Factors that will influence industry in 2020 include: fossil fuel prices and taxes, environmental regulations, growth in alternative processing technologies such as biotechnology, recycling, use of total life cycle evaluations in decision-making processes, information technology, international competition, and industrial growth in Asia, Europe, and North America. Four potential scenarios were presented based on different rates of change in each of these variables. Changes that could be expected in process streams and the top fifty chemicals produced in the United States were also discussed.

Paul Bryan, Council of Chemical Research Vision 2020 committee chair for Process Science and Engineering Technology, defined the brainstorming process and led a discussion of the situational analysis for the chemical industry in 2020. Workshop participants concluded that although no single scenario for this industry's future is likely to be correct, several key factors are expected to drive the need to change industrial practices. Assumptions to be used in the brainstorming sessions included: (a) the public demand for increases in pollution prevention/reduction and public safety, (b) significant increases in the cost of fresh water, (c) increases in raw materials costs, (d) increased energy costs, and (e) more open access to and availability of information. To remain competitive in the future, the industry will have to (a) meet tighter product specifications, (b) reduce investment costs, and (c) increase the flexibility of plant operations.

Three brainstorming groups according to technical backgrounds and area of expertise: crystallization, distillation, and extraction. Industry volunteers facilitated breakout sessions for each technical area. The groups were asked to review the situational analysis of the industry discussed previously and to (a) identify unique areas for the individual technical areas, (b) identify technical barriers to reaching the chemical industry vision, and (c) identify and prioritize by need and within time-frames the research required to overcome these barriers. The three groups looked at both existing processes/products and processes/products expected by the year 2020. Each group was asked to examine the future of its particular technology in light of competing technologies and the various possible scenarios.

Separations III

The third separations workshop was held on March 9–11, 1999 in St. Louis, Missouri. It focused on bioseparations and was co-sponsored by BF Goodrich, CWRT, DuPont, Monsanto, US DOE/OIT, and Oak Ridge National Laboratory. The workshop was organized by Earl Beaver, Tom King of US DOE/OIT, Sharon Robinson, and William Scouten of Utah State University, and was hosted by Monsanto. The workshop agenda is part of this Appendix, and the participants are also included in Appendix B.

Presentations at the kick-off dinner on May 9 and welcoming talks on May 10 set the stage for two days of brainstorming sessions. Earl Beaver, Jim McLaren, President of Inverizon International, Inc., and Henry Kenchington, Chemical Team Lead at the US DOE/OIT

Office of Industrial Technologies, gave presentations summarizing the status of the Vision 2020 programs for the chemical and agricultural industries and US DOE "Industries of the Future" partnership program. They indicated that the workshop results will be used to develop roadmaps for the next steps in the implementation of *Technology Vision 2020: The U.S. Chemical Industry* and *Crop/Renewables Vision 2020* as well as "visions" for other energy- and material-intensive industries. The workshop results will also guide the future direction of the US DOE/OIT partnerships program with material- and energy-intensive industries.

Forty-seven bioprocessing and separations experts from industry, academia, and government participated in brainstorming sessions to identify future research needed to expand the use of bioprocessing in the chemical and related industries. The workshop format was similar to that of Separations II.

The workshop group used the following general definition of bioseparations: separation issues and processes related to purification of biological-based feed stocks and products whether directly from a biological material via a biocatalyst or from conventional transformation. Participants focused primarily on downstream processing for chemical production rather than conversion of waste streams to energy, although displacement of petroleum-based energy was deemed desirable. Attendees worked in three brainstorming groups according to their technical backgrounds and areas of expertise. The brainstorming sessions where focused around three types of feed streams: agricultural corps, forestry products, and all other biomass. Industry volunteers chaired and Energetics, Inc. facilitated the breakout sessions. The groups were asked to review the situational analysis of the industry in its present and future state, and develop typical feed stream compositions for bio-processes in 2020. They (a) identified unique areas for the individual technical areas, (b) identified technical barriers to reaching the chemical industry vision, and (c) identified and prioritized by need and within time-frames the research required to overcome these barriers. The groups looked at both existing processes/products and processes/products expected by the year 2020. Each group was asked to examine the future in light of competing technologies and the various possible scenarios. The feed streams identified by the breakout groups are given in tables in this appendix. Technology barriers and research needs are summarized in Section III, and detailed information by breakout group is given in Appendix C. The feed stream compositions for agricultural corps were based on information available in Agricultural Vision 2020 documents: *Plant/Crop-Based Renewable Resources 2020* (DOE/GO-10098-385, January 1998) and *The Technology Roadmap for Plant/Crop-Based Renewable Resources 2020* (DOE/GO-10099-706, February 1999). The breakout groups developed specific feed compositions for all other biomass and forestry products that are given in Tables A.1 and A.2, respectively.

Separations IV

The fourth separations workshop was held on October 20–22, 1999 in Gatlinburg, Tennessee. It was held in conjunction with the *11th Symposium on Separation Science & Technology*, and was co-sponsored by CWRT, US DOE/OIT, Rohm and Haas, and Oak Ridge National Laboratory. The workshop was organized by Earl Beaver, Tom King, Sharon Robinson , and Paul Bryan, and was hosted by ORNL. The workshop agenda is part of this Appendix, and the names of the participants are also included in Appendix B.

Twenty-eight chemical processing and separations experts from industry, academia, and government participated in brainstorming sessions to identify future research needed to address dilute solutions in the chemical and related industries. The workshop format was similar to that of Separations II and III. The theme for the fourth workshop was dilute solutions, but an effort was made to include separations technologies that were not specifically covered in previous workshops, including ion exchange, leaching, filtration, hybrid systems, and field-enhanced systems.

The stage for two days of brainstorming sessions was set by technical presentations on the night of October 19 and on October 20. Earl Beaver coordinated the technical discussions and gave the ground rules for the brainstorming breakout sessions. Jack Vinson of Searle and Henry Kenchington, Chemical Team Lead at the US DOE/OIT Office of Industrial Technologies, gave presentations summarizing the research needs for separations in the pharmaceutical industry and US DOE "Industries of the Future" partnership program, respectively. Paul Bryan discussed "Hindsight 2020", while Vincent Van Brunt, University of South Carolina, and Rich Noble, University of Colorado, summarized results of previous workshops on separations from dilute solutions in 1985 and 1991, respectively.

The workshop attendees participated in three brainstorming groups according to their technical backgrounds and areas of expertise. The sessions were focused on three types of feed streams: contaminants from organic streams, ionic species from aqueous streams, and organics from aqueous streams. The groups defined dilute solutions as streams with species present in concentrations of one weight percent or less. For ionic species in aqueous streams, this centered on dissolved species in the aqueous phase. Complicating factors such as the presence of minute quantities of organics, chelated species, and phase

Table A.1 Biomass Feed Streams for Bioseparations

Bioprocessing Stream	Temperature	Salts Content	pH	Composition	Volume
1. *Fermentation: Plant*	*10–60°C; down streams in fermentation processes are typically 'cool'*	*1 to 3 wt% of stream could be salts. Trace minerals (such as copper, manganese) and a mixture of mineral salts driven by changes in pH will be present (thus, ammonium, sulfate concentrations, etc., may be significant.*	*Tight control is required for most bioprocesses* *pH Range: 5 to 8*	*1–10% cell biomass* *0.1 to 20% product* *~80% spent broth (which would include acids, alcohols and microbial byproducts)* *May include 5% or more extraction solvent.*	*10^2 to 10^4 liters/day*
2. *Fermentation: Microbial/fungal*	*10–60°C*	*Similar to above*	*pH Range: 4 to 9*	*Similar to above*	*10^4 to 10^8 gallons/day*
3. *Fermentation: Mammalian*	*10–40°C*	*Similar to above*	*pH Range: 5 to 8*	*Similar to above*	*10^2 to 10^4 liters/day: note that this value is substantially smaller than the other two types of fermentation streams*
4. *Predigested Biomass*	*Ambient. 11–21°C*	*Minimal/low/trace* *Considered relatively unimportant*	*Generally 6.8 to 7.1, but can be run as low as 5 or as high as 8*	*1– 30% dissolved solids* *This stream is likely to have a high level of dissolved solids. Examples are 2 to 4% for municipal waters; food at 1%, animal at 5 to 10%.* *Many of these levels will be affected by regulatory limits* *Microbial bio-mass, ammonium, phosphorous, etc. are of concern.*	*High* *10 to 100 tons/day on a typical farm* *Example: one cow can produce 80 gallons/day of urine.*
5. *Sludge (biosolids)*	*Ambient. This will be somewhat dependent upon whether a thermophilic treatment is being used.*	*Very low* *Specific cases where high salt discharges are possible were noted, included desalting of petroleum.*	*pH Range: 5 to 8*	*1–2% for municipal wastewater streams before going through dewatering* *1–10% for industrial wastewater streams* *There might be potential pathogens present, as well as concentrated metals and toxins in some of these streams.*	*High for municipal at 10^3 to 10^6 million gallons/day* *Varied for industry*
6. *Food Processing Waste (plant)*	*Ambient*	*0 to 10%. Somewhat variable*	*pH Range: 5 to 8*	*Carbohydrates such as starch, cellulose*	*10^4 to 10^7 pounds/day*
7. *Food Processing Waste (animal)*	*Ambient*	*0 to 10%. Somewhat variable. High salt example of whey production was given as an example*	*pH Range: 5 to 8*	*Carbohydrates such as fats, protein (keratin, grease, oil, cartilage), bone meal* *Very little fat should be coming out in waste streams because of their high energy content/value. Overall, food (animal waste) will not generate large waste streams*	*10^4 to 10^6 gallons/day*

(Continued on next page)

Appendix A: Table A.1 Biomass Feed Streams for Bio-Separations (Continued)

Bioprocessing Stream	Temperature	Salts Content	pH	Composition	Volume
8. Plants for Chemical Production	*Ambient*	*Very low*	*~7*	*1–10% product and the balance will be plant dry weight* *This is an emerging technology, including plants used for pharmaceutical production*	*Variable* *Somewhat dependent on how the process would compete with fermentation* *10^4–10^8 pounds per year*
9. Phytoremediation Plant Streams	*Ambient*	*Very low*	*~7*	*0.1 to 3% heavy metals* *plant material residues* *recalcitrant refractory compounds, that are more likely to be taken up but remain relatively unaltered*	*Very low in the 5 to 7 tons/acre range*
10. Marine biomass	*'Cooler' ambient*	*1 to 3%* *May be dependent on osmotic relationship with ocean*	*6.8*	*High water* *1 to 45% product* *balance: plant residue*	*10^4–10^8 pounds per year of product*
11. Municipal Solid Waste	*Not applicable*	*Not applicable* *Recycling by Year 2020 may mean differentiated streams with widely varied properties*	*Not applicable*	*40% cellulose* *10% plastics* *10% metals* *10% glass* *other carbohydrates*	*Should be lower than 6 pounds per day per person by Year 2020*
12. Natural fibers (e.g., cotton, wool)	*Ambient*	*Not applicable*	*Not applicable*	*Protein, cellulose*	*10^7 pounds/day*

changes were identified and considered. Industry volunteers chaired and Energetics, Inc. facilitated the breakout sessions. The groups reviewed the situational analysis of the industry in its present and future state, and developed typical feed stream compositions for 2020. They (a) identified unique areas for the individual technical areas, (b) identified technical barriers to reaching the chemical industry vision, and (c) identified and prioritized by need and within time-frames the research required to overcome these barriers. The three groups examined existing processes/products and processes/products expected by the year 2020. Each group also examined the future in light of competing technologies and the various possible scenarios. The technology barriers and research needs are summarized in Section III, and detailed information by breakout group is given in Appendix C.

Separations 2020: Adsorption, Membranes, Separative Reactors

Workshop I Agenda
February 4–6, 1998
New Orleans, LA

Time	*Activity*	*Moderator*
PROGRAM—DAY 1 Wednesday, February 4, 1998		
7:00 A.M.	***INTRODUCTION***	*Energetics, Inc.*
8:00 A.M	*Registration & Breakfast*	*Jack Weaver, CWRT*
8:15 A.M.	*Introduction & Opening Remarks*	*Darryl Hertz, M.W. Kellogg*
8:30 A.M.	*Review of Workshop Logistics & Agenda*	*Earl Beaver, Monsanto*
9:00 A.M.	*Sustainability: The Future of Pollution Prevention*	*Jimmy Humphrey, J.L. Humphrey & Associates*
	Overview of Emerging Adsorption, Membrane, & Separative Reactor Technologies for Process Pollution Prevention	
10:00 A.M.	***ADSORPTION TECHNOLOGY***	*George Keller, Union Carbide-retired*
10:30 A.M.	*Introduction to Adsorption Technology* *Panel Presentations & Discussion*	*Moderator: Erik Sall, Monsanto* *Panelists: John Crittenden, MTU;* *Kent Knaebel, Adsorption Research Inc.;* *Douglas Ruthven, Univ. of Maine*
11:00 A.M.	*BREAKOUT SESSIONS*	
12:30 P.M.	*LUNCH*	
1:30 P.M.	*Conclusions Panel for Adsorption*	*George Keller, Union Carbide-retired*
2:15 P.M.	*Design and Optimization of Water & Effluent Systems*	*Nick Hankins, Aspen Tech*
2:45 P.M.	*BREAK*	
3:15 P.M.	*Process Integration for Pollution Prevention*	*Russell Dunn, Solutia Inc.*
3:45 P.M.	*Vision 2020: The DOE/OIT Partnership with Industry*	*Denise Swink, US DOE/OIT*
4:15 P.M.	*Invitation to CWRT Vision 2020 Roadmapping Workshop*	*Charles Russomanno, US DOE/OIT*
4:25 P.M.	*Review of Day 2 Agenda*	
4:30 P.M.	*ADJOURN*	
PROGRAM—DAY 2 Thursday, February 5, 1998		
7:00 A.M.	*Breakfast*	*Darryl Hertz, M.W. Kellogg*
8:00 A.M.	*Review of Workshop Logistics & Agenda*	
8:15 A.M.	***MEMBRANE TECHNOLOGY***	*Edward Cussler, Univ. of Minn.*
8:45 A.M.	*Introduction to Membrane Technology* *Panel Presentations &Discussion*	*Moderator: Gregory Keeports, Rohm & Haas* *Panelists: David Shonnard, MTU;* *Richard Baker, Membrane Technology & Research, Inc.;* *Kamelesh Sirkar, NJIT;* *Pushpinder Puri, Air Products & Chemicals*
9:30 A.M.	*BREAKOUT SESSIONS*	
11:00 A.M.	*Conclusions Panel*	
12:00 P.M.	*LUNCH*	

Time	***Activity***	***Moderator***
1:00 P.M.	***SEPARATIVE REACTORS TECHNOLOGY***	*Anna Lee Tonkovich, PNNL*
1:30 P.M.	*Introduction to Separative Reactors* *Panel Presentations & Discussions*	*Moderator: Kerry Irons, Dow Chemical* *Panelists: Jeffrey Siirola, Eastman Chemical; Jimmy Humphrey, J.L. Humphrey & Associates; Robert Carr, Univ. of Minn.*
2:00 P.M.	*BREAKOUT SESSIONS*	*Anna Lee Tonkovich, PNNL*
4:00 P.M.	*Conclusions Panel for Separative Reactors*	
4:45 P.M.	***CONFERENCE CONCLUSIONS & WRAP-UP***	
	Conclusion of Separation & Separative Reactor Technologies Monograph	*Peter Radecki, CenCITT/MTU*
5:00 P.M.	*Separation Conference Conclusion & Wrap-up*	*Joseph Rogers, CWRT*
PROGRAM—DAY 3 Friday, February 6, 1998		
7:00 A.M.	*Breakfast*	
	VISION 2020 ROADMAPPING WORKSHOP	
7:30 A.M	*Introduction & Review*	*Jack Weaver, CWRT & Darryl Hertz, M.W. Kellogg*
7:45 A.M.	*Introduction to Roadmapping Exercise*	
8:00 A.M.	*Roadmapping Preview for Adsorption Technology*	*Bruce Cranford, US DOE/OIT*
8:10 A.M.	*Roadmapping Preview for Membrane Technology*	*Erik Sall, Monsanto*
8:20 A.M.	*Roadmapping Preview for Separative Reactor Technology*	*Kerry Irons, Dow Chemical*
	BREAKOUT SESSIONS—ADSORPTION, MEMBRANES, AND SEPARATIVE REACTORS	
8:30 A.M.	*Agreement on Broad Goals*	
9:45 A.M.	*Identification of Barriers to Process Waste Reduction*	
10:30 A.M.	*Identification of Research Needs & Potential Approaches*	
11:30 A.M.	*LUNCH*	
12:30 P.M.	*Building Roadmaps*	
2:30 P.M.	*Building Detailed Action Plans*	
	ROADMAPPING CONCLUSIONS & WRAP-UP	
3:00 P.M.	*Results of Adsorption Technology Breakout Group*	*Erik Sall, Monsanto*
3:15 P.M.	*Results of Membrane Technology Breakout Group*	*Gregory Keeports, Rohm & Haas*
3:30 P.M.	*Results of Separative Reactor Technology Breakout Group*	*Kerry Irons, Dow Chemical*
3:45 P.M.	*Planning Future Follow-up*	*Joseph Rogers, CWRT & Charles Russomanno, US DOE/OIT*
4:00 P.M.	*ADJOURN*	

Separations 2020: Crystallization, Distillation, Extraction

Workshop II Agenda
May 11–13, 1998
Oak Ridge, TN

Monday, May 11

8:00–12:00	Registration—Main Lobby
8:30–11:30	Optional tour of Oak Ridge National Laboratory
11:00–12:00	Planning Meeting with Facilitators, Scribes, and Recorders–Salon C
12:00–1:00	Working lunch (covered by registration)–Salon B
1:00–1:30	Welcome by Gil Gilliland, Associate Laboratory Director, and Tony Schaffhauser, Energy Efficiency and Renewable Energy Program Director, Oak Ridge National Laboratory–Salon C
1:30–2:00	OIT Partnership–Denise Swink, Deputy Assistant Secretary, Department of Energy, Office of Industrial Technology–Salon C
2:00–3:30	The World of 2020–Earl Beaver, Director, Waste Elimination, Monsanto–Salon C
3:30–3:45	Define brainstorming process–Paul Bryan, Council for Chemical Research Vision 2020 Committee Chair for Process Science and Engineering, Union Carbide–Salon C
4:45–5:00	Break
5:00–7:00	Reception (hosted by ORNL and CWRT)–Salon A
	Dinner on own

Tuesday, May 12

7:30–8:00	Continental breakfast (covered by registration)–in breakout rooms
8:00–12:00	Parallel brainstorming sessions on Crystallization (Salon A), Distillation (Salon C), and Extraction (Salon B)
10:00–10:15	Break
12:00–1:00	Working lunch (covered by registration)–Salon C
1:00–4:30	Continue brainstorming sessions (Same as morning)
3:00–3:15	Break
4:30–5:00	Summary results (Salon C)
6:30	Optional dinner at Bleu Hound (Dutch treat)–meet in Lobby at 6:15 pm

Wednesday, May 13

7:30–8:00	Continental breakfast (covered by registration)–in brainstorming rooms
8:00–12:30	Continue brainstorming sessions (Crystallization–Salon A, Distillation–Salon C, and Extraction–Salon B)
10:00–10:15	Break
12:30–1:30	Working lunch (covered by registration)–Salon C
1:30–3:00	Summarize results of brainstorming sessions and wrap-up–Salon C

Separations 2020: Bioseparations

Workshop III Agenda
March 9–11, 1999
St. Louis, MO

Tuesday, March 9

4:00–6:00 pm	Registration
6:00–7:30	Kickoff dinner
7:30–8:30	Presentations by Earl Beaver, Director of Waste Elimination, Monsanto; and Hank Kenchington, Department of Energy's Office of Industrial Technologies

Wednesday, March 10

7:30–8:00	Continental breakfast
8:00–9:00	Welcoming talks by Earl Beaver, Director of Waste Elimination, Monsanto; Jim McLaren, President, Inverizon International, Inc.
9:00–9:20	Instructions for breakout sessions
9:20–10:30	Discuss current and future state-of-the-art
10:30–12:00	Brainstorming sessions to define technology barriers
12:00–1:00	Working lunch
1:00–4:00	Brainstorming sessions to define research needs
4:00–4:40	Recap of day's work
6:30–8:30	Optional dinner

Thursday, March 11

7:30–8:00	Continental breakfast
8:00–8:15	Morning recap by Earl Beaver, Director of Waste Elimination, Monsanto
8:15–10:20	Brainstorming session to define timeline for research needs
10:20–12:00	Wrap-up session
12:00–1:00	Working lunch
1:30–4:30	Optional tour of Monsanto Chesterfield Life Science Research

Separations 2020: Dilute Solutions

Workshop IV Agenda
October 20–22, 1999
Gatlinburg, Tennessee

Tuesday, October 19

5:00–8:00	Early registration–Glenstone Lodge

Wednesday, October 20

7:30–5:00	Registration–Glenstone Lodge
8:30–4:00	*Eleventh Symposium on Separation Science Technology–Park Vista Hotel*
8:30–11:45	Industrial Separations Technical Session
1:30–4:45	Separations for Dilute Solutions Technical Session
5:00–6:30	*Reception–Glenstone Lodge, Highlander Room*
8:00–10:00	*Kickoff Session: The Future of Separations from Dilute Solutions–Park Vista*
8:10–8:10	Welcome–Sharon Robinson, Oak Ridge National Laboratory
8:10–8:30	USDOE/OIT Efforts in Vision 2020 and the Importance to Separations; Hank Kenchington, DOE Office of Industrial Technologies
8:30–9:15	Present & Future Needs for Separations in the Pharmaceutical Industry; Jack Vinson, Searle
9:15–10:00	Group Discussion—Earl Beaver, Practical Sustainability

Thursday, October 21, Glenstone Lodge–Azalea Room

7:30–8:00	Continental breakfast
8:00–8:15	Welcome–Earl Beaver
8:15–8:45	Review of previous workshops by Vincent Van Brunt, University of South Carolina, and Rich Noble, University of Colorado
8:45–9:15	Breakout Sessions: Discuss current and future state-of-the-art
9:15–10:30	Breakout Sessions: Identify technology barriers
10:30–10:45	Break
10:45–12:00	Breakout Sessions: Analyze/prioritize technology barriers
12:00–1:00	Working lunch
1:00–2:30	Breakout Sessions: Identify R&D needs
2:30–3:00	Break
3:00–4:15	Breakout Sessions: Analyze R&D needs
4:15–5:00	Recap of day's work
6:30–8:30	Dinner–Hindsight 2020, Paul Bryan, GE Plastics

Friday, October 22, Glenstone Lodge–Azalea Room

7:30–8:00	Continental breakfast
8:00–8:15	Morning Recap
8:15–10:00	Breakout Sessions: Continue analysis of R&D needs
10:00–10:20	Break
10:20–11:30	Breakout Sessions: Finish analysis of R&D needs
11:30–12:30	Working lunch
12:30–3:00	Final summary session and wrap up

APPENDIX B. WORKSHOP PARTICIPANTS

Workshop Participants by Technology Area*

Name	Technology Area	Organization
Adler, Steve	A, C, O	CWRT
Albares, Greg	O	Owens Corning
Apel, Bill	O	Idaho Nat'l Env. & Eng. Lab
Asher, Bill	O	SRI Consulting
Baker, Jim	O	CenCITT
Baker, Richard	M	MTU
Barton, John	E, O	Oak Ridge National Lab
Beaver, Earl	S, E, O	Monsanto
Berger, Scott	O	Owens Corning
Bodnaruk, Dan	A	US DOE/OIT
Bontha, Jagan	M	PNNL
Bordacs, Krisztina	O	SmithKline Beecham
Borsey, Bill	M	Oak Ridge Ctr./ Man. Tech.
Bowden, Greg	O	Celanese
Bradford, Marion	O	A. E. Staley
Bray, Ronald	C	SRI Consulting
Brosey, Bill	C	Lockheed Martin
Bryan, Paul	M, D	Union Carbide
Burton, Stephanie	O	Rhodes Univ., S. Africa
Butner, Scott	O	PNNL
Byers, Bill	O	CH2M Hill
Byers, Charlie	D	IsoPro International
Carr, Bob	S	Univ. of Minnesota
Chambers, Greg	O	General Electric
Chen, Norman	E	FMC Corporation
Cheryan, Munir	O	Univ. of Illinois
Chow, Michael	O	Rhône-Poulenc
Cichy, Paul	M	Rohm & Haas
Clevenger, Len	O	Dow Chemical
Cockrem, Mike	O	KiwiChem International, Inc.
Connor, John	D	Nofsinger, Inc.
Constable, David	S	SmithKline Beecham
Cranford, Bruce	O	US DOE/OIT
Crittenden, John	A, O	MTU
Cunningham, Virginia	O	SmithKline Beecham
Danner, Herbert	O	IFA-Tulln, Austria
Datta, Rathin	M	Argonne National Lab
Davison, Brian	O	Oak Ridge National Lab
Dien, Bruce	O	NCAUR, ARS
Dobbs, Greg	M	United Technologies
Doody, Dennis	S	Bristol Myers
Eiteman, Mark A.	O	Univ. of Georgia
Eldridge, R. Bruce	D	Univ. of Texas at Austin
Evans, Robert	O	NREL
Fair, James R.	D	Univ. of Texas at Austin
Farone, John	D	Dow Chemical
Figuly, Garry	O	E. I. DuPont
Flammino, Tony	A	Merck
Fort, Garth	O	Monsanto Chemicals
Frank, Timothy C.	C	Dow Chemical
Gencer, Mehmet	O	B. F. Goodrich
Glatz, Donald J.	E	Koch Process Tech.
Gold, Harris	A	Foster Miller
Hamilton, Bill	O	Merck
Handley, John	O	Eastman Chemical
Harten, Teresa	A	US EPA
Helling, Rich	S	Dow Chemical
Hertz, Darryl	M, O	M.W. Kellogg Co.
Hettenhaus, Jim	O	CEA
Holbrook, Tim	O	Camp Dresser & McKee
Hsiung, Tom	M	Air Products
Huestis, David	O	SRI Consulting
Hunter, Jesse	O	Bristol Myers Squibb
Irons, Kerry	S, O	Dow Chemical
Jarvinen, Gordon	M	LANL
Jubin, Bob	C	ORNL
Jurgensen, John	A	Dupont Dacron
Kaempf, Doug	D	US DOE/OIT
Kanel, Jeffrey S.	E	Union Carbide Corp.
Kaufman, Erik N.	O	Oak Ridge National Lab
Keeports, Greg	M, O	Rohm & Haas
Keller, George	S	Consultant
Kelley, Steve	M, O	NREL
Killat, George	S	Dow Chemical
King, David	M	NIST
King, Kathy	A	Rohm & Haas
Knaebel, Kent	A	Adsorption Research
Krause, Ted	M, O	Argonne Nat. Lab.
Krishnamurthy, Krish R.	D	BOC Gases R&D
Krishnan, Mahesh	O	Oak Ridge National Lab
Kulesa, Gloria	O	U.S. DOE
Kunesh, John G.	D	Fractionation Research, Inc.
Kurdikar, Devdatt L.	E	Monsanto
Laugone, Parta	O	Univ. of Rio de Janeiro, Brazil
Li, David	M	Air Liquide
Lockett, M.J.	D	Praxair Inc.
Magrini, Kim	O	NREL
Marr, Dave	M	Akzo Nobel Chemicals
Martin, Carol R.	E	Eastman Chemical
Maskarinec, Mike	E	Oak Ridge National Lab.
Maves, Fred	O	3M
Meyer, Don	O	Nofsinger, Inc.
Midler, Mike	C	Merck & Co.
Mielenz, Jonathan	O	Eastman Chemical
Miller, Robert	M	Air Products
Mills, Ken	S	Norton Chemical Process
Morris, Virginia	O	AD Little
Motwani, Jay	O	CH2M Hill
Muhlebach, George	S	CWRT
Myers, Alan	A	Univ. of Pennsylvania
Nilsen, David	E	US DOE Albany Research Ctr.
Nofsinger, Rowland	C	Nofsinger, Inc.
Ong, SayKee	M	Iowa State Univ.
Oolman, Timothy	C	Cargill
Ou, John D. Y.	E	Exxon Chemical
Panchal, Chandrakant B.	E	Argonne National Lab.
Paulson, Jim	M	US DOE/OIT
Pelligrino, John	M	NIST
Pereira, Candido	A	Argonne National Lab.
Peterson, Eric	M	Idaho Nat. En. & Envir. Lab.
Peterson, Gene	O	Nat'l Renewable Energy Lab.
Ponciroli, Dana	O	CWRT
Puri, Pushpinder	M	Air Products
Pye, Rob	M	LANL
Radecki, Pete	A, O	CenCITT/MTU
Rakestraw, Julie	E	E.I. DuPont de Nemours
Ramsden, Steve	O	Grain Processing Corporation
Reynolds, John	M	Lawrence Livermore
Riggs, James	D	Texas Tech. Univ.
Ritz, Jon	O	BF Goodrich
Robbins, Lanny A.	D	Dow Chemical
Robinson, Sharon	S, O	ORNL
Rogers, Joseph E. L.	M, O, C	CWRT
Rogers, Robin	E	Univ. of Alabama
Roundhill, Max	A	Texas Tech. Univ.
Rousseau, Ron	C	Georgia Inst. of Tech.
Russomanno, Charles	S, O	U.S. DOE

A = adsorbents, C = crystallization, D = distillation, E = extraction, M = membranes, S = Separative reactors, O = other
(Gatlinburg, CWRT General Meeting, Richland)

Name	Technology Area	Organization	Name	Technology Area	Organization
Ruthven, Douglas	A	Univ. of Maine	Stone, Mark	M	Idaho Nat'l. Env. & Eng. Lab.
Sall, Erik	A, O	Monsanto	Thompson, Tyler	S	Dow Chemical
Sauer, Nancy	S	LANL	Tipping, Jim	S, O	ICI/CWRT
SaztAnna, Geraldo L.	O	Coppe/VFRF/Brazil	Tonkovich, Lee	S, O	PNNL
Schmidt, Tom	M, D	ORNL	Tran, Thanh	S	Argonne National Lab.
Schnipp, Carolyn	D	Univ. of Texas at Austin	Tsai, Shih-Perng	O	Argonne National Lab.
Scouten, Charles	D	Amoco	Van Brunt, Vincent	E	Univ. of South Carolina
Seale, Jerry	S	Eastman Chemical	Vandegrift, George	S	Argonne National Lab.
Seibert, Michael	O	Nat'l. Renewable Energy Lab.	Vinton, Claire	O	Argonne National Lab.
Shonnard, David	M	MTU	Vitolo, Michele	O	Univ. of S. Paulo, Brazil
Short, David	O	DuPont, Inc.	Wang, Ping	O	Oak Ridge National Lab.
Siebert, Frank	E	Univ. of Texas at Austin	Watson, Jack	A, O, E	ORNL
Siirola, Jeff	S, D	Eastman Chemical	Weaver, Jack	O	CWRT
Smith, Barbara	A, O	LANL	Weiner, Steve	S, O	PNNL
Smith, Ron	A, O	SRI Consulting	Wijmans, Hans	M	MTR
Sneeringer, Mark	O	General Electric	Woinsky, Sam	M, O	EPRI
Sridhar, Jaynanth	O	Univ. of Georgia	Wooley, Bob	A	NREL
Starr, Jack	O	Cargill Dow Polymers	Yeoman, Neil	D	Koch-Glitsch, Inc.
Steele, Bill	D	Oak Ridge National Lab.			

Separations 2020: Bioseparations Workshop Registration List

March 9–11, 1999
Sheraton West Port Hotel, St. Louis, MO

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APPENDIX C. TECHNICAL BARRIERS, R&D NEEDS, AND OTHER ACTION ITEMS

This appendix provides a detailed listing of the technical barriers and research needs identified in the four workshops organized by brainstorming session. Key barriers and research needs are those that received enough votes to score a relative high (H) or medium (M). Barriers and needs were ranked low (L) if they received a small number of or no votes. Tables in this appendix also include research-related needs identified during the workshop.

APPENDIX C: Table C.A.1 Technical Barriers for Adsorbents

(H= High Priority, M= Medium Priority, L= Low Priority)

Process Systems	Materials	Fundamental Data	Institutional Issues	Risk	Cost Issues	Other
Disposal of metals and other environmentally unacceptable materials from adsorption systems (M)	*Difficulty in tailoring adsorbents to handle complex streams* (H)	*Lack of predictive methods for mass transfer, adsorption equilibria, and other physical data* (H)	*Technology underutilized due to users' lack of understanding* (H)	*Perceived high technical risk connected to investing in this technology* (M)	*Capital costs too high* (M)	*Inability to integrate adsorption as presently marketed into all parts of a process that could benefit from technology* (L)
Trade-off required between ability to adsorb and heat/mass transfer requirements to desorb (working capacity) (L)	*Poor physical properties* (L)	*Scarcity of physical property data applying to different geometries and process conditions* (M)	*Inability to integrate technical solutions and cost information across institutional and organizational lines* (M)	*Lack of adequate research funds* (L)	*Lack of adequate cost comparison based on a life-cycle view* (L)	*No identification of areas of important industrial applications* (L)
Sometimes the materials concentrated on an adsorbent can lead to an undesirable or unintended reaction (L)	*Reduce/minimize adsorbent use through improved selectivity* (L)	*Relating physical properties (pore size, surface chemistry) to needs* (L)	*Lack of life cycle perspective by users* (M)	*Discomfort with replacing thermal technology with physical mechanisms* (L)		
Lack of flexibility of adsorption systems vs. other separations (L)	*Inadequate adsorbent stability at system temperatures and other process conditions* (L)		*Small-scale applications of one-of-a-kind, tailor-made adsorbents prevent development of standardized approaches* (L)	*Most systems utilizing adsorption are small-scale, and scale-up is unreliable* (L)		
Disposal of effluent from adsorption processes (L)	*Lack of adsorbents that can handle high pressure drop and velocities* (L)		*Over-emphasis on sales rather than added value* (L)	*Inability to use adsorbents for hazardous waste reclamation* (L)		
Handling of solids more difficult than liquids handling (L)			*Conflicting goals: hazardous waste reduction vs. other process considerations* (L)			
			Lack of predictability of government regulations (L)			

APPENDIX C: Table C.A.2 Research Needs and Other Action Items for Adsorbents

(H= High Priority, M= Medium Priority, L= Low Priority)

Time - Frame	Materials	Process Systems	Predictive Modeling	Demonstrating Commercial Feasibility	Education/ Information Transfer	Structural/ Institutional
All (Ongoing Processes)	*Develop new adsorbents for high selectivity in complex mixtures (e.g., using combinatorial chemistry approach) (H)*	*Integrate materials research and process development (M)* *Integrate materials research and process development (L)*	*Collect/correlate data on equilibrium and kinetics for a variety of adsorbents (M)*		*Create incentives for the adsorbents regeneration business (L)* *- look at government cost- sharing or loan guarantees for this technology* *- investigate consequences of tax code changes to allow companies to depreciate capital investment more rapidly* *Utilize multi-disciplinary approach (e.g., in workshops) to drive innovation (L)*	*Fund a national institute to fund/coordinate research (L)* *Give R&D management a stronger voice in corporate decision-making (L)*
Near-Term (0-3 Years)	*Develop more and better adsorbent forms and geometries (M)* *Reduce manufacturing cost per unit of adsorbent performance (M)* *Application of adsorbents to improve process chemistry (L)* *- remove inhibitors*	*Need for control of continuous chromatography (L)* *Research on disposal of regeneration waste (L)* *Evaluate fluid bed adsorbent process (L)* *In-bed process sensors (L)*		*Demonstrate adsorption technology on important process streams to promote use of the technology (M)* *Identify and understand target markets (L)* *Determine what is in use or planned in industry (L)*	*Develop comprehensive information source to identify waste stream opportunities (M)* *- specific as opposed to general*	

Time - Frame	Materials	Process Systems	Predictive Modeling	Demonstrating Commercial Feasibility	Education/ Information Transfer
Mid-Term (3-10 Years)	*Develop switchable adsorbents using non-thermal desorption energy (M)* *Develop improved high performance conductors (M)* *Develop adsorbents with stability to extreme conditions such as acidity, high temperature (>300°C) (L)*	*Consider non-conventional ways to desorb adsorbed molecules (e.g., microwave, sonic energy) (M)* *Develop new control scheme to allow integration of rapid cycle adsorption and innovative regeneration (L)* *Integrate into hybrid processes (L)* *More dynamic systems and improved solids handling (L)* *Develop a continuous process for concentrating dilute/ aqueous/ heterogeneous/ gaseous streams to enable recycle of carrier (L)* *Novel processes for contacting products with adsorbents (e.g., fluid / moving beds) (L)*	*Generate new physical property data (L)*	*Process design tool to allow technology comparisons on an equal basis (H)* *Develop facilities to demonstrate applications (L)* *- portable pilot plant*	*Create adsorbent handbook of physical properties (H)* *Integrate into chemical engineering curriculum (L)*
Long-Term (10+ Years)	*Develop non-conventional adsorbents (M)* *- micelles* *- liquid crystals* *- enzymes* *- colloids* *Develop molecular recognition methodology for selectivity (L)* *Develop more effective adsorbents along with new substrates (L)*	*Get adsorbents into the environment for clean-up conversion (L)*	*Develop molecular modeling tools to predict interaction of molecules with adsorbent surfaces (M)* *Develop predictive model to correlate physical properties with performance (L)*		*One stop shop for marketing (L)*

APPENDIX C: Table C.B.1 Technical Barriers for Crystallization

(H= High priority, M= Medium priority, L= Low Priority)

Process Control	Analytical	Economics	Equipment & System Design	Education	Physical Properties	Process Modeling
Particle size control is inadequate (M) *Lack of adequate deliquoring & filtering capabilities* (M) *Lack of control systems to handle feedstock complexity and variability* (M) *Lack of adequate solvent recovery process* (L) *Lack of adequate process control systems* (L) *Single purpose versus multi-use crystallization vessels* (L)	*Lack of means to measure super-saturation* (H)	*Lack of market demand for high purity organic intermediaries* (L) *Capital costs are too high* (L) *Development time for crystallization process is too long* (L)	*Need for more continuous crystallizers* (M) *Lack of devices to reliably classify sizes* (L) *Throughput of scraped wall crystallizer is too long* (L) *Build up of gypsum on surfaces* (L) *Heat transfer rates are too low* (L) *Kinetic data for crystallization need to be increased* (L) *Mixing efficiency needs to improve* (L) *Separation of ice crystals from juice concentrate is inadequate* (L)	*Lack of crystallization knowledge by chemical engineering graduates* (H) *Lack of knowledge of solids and solids handling* (M) *Lack of understanding of crystallization at the bench chemist level in early stages of development cycle* (L)	*Lack of understanding of polymorphs* (H) *- mechanism for crystal growth* *- dewatering* *- filterability* *Lack of physical property databases* (H) *Lack of molecular modeling* (M) *Understanding of long-chain molecules is inadequate* (L)	*Lack of data for simulation* (M) *Lack of adequate means to predict continuous process performance from batch, bench or pilot scale* (L) *CFD not adequate for crystallization purposes* (L) *Lack of adequate methods to convert from batch to continuous systems* (L) *Toxicity of some solvents hampers use of crystallization* (L)

APPENDIX C: Table C.B.2 Research Needs and Other Action Items for Crystallization[1]

(H= High priority, M= Medium priority, L= Low priority)

Time-Frame	Process Systems (L)	Economics (L)	Equipment & System Design (M)	Education/ Information Transfer (L)	Fundamental Data (H)	Predictive Modeling (M)
All (Ongoing Processes)						*Improve process modeling to permit for better scale-up capabilities* (H)
Near-Term (0-3 years)	*Develop improved on-line monitor for particle size* (L) *Develop spectroscopic monitors for measuring degree of super-saturation* (M)	*Develop standardized design for reactor vessels* (L)	*Develop micro-mixing modeling* (L)	*Involve engineering early in the product development cycle* (M)	*Develop methodology for estimating solid/liquid equilibrium* (H)	*Extend use of CFD modeling to crystallizer design, multi-phase flow, and micro-mixing* (L)
Mid-Term (3-10 years)	*Design continuous equipment to replace batch equipment* (M) *Develop improved methodology for identifying crystal modifiers* (L) *Develop feed-forward on-line process control based on impurity measurements in feedstock* (L)		*Develop better understanding of fouling mechanism* (L) *Develop cost- effective surface modification* (L) *Obtain better description of flow through particulates* (L) *Improve filter- cake washing capabilities* (L) *Develop novel continuous crystallizer designs which discourage fouling deposits* (L)	*Alter educational curriculum to emphasize fundamental knowledge of solids handling* (L) *Modify education curriculum to include more practical industrial content* (L)	*Establish theoretical basis for effect of impurities on solubilities* (L)	*Develop kinetic data for modeling* (L) *Develop models of crystallization mechanism* (H) *- polymorph* *- size* *- shape*
Long-Term (10+ years)			*Automate crystallizer design based on fundamental material properties* (H)		*Develop molecular modeling methodology to determine solid/liquid equilibrium* (H)	

[1] Participants prioritized both categories and individual needs within each category.

APPENDIX C: Table C.C.1 Technical Barriers for Distillation[1]

(H= High Priority, M= Medium Priority, L= Low Priority)

Physical Fundamentals (H)	Equipment Performance (M)	Education/Information Transfer (M)	Operations Optimization (L)	Other (M/L)
Lack of accurate real stage efficiency calculation *Lack of adequate mixing characterization* *Lack of understanding of distillation phenomena* *Lack of adequate vapor liquid imaging techniques* *"Bad actor" (foam) separation is inadequate* *Lack of ability to measure multi-phase traffic* *A better understanding of mass transfer and multi-phase flow is required* *A better understanding of the processes of phase formation, mixing, interface area formation, and mass transfer, etc. is required* *Lack of adequate data on bubble formation*	*Flow control on trays is inadequate* *Liquid distribution in packed beds is inadequate* *Scanning methods for tower operation troubleshooting are inadequate* *Lack of non-fouling distributors* *Lack of active devices for phase disengagement* *Lack of adequate means to prevent fouling in distillation towers* *Lack of methods for handling multi-phase feeds* *Equipment size-determining rate processes need to be re-evaluated* *Hybrid column internals are required* *Means of reducing stage spacing to less than 2 inches are required*	*Companies and vendors will not share information* *Industrial R&D funds are being reduced* *Universities and national labs are not emphasizing distillation research* *Universities are reducing courses in distillation*	*Lack of reliable plant data* *Lack of proper instrumentation* *Lack of good large-scale test facilities* *Operators lack tools* *Risk-avoidance by supervisors/management* *Better process control is required* *Steady-state simulations are needed that can match plant operation* *Too much plant variability* *- feed* *- steam pressure* *- column pressure* *Need to optimize across plant, not just one column or train*	*Applications* *- lack of system specific needs* *Lack of hybrid systems* *- lack of design tools* *- lack of experimental capability* *- lack of experience with operation and process control* *Computer modeling capabilities* *- lack of thermodynamic and physical property data for some systems* *- non-equilibrium models lack accuracy, generality, and ease of use*

[1] Participants prioritized categories and not individual needs within each category.

APPENDIX C: Table C.C.2 Research Needs and Other Action Items for Distillation

(H= High Priority, M= Medium Priority, L= Low Priority)

Time-Frame	Fundamental Data	Process Systems	Operations Optimization	Education/Information Transfer
All (Ongoing Processes)				*Modify education curriculum to emphasize distillation (L)* *Create incentives for distillation research (L)* *Develop mechanisms to increase industry/ government/university collaboration (L)*
Near-Term (0-3 years)	*Develop sensors for measuring basic distillation phenomena (H)* *Develop database of mass transfer and hydrodynamic data (H)*	*Develop column internals imaging equipment (M)* *Develop better simulators (M)* *Develop database of existing packing/trays (M)* *Develop tools to predict composition from column temperature (M)*	*Develop more reliable instrumentation (L)* *Develop better simulators (L)* *Demonstrate optimization of single column/train (L)*	
Mid-Term (3-10 years)	*Improve understanding of basic distillation phenomena (H)* *- mixing* *- interfacial area* *- mass transfer* *- multi-phase flow* *Develop fundamentals-based model for predicting mass transfer and hydrodynamics in complex "difficult" systems (H)*	*Develop sensors for multi-phase flow (M)* *Develop understanding of factors affecting vapor/liquid distribution (M)* *Develop better understanding of three- and four-phase flow in packing/trays (M)* *Develop in situ sampling methods (M)* *Develop better process gas chromatographs (M)* *Develop novel phase separation methods (M)*	*Demonstrate plant-wide optimization (L)*	
Long-Term (10+ years)			*Demonstrate refinery-wide optimization (L)*	

APPENDIX C: Table C.D.1 Technical Barriers for Extraction[1]

(H= High Priority, M= Medium Priority, L= Low Priority)

New Technologies Development (H)	Understanding Fundamentals (H)	Retrofitting Existing Equipment/Solvents (M)	Third Phase/Unwanted Reactions (M)	Other (L)
Materials: *- better solvents* *- more selectivity for target metals* *- more selectivity for other compounds* *- better understanding of existing solvents* *- better methodology for selecting new or existing solvents* *Equipment* *- better design capabilities* *- better interfacial sensors* *- better drop size determinations* *Processes* *- improve efficiency to reduce dilute streams* *- improve downstream recovery of pure extractant* *- better coalescence* *- better process control* *- improve aqueous/aqueous two-phase extraction*	*Improve understanding of surface/interfacial chemistry to prevent rag layer formation* *Need dynamic modeling for controlling processes* *Need better equilibrium models* *Inadequate ability to predict coupled processes* *Better interfaces are required for computational fluid dynamic type codes to produce a visualization tool*	*Need better capabilities to design retrofits for existing equipment and solvents for:* *- altered conditions* *- altered streams* *- altered capacities* *Need better capabilities to predict performance of existing equipment and solvent to allow de-bottlenecking of process*	*Need methods for eliminating rag layer formation* *Need better methods for dealing with solids in extraction streams* *- existing solids* *- solids that form during processing* *- cell biomass* *- fermentation broth* *- rust* *- catalyst* *- larger particulate contaminants* *Eliminate unwanted reactions* *Treatment of extreme waste streams (due to chemical reaction)*	*Develop better educational textbooks, references, and basic operating guidelines* *Reduce environmental impacts* *Capability to extrapolate data between contactor types* *Lack of cost data and flow sheet optimization capabilities based on total life cycle costs* *Capability to make balanced decisions for safety related activities* *Capability to design hybrid processes for reaction with extractive separations in one unit operation for enhanced production*

[1] Participants prioritized categories and not individual needs within each category.

APPENDIX C: Table C.D.2 Research Needs and Other Action Items for Extraction[1]
(H= High Priority, M= Medium Priority)

Time-Frame	New Technologies Development (H)	Fundamental Data (H)	Retrofitting Existing Equipment/Solvents (M)	Third Phase/ Unwanted Reactions (M)	Education/Information Transfer (M)
Near-term (0-3 years)	*Develop interfacial sensors*	*Physical properties & interfacial phenomena* *- emulsion phenomena* *- coalescence phenomena* *- Marangoni phenomena* *Measure interfacial tension with mass transfer* *- diffusion coefficients* *- density* *- viscosity* *Dynamic CFD modeling* *- drop breakage and coalescence frequency* *- large-scale homogeneous* *- interfacial and drop convection* *- effect of surfactants and contaminants* *- two-phase flow with breakage and coalescence* *- tray efficiency* *- drop dynamics and hydrodynamics*	*Develop models of existing systems* *Perform side-by-side comparison of existing and new processes; use to evaluate models*	*Determine effects of third-phase formation on extraction efficiency* *Develop interface controls to minimize third-phase formation*	*Increase undergraduate courses in extraction* *Increase internal communications within companies*
Mid-term (3-10 years)	*Develop highly selective solvents*	*Develop methodolgy to predict effect of surfactants and contaminants* *Develop equilibria models* *- electrodynamic effects* *- quantum-mechanical effects* *- diluent effect* *Multi-component solutes* *- fractional extraction* *- multi-component* *- extraction*	*Design large-scale homogenous extraction systems*	*Develop additives, etc., to eliminate unwanted reactions* *Determine effect of rag layers on drop coalescence at interface* *Develop structured packing with understanding of time-dependent wetting of materials* *Develop chemical coalescence aids* *Develop new devices for decantation* *Develop external field-enhanced decantation* *Quantify solids that each extract type could handle*	
Long-term (10+ years)	*Develop recovery processes*		*Commercialize large-scale homogenous extraction systems*	*Determine mechanisms for third-phase formation*	

[1] Participants prioritized categories and not individual needs within each category.

APPENDIX C: Table C.E.1 Technical Barriers for Membranes

(H= High Priority, M= Medium Priority, L= Low Priority)

Materials	Process Systems	R&D Climate/ Practices	Government Policy	Other
Inadequate selectivity for hydrogen sulfide and carbon dioxide (M)	*Membranes must fit real world (dirty) conditions (H)*	*Lack of cross-cutting fertilization among technologies and companies (H)*	*Cost of energy is too low (H)*	*Insufficient funds to take technology from bench to demonstration to commercial scale (H)*
High capital cost of robust bi-polar membranes (M)	*Existing membranes do not have cost-effective capacity (prohibitive scale-up economics) (H)*	*Too much focus on materials versus manufacturing technology (M)*	*Not enough positive incentives to drive improvements (M)*	*Too much focus on present commodity chemicals versus chemicals likely to be produced in the US in 2020 (H)*
Inadequate chemical specificity of membrane (M)	*High manufacturing costs for membranes/membrane systems (M)*	*High tolerance for poor technical performance (L)*	*Investment tax policy is not conducive to risk and new technologies (L)*	*Large risk-aversion to using membranes (M)*
Lack of in situ healing of membrane defects (M)	*Pervaporation systems/modules are too expensive (M)*	*Excessive R&D time for commodity chemicals (L)*	*Lack of key political interest (L)*	*Membranes that permit operation at lower temperatures with more favorable equilibrium conditions have inadequate flux-rate (L)*
Existing membranes do not have cost-effective capacity (L)	*Lack of membranes and modules for specific applications (L)*		*Fear of working with government (L)*	*Lack of financial and cultural infrastructure to use existing technology (L)*
Prohibitive scale-up economics (L)	*Lack of structural robustness for large modules (L)*			*Decision-makers do not understand membrane technology*
Driving force problem for dehydration systems (L)	*High cost of membrane modules for azeotropes (L)*			*Venture capitalists not interested because of small returns (L)*
Excessive methane losses (L)	*Lack of commercial membrane acceptance for some applications (L)*			*Probability of long-term sustainability of investment is low (L)*
Expensive capital/operating costs (L)	*Lack of scale-up for large processes (complete multi-stage flash for huge water treatment) (L)*			
Recovery value is too low (L)	*Lack of knowledge for use of electric fields and other novel system mechanisms at the commercial scale (L)*			
Thermodynamic constraints limit recovery (L)	*Physical constraints of current membranes at high temperatures (L)*			
Lack of recognition for membranes in the US engineering community (L)	*Lack of continuous membrane manufacturing capability (L)*			
Low separation factors (L)	*Need better technology-module design (L)* *- physical constraints* *- seals* *- pore sizes* *- inefficiency* *- module manufacturing*			
Lack of understanding / facilitated transport (chemistry) (L)	*Manufacturing technology lacking for automatic/low cost assembly (L)*			
Membranes which remove aromatics leaving paraffins behind (L)				
Membranes to make 50% oxygen from air at reasonable economics are needed to reduce cost by a factor of 2-3 (L)				
Prohibitive oxygen-enriched scale-up economics (L)				
Prohibitive scale-up economics for large volumes (L)				
Membranes must fit "real world" dirty situations (L)				
Capital cost is linear (no economy of scale for high volumes) (L)				
Reaction systems require specific designs for chemistry (technology base is narrow) (L)				
Over-engineering of new systems diminishes cost advantages (L)				

APPENDIX C: Table C.E.2 Research Needs and Other Action Items for Membranes

(H= High Priority, M= Medium Priority, L= Low Priority)

Time-Frame	Materials	Process Systems	Predictive Modeling	Applied & Basic R&D Needs	Other
All (Ongoing Processes)	*Improve long-term performance (interim products here feed other activities) (M)* *- anti-deterioration* *- schemes for regenerating activity* *- anti-fouling* *- anti-flux decline*	*Prove robustness on real streams (H)* *Integrate membrane technology with other processes (M)* *- systems approach tied to another technology* *- target augmenting existing system* *Improve operating efficiency and lower maintenance of existing membrane systems (increase efficiency via maintenance procedures) (M)* *Develop bigger cheaper modules (manufacturing technology)* *- develop entirely new concepts (L)* *Membrane platform base module/membrane designs that can be modified to suit many applications (L)* *Enhance pre-treatment of feeds (L)* *- method to prevent fouling of membrane* *- methods must maintain attractive economics* *Applications development to interchange membranes/substrate in multiple applications (L)* *Investigate sealants and practical applications in situ (e.g., hollow fiber angioplasty) (L)* *Develop low-cost sensors to indicate module problems (L)* *Sensors for membrane manufacturing processes (L)* *Perform replacement change-out of membrane module quickly (L)*	*Develop modular modeling tools (L)*	*Develop thermodynamic data for simulation of separations (L)* *Need to pursue R&D to develop more effective and reliable designs, including scale-up (L)* *Understand process-specific impact process of temperature and pressure on membrane applications (L)* *Couple economic analysis with R&D from inception (L)* *Lower R&D applications development expense (each application is unique and R&D is costly) (L)* *Run R&D tasks in parallel to reduce development times (L)* *Improve efficiency of distillation (L)* *- break azeotropes using membranes* *Focus on recycle and slip-streams rather than through-streams (L)* *Reduce time to when needed (L)*	*More thoroughly examine the future chemical industry to tailor membranes to it (M)* *Coordinate industry/academia/ government R&D (L)* *Revise funding strategies (L)* *- intelligently targeted funding* *- government funding for only economically viable processes* *Commercialize risk insurance using either a public or private entity (L)*

Time-Frame	Materials	Process Systems	Predictive Modeling	Applied & Basic R&D Needs	Other
Near-Term (0-3 Years)	*Cost-effectively increase surface area per unit volume of membrane (H)* *Develop high-temperature membranes (time-frame depends on application) (M)* *- selectivity and throughput* *- pore-size distribution* *Conduct process design and application development of existing materials into operating plants to prove reliability (L)* *Increase selectivity in membrane without reducing sensitivity or flux (L)* *Enhance structural stability (L)* *Improve membrane throughput flux (L)* *Apply existing materials in new ways for membranes (L)*	*Overcome scale-up difficulties for industrial streams (M)* *- fouling, oil mists, etc.* *Develop better sealing strategies for high temperature & pH balance (M)* *Design automated module assembly (M)* *Design automated module assembly (L)* *Develop better sealing strategies (especially for high temperatures, pH, etc.) (L)* *- improve adhesives and sealants* *Pursue multiple-module design/cycles/staging (L)* *Develop high efficiency module designs (eliminate bypassing and leakage), requiring understanding of fluid dynamics and mass transfer (L)* *Devise fabrication approaches in design (L)*	*Develop process simulation packages for membranes (e.g., hybrid modules) (M)* *- more specific modes* *- generic modules/training modules* *Improve modeling capability for more realistic systems (L)* *- better mechanistic understanding of transfer properties* *- easy to use software* *- modeling tools needed at process development stage* *Design tools for use in process design early on using pilot plant data (L)*	*Develop methods to shorten acceptance time by industry (L)* *Create government-funded demonstration facility operated by industry consortium (L)* *Membranes to reduce multiple solvent use for pharmaceuticals (L)* *R&D to understand system susceptibility (take safeguards to make membranes reliable) (L)* *Start long-term performance testing as soon as possible (L)* *Explore alternative applications for existing membranes (L)* *Develop long-term applications for other industries (L)*	*Find high potential applications in specialty chemicals (e.g., pharmaceuticals) and in "Top 100 Chemicals" (H)* *Customized delivery of reactants (L)* *Chemical reaction optimization (L)* *Facilitated transport (L)* *Hybrid systems (L)* *Membranes and electro-chemistry applications (L)* *Utilize available information exchange to share knowledge (Internet) (L)*

APPENDIX C: Table C.E.2 Research Needs and Other Action Items for Membranes (cont'd.)
(H= High Priority, M= Medium Priority, L= Low Priority)

Time-Frame	Materials	Process Systems	Predictive Modeling	Applied & Basic R&D Needs	Other
Mid-Term (3-10 Years)	*Investigate novel material concepts: (M)* *- nano-composites* *- chemically resistant properties/ characterizations* *Conduct applications development of ionic membranes in aqueous systems (bipolar) (M)* *Design/develop mixed organic/inorganic composites (mixed matrix) membranes (L)* *Design processes to modify materials/tailor properties for membrane in situ (L)* *Explore innovative new chemistries with membranes to replace traditional chemical processes (cheap peroxide) (L)* *Develop multi-function membranes (L)* *Create nano-filter selectivity with micro-filter productivity (L)* *Develop molecular sieve membranes (L)* *Develop recyclable membranes (L)* *- develop disposable membranes*	*Develop scaleable, low-cost manufacturing techniques (M)* *Step-change in ability to create surface area (M)* *Develop co-extrusion manufacturing techniques (fundamentals) (L)* *- hollow fibers* *Create a large, reproducible module for high flows (L)* *Develop intelligent controls and monitoring (L)* *- chemical/physical/ operating conditions* *Cleanly manufacture membranes (L)*	*Develop an expert database system in process design to avoid duplication (L)* *Increase understanding of surface energy interactions (L)*	*Develop membranes for fuel cells (L)* *Pursue sophisticated design approach to trade-off membrane technology vs. fluid dynamics (L)* *Develop long-term durable membrane modules (L)*	*Continue to work for government-funded demonstration facility operated by industry consortium (L)*

Time-Frame	Materials	Process Systems	Predictive Modeling	Applied & Basic R&D Needs	Other
Long-Term (10+ years)	*Develop new materials for separating hydrophilic compounds from dilute streams (M)* *- covers the entire R&D spectrum* *Develop membranes with single component recognition (i.e., hydrogen sulfide/carbon dioxide separations) (L)* *Develop regenerable/ repairable membranes (fouling, torn, damaged) rather than replace in situ (R&D should be application-specific) (L)* *Develop amorphous membranes (L)*	*Design manufacturing technology for inorganic modules (ten-fold cost reduction) (L)* *Enhance membrane performance via secondary controls (electric fields, etc.) (L)*			

APPENDIX C: Table C.F.1 Technical Barriers for Separative Reactors

(H= High Priority, M= Medium Priority, L= Low Priority)

Technical Gaps	Technology Transfer	General
Lack of simulation and scale-up capability (experience, lack of models) (H)	*Lack of multi-disciplinary team approaches to process integration (H)*	*New technologies are typically held to higher standards than existing (H)*
Lack of validated thermodynamic and kinetic data (H)	*Lack of commonality of problem because technology is application-specific (M)*	*Lack of R&D resources from industrial community (M)*
Lack of materials (e.g., integrated catalysts) with activity, selectivity, permeability, stability, and manufacturability (H)	*Separative reactors still a science rather than a technology. Lack of demonstration on a reasonable scale (prototype) (M)*	*Physical limitations to matching chemical reactors and separation technology (M)*
Lack of high-level process synthesis methodology (H)	*General lack of appreciation /understanding of potential of separative reactors (L)*	*Scale-up issues (experience, lack of models, etc.) (L)*
Radically different nature of operating systems (L)	*Lack of specific problem to address (i.e., which reaction?) (L)*	*Chemistry can change when the reactor changes. Products/processes may no longer be qualified (L)*
Difficulty of controlling distribution of reactive components in reactor (L)	*Considered as unproved technology by industry (L)*	*Large amount of existing capital already in place. Economic uncertainties of new versus established technologies (L)*
Lack of process control knowledge (L)	*Potentially resulting in loss of flexibility/degrees of freedom in process design (L)*	*Unproved reliability of the technology, real or perceived, presents a fear of risk in using new technologies (L)*
Process engineering paradigm for separative reactors missing (L)		*Short product development time makes it difficult to develop specific separative reactors and to introduce new technology (L)*
Inability of needed scientific breakthroughs in multiple disciplines to converge in compatible time-frame (L)		*Reluctance of companies to spend capital to reduce energy and waste due to lack of economic justification (L)*
Lack of understanding of the interaction of process parameters (L)		*Full costs for energy and raw materials are not carried leading to an unfair advantage for old technologies (L)*
Need for multi-disciplinary action (L)		*Lack of information on process economics (e.g., PEP spreadsheet) (L)*
Limitation of available materials (L) *- sufficiently high selectivity* *- able to operate in harsh environments*		*Lack of early process screening to qualify new process technologies (L)* *- science needs to be done efficiently (lack of early economic and process evaluation)*
		Lack of short- and long-term funding to support team approaches (L)
		Lack of information on the specific needs of manufacturing operations (L)
		Different priorities and cultures in manufacturing operations and R&D (L)
		Lack of industrial involvement (L)
		Development time to new products is shortened; less time to introduce new technology (L)
		Products may no longer be qualified if the process is changed (L)

APPENDIX C: Table C.F.2 Research Needs and Other Action Items for Separative Reactors

(H= High Priority, M= Medium Priority, L= Low Priority)

Time-Frame	Materials	Process Systems	Demonstrate Value	Fundamental Data
All (Ongoing Processes)	*Perform basic research for new chemical pathways using separative reactors (M)* *Develop new materials; new adsorbents; new membranes; high-activity, low-temperature catalysts (M)* *- more selective* *- able to operate in harsh environments* *Develop catalysts (including bio-catalysts) to better match operating conditions (L)*	*Conduct pilot and industrial scale demonstrations (M)* *Develop equipment with processing flexibility (L)*		*Develop reactive 3-D modeling (M)* *- couple computational fluid dynamics with kinetics* *- user-friendly systems needed* *Establish a program to develop better thermodynamic and kinetic data (L)* *- well-funded, coordinated, sustained* *- balance of experiment and modeling* *- prioritize key chemical reaction chains* *Include in chemistry and chemical engineering curricula (L)*
Near-Term (0-3 Years)		*Develop methods to convert existing equipment to separative reactors (M)* *Develop a systems approach (integrate research and engineering) (L)* *Evaluate existing technologies for retrofit (L)* *Evaluate the impact of recycling and reusing within the process (L)*	*Perform broad analysis of possible combinations of reactor types and separation technologies (H)* *- go beyond combinations presently known* *- include separator types, reactor types, chemistry* *Define the potential applications map (H)* *- prioritize key chemical reaction chains* *- define common model reactions* *Develop early stage economic evaluation tools (incorporating full cost accounting) (M)* *Better define environmental issues to be solved by separative reactors (L)*	*Develop analytical chemical techniques needed to get the data to model the reactors (L)* *Develop improved on-line, real-time sensors to enable sufficient process control (L)*

Time-Frame	Materials	Process Systems	Demonstrate Value	Demonstrate Feasibility	Fundamental Data
Mid-Term (3-10 Years)	*"Green" technology initiative for pharmaceuticals to deal with solvent use / impact (M)* *Develop alternate solvents (L)* *- designer* *- ionic*	*Develop separation devices with wider operating ranges (M)* *Develop new alternative reactor designs (L)* *Develop new process designs for improved thermal management (L)* *Develop alternate reaction initiation schemes (e.g., microwave plasma) (L)*		*Develop "poster child" -- industrial-scale demonstration of an important process that can be run with lower energy (L)*	*Develop new control equipment and algorithms (L)* *Develop high-level process synthesis modeling (L)*
Long-Term (10+ Years)		*Develop methods for using imperfect materials (e.g., catalytic membranes) (L)*			*Continue development of high-level process synthesis modeling (L)*

APPENDIX C: Table C.G.1 Technical Barriers to Ion Exchange

(H = High Priority, M = Medium Priority, L = Low Priority)

Fundamental Science and Data	Materials	Risk	Cost Issues
Lack of fundamental data properties for modeling (M) *Kinetics, thermodynamics (including thermodynamic limits), solubilities, organic/ inorganic species* *Mechanical properties*	*Material limitations (H)* *Loading capacity, stability* *Selectivity and specificity, such as separating metals in presence of organics and chelating agents* *Mechanical stability* *Lack of good regeneration methods (M)*	*Perceived high technical risk connected to investing in this technology (M)*	*Capital costs too high (H)*

APPENDIX C: Table C.G.2 Research Needs for Ion Exchange

(H = High Priority, M = Medium Priority, L = Low Priority)

Time-Frame	Materials	Process Systems	Fundamental Science and Modeling	Demonstrating Feasibility
All (Ongoing Processes)	*Develop new materials with high selectivity, capacity, and kinetics (H)*	*Integrate materials research and process development (M)*	*Develop improved synthesis chemistry (M)* *Develop improved modeling techniques to design ion exchangers (M)*	
Near-term (0–3 years)	*Develop more and better ion exchange forms and geometries (M)*	*Improve regeneration methods (H)*		*Demonstrate technology on important process streams to promote use of the technology (M)*
Mid-Term (3–10 years)	*Reduce manufacturing cost of ion exchangers (H)*	*Develop nonstandard ion exchange equipment (M)*		
Long-term (10+ years)	*Develop nonconventional ion exchange materials (M)*	*Develop hybrid ion exchange systems (H)*	*Develop advanced molecular modeling tools (M)*	

APPENDIX C: Table C.H.1 Technical Barriers for Bio-separations of Agricultural Crops

(H = High Priority, M = Medium Priority, L = Low Priority)

Separations	Processing	Economic/Institutional/ Regulatory	Fundamental Understanding	Feedstock
Difficulty separating desired products from other with similar compound and achieving high purity. (H) *Low concentration in fermentation broth. (H)* *Reaching high purity without conventional methods (e.g., distillation, crystallization). (H)* *Difficulty of removal of water from the feed and in the process. High water use requirement. (H)* *Solids handling is inherently more expensive than liquid handling and most bio-separations involve a solid liquid separation. (H)* *Lack of technologies to separate salt from the component you are interested in. (M)* *Industrialization of bio-separation in the main chemical industry. (L)* *Downstream processing for polymer solutions is difficult, energy-intensive, and expensive. (L)* *Protein-rich materials with broad molecular weight range are difficult to separate. (L)* *Solid separation (as in microbial mass) is difficult from fermentation. (L)* *Separation processes must be compatible (e.g., low temperature) with the biological products. (L)* *Process water or solvent reuse and reprocessing. (L)*	*Product inhibition and fermentation productivity. (H)* *Lack of technology for turning carbohydrates into effective building blocks. (L)* *Complex organic nutrient requirement for fermentation. (L)* *Handling of the bulk material, or the by-products. (L)*	*Cost and risk of process research is high and returns are uncertain. (H)* *Lack of knowledge what it cost to make a chemical from petroleum. (L)* *Current cost of energy is low. No knowledge about future. (L)* *High energy and capital cost of separations for the processes. (L)* *Short-term focus of chemical companies, other companies is developing separation technologies. (L)*	*Lack of accessibility of physical properties for biological derived chemicals. Critical tables, solubility, distribution coefficients, mathematical modeling. (H)* *Lack of on-line instrumentation for monitoring separations in fermentation. (L)* *Lack of mathematical models for bio-separation. (L)* *Science in bio-separation is still empirical rather than predictive. (L)*	*Fractionation of multi-component feeds. (M)* *Cross-contamination of natural and engineered crops. (L)*

APPENDIX C: Table C.H.2 Research Needs for Bio-separations of Agricultural Crops

(H = High Priority, M = Medium Priority, L = Low Priority)

Time-Frame	Existing Technologies	New Technologies	Fundamental Data	Biological Process Design	Economic/ Institutional/ Regulatory	Waste Management
All (Ongoing)	*Develop means to get catalytic polymer grade purities with biological feed stock (L)*	*Develop means to get catalytic polymer grade purity with biological feed stock (L)*	*Develop fundamental property data.(H)* *Fundamental R&D to make carbohydrates into useful building blocks. (L)*	*Robust bio-catalysts not inhibited by by-products or pH. High-yield catalysts biological or conventional catalysts.(H)*	*Establish national policy to get all the government agencies to work from the same agenda for bio-processing renewables (L)*	
Near-Term (0-3 Years)	*Carefully characterize capabilities of mass transfer equipment for biological feed stock.(M)* *Develop new line of sensors, analytical techniques that are robust for bio-processes (M)*		*Develop computational techniques for predicting candidates for solvent screening.(M)* *Simple and economic models for bioseparation processes. (M)* *Characterize physical properties of feed stock components to suggest separations approach. (L)*	*Explore monomers that can be made from fermentation and possible products that could be marked (L)*	*Establishment of focused research programs. (L)* *Communicate with plant scientist and chemists on separation issues. (L)* *Notify academic community about specific problems the industry is facing in bio-separations. (L)*	
Mid-Term (3–10 Years)	*More and better process separation equipment for solids handling. (M)* *Easily regenerable sorbents (L)* *Improved membranes to increase flux, eliminate fouling.(L)* *Develop membrane to pass dilute product rather than the water. (L)*	*Facilitated transport membrane to separate "like" molecules. (H)* *Develop highly selective adsorbents/ desorbents.(H)* *Continuous separation process using selective separation media.(L)*		*Develop hybrid reactors for simultaneous separations. (M)* *Develop novel, improved bio-reactor design to improve yields. (L)* *Eliminate the need for organic nutrient addition and byproduct formation. (L)* *Biological and biochemical reaction and separation in nonaqueous system (L)* *Development of robust industrial organisms. (L)*		*Better water purification and reuse. Water from different sources. Zero discharge. (H)* *Explore new ways to turn by-products into energy sources. (L)*
Long-Term (10+ Years)		*Development of next generation, lower energy, dehydration systems to remove water. (M)* *Methods (and models) for compartmen-talization of plant components containing the desired product (L)*				

APPENDIX C: Table C.H.3 Technical Barriers for Bioseparation of All Other Biomass

(H = High Priority, M = Medium Priority, L = Low Priority)

Feedstock Challenges	Process and Equipment Design/Control	Product Extraction and Recovery	Waste Management
Nonlocalization of desired chemical in plant tissues (L) *Feedstock variability leads to less pure product streams (L)*	*Inability to have closed-loop systems (M)* *Lack of continuous fermentation processes (L)* *Lack of physical properties (L)* *Scale-up issues prevent many successful bench scale processes from being implemented at larger scales (L)* *Microbial/viral contamination (L)* *Lack of interaction between customer, vendor, producer (L)* *Lack of multi-disciplinary interaction for process optimization (L)* *Need new sorbent materials and materials processing technologies (L)*	*Lack of specificity for current separation technologies (H)* *Too many purification steps for current processes (M)* *Product removal from water is difficult (M)* *Separation of commodity chemicals from green plants is not well developed (M)* *There are few effective small-scale plant separations (L)* *Physical separation of plant materials is not optimized (L)* *Poor extraction leads to disposal problems (L)*	*CO_2 recovery/emissions (M)* *Noxious odors must be removed from air streams (L)*

APPENDIX C: Table C.H.4 Research Needs for Bio-separations of All Other Bio-mass

(H = High Priority, M = Medium Priority, L = Low Priority)

Time-Frame	New Technologies	Equipment/Process Design	Materials Development	Fundamental Data	Economic/ Regulatory/ Institutional	Waste Management
All (Ongoing)	*Processes for selective fractionation (M)* *New methods to separate chiral molecules (L)* *Large scale separation of enzymes (L)*	*Control of viral contamination (M)*		*Accessible physical property databases (L)* *Thermo-physical* *Thermo-chemical* *Enzyme–substrate interaction*	*Share risk of scale up through consortium partnerships (L)* *Foster govern-ment/ industry collaborations (L)*	*Efficient separation of nitrates and phosphorous from waste streams (L)* *Downstream processing of spent biomass (L)*
Near-Term (0–3 Years)	*Methods for removing interfering molecules prior to using traditional chemical separation (M)* *Removal of organic solvents from water (L)* *Separate genetically engineered materials (L)*	*Processes to separate and recover byproducts (L)*			*Reduce regulatory impact of greenhouse gas emissions (L)*	
Mid-Term (3–10 Years)	*Processes for selective fractionation (M)*	*Need to develop closed-loop fermentation processes (H)* *Direct separations from fermentation broth to product (M)* *Need for separative reactors (non-membrane) (M)* *Design better solid fermentations (L)*	*Membrane adsorbent material development (H)* *Ionic liquids* *Solid polymers* *Tailor molecular design of adsorbents (L)* *Develop new molecules for biocatalysis (L)*	*In vitro synthesis/ processing (M)* *Synthesize narrow molecular weight ranges (M)* *Understand mass transfer characteristics by applying computational fluid dynamics (L)* *Localize products in specific part of a plant (L)*		

APPENDIX C: Table C.H.5 Technical Barriers for Bioseparations of Forest Products

(H = High Priority, M = Medium Priority, L = Low Priority)

Feed Stock	*Fundamental Data*	*Processing*	*Economic/Institutional*	*Crosscutting*
Variability of feed stocks (M) *Difficult to delignify (L)* *Multiple unit operations for feed preparation (L)* *50% of tree is wasted (L)*	*Inadequate membranes (H)* *Inefficient bio-catalysts (H)* *Lack of physical property data (H)* *Lack of genetics knowledge (L)* *Separation of lignin from black liquor (L)* *Need new chemical synthesis routes (L)*	*Separations from dilute solutions (H)* *Low solids content of black liquor (L)* *Need improved membranes for solids separations (L)* *High energy consumption (L)* *Need separations processes other than gasification (L)*	*Black liquor is not considered a feed stock for chemicals (L)* *Communication between Forestry Products and other fields (L)* *Need preliminary cost estimates early in process development (L)* *Alternative uses of forest products are not being considered (L)* *Industry not receptive to new approaches (L)*	*Lack of on-line, real-time sensors and controls (M)* *Lack of process modeling capabilities (M)* *Low value of waste streams (L)*

APPENDIX C: Table C.H.6 Research Needs for Bioseparations of Forest Products

(H = High Priority, M = Medium Priority, L = Low Priority)

Time - Frame	Feed stock	Models and Databases	Separations Processes	Biocatalysis	Economic/ Institutional/ Regulatory
Near-Term (0–3 years)		*Modeling systems are needed. May not have all the data needed. (M)* *Identify components in bio-streams to obtain higher value products. (L)*	*High temperature/composite/new materials membranes. (M)* *Better molecule configuration in membranes to fouling abatement. (M)* *Continuous methods* *Extractive fermentation* *Reactive extraction (L)* *Handle foaming and solids in extraction (L)* *Eliminate fouling in membranes (L)*	*Genetic engineering of extremophiles. (M)* *Enhance stability (L)*	*Foster joint federal/ industrial funding (L)* *Intermediate research* *Physical properties measurement/ modeling* *Establish dialogues between industries (L)*
Mid-Term (3–10 years)		*Measurements of and predictive methods for physical properties. (H)* *Modeling systems are needed. May not have all the data needed. (M)* *Comprehensive physical property database for Forestry Products. (M)*	*Smart membranes and separations systems for low concentration / high value products. (H)* *Membranes for selective chemical separations. (M)* *New extractants. (M)* *Combine membranes & ion exchange chromatography for processing under extreme conditions. (M)* *Minimize unit operations (L)* *Develop "smart" bioreactors (L)* *Develop better enzymatic recovery systems (L)* *Adsorbents with molecular recognition (L)*	*Genetic engineering of extremophiles (M)* *Better lignin degradation (L)* *Better cellulose expression (L)*	
Long-Term (10+ years)	*Genetic engineering of trees to optimize what you want (e.g. use sap instead of destroying whole tree, shape of tree). (M)* *Understand factors determining cellulose crystalinity (L)* *Understand lignin synthesis (L)*	*Develop predictive models for adsorption-type separations (L)*	*New techniques for separations of dilute streams (or combination of techniques). This includes high efficiency separations. (H)* *Separation methods for specific sugars in feedstock (L)*		

APPENDIX C: Table C.I.1 Technical Barriers to Separations from Dilute Solutions: Ionic Species from Aqueous Streams (H = High Priority, M = Medium Priority, L = Low Priority)

Fundamental Science and Data	Constraints on Current Processes	Implementation and Evolution	Institutional/Educational
Lack of fundamental property data properties for modeling (H) *Kinetics, thermodynamics, solubilities, organic/inorganic species* *Mechanical properties* *Limitations of current selectivity and specificity (M)* *Materials limitations (L)* *Temperature range, corrosion resistance, other mechanical properties* *Loading capacity, stability* *Technology limits for separating metals in the presence of organics and chelating agents (L)* *Lack of process measuring and analytical equipment for specific species and concentrations (L)*	*Low value per gallon, high capacity cost to handle dilute streams (H)* *Long residence times in contactor (M)* *Lack of processes to eliminate generation of neutralized solvents (M)* *Lack of technology to recover ions from strong acids and bases (L)* *- Thermodynamic limits* *Lack of processing capabilities for treatment of multiple components in stream (L)* *Attrition cost of separation media is greater than recovery values (L)* *- Solvent extraction losses*	*Cost and time of developing technology through pilot scale testing (H)* *Limitation on integrating new and conventional separation techniques (L)* *Small scale flexible techniques* *Hybrid systems* *Variable feed conditions* *Estimating costs of different technologies (new versus current) (L)*	*Lack of funding for frontier R&D (L)* *Short-term results mentality* *"Use-what-you-know" mentality (L)* *Risk of contaminating product stream not acceptable in testing (L)*

APPENDIX C: Table C.I.2 Technical Barriers to Separations from Dilute Solutions: Organics from Aqueous Streams (H = High Priority, M = Medium Priority, L = Low Priority)

Fundamental Understanding	Modeling	Technologies	Materials and Equipment	Institutional/ Educational
Lack of ability to manage interfacial phenomena (H)	*Inaccurate predictive tools (H)*	*Inability to design mass separating agents(H)* *Lack of recovery methods for low-value solutes (L)* *Lack of processes to handle hydrophilic solutes (L)*	*Lack of scale-up methods (H)* *Lack of on-line analysis (M)* *Salt buildup (M)* *Lack of flexible plants (M)* *Improve analytical capabilities (L)*	*Public perception (H)* *Low value and high processing costs reduce incentives to treat dilute solutions (M)*

APPENDIX C: Table C.I.3. Technical Barriers to Separations from Dilute Solutions: Contaminants from Organic Solutions (H = High Priority, M = Medium Priority, L=Low Priority)

Fundamental Understanding	Modeling	Technologies	Materials Development	Institutional/Educational
Back to basics approach to understanding separations(H) *Molecular* *Engineering* *Ecosystem* *Lack of molecular level understanding and control of material synthesis (M)* *Difficulty in predicting thermodynamic limits of dilute solutions (M)* *Liquid–liquid systems* *Solid–liquid systems* *Lack of understanding of accessible solvent alternatives (L)*	*Scale-up issues are poorly understood (H)* *Molecular-level prediction of new separations technologies is difficult (M)* *Old models developed for the chemical industry do not work for new applications in other industries (e.g., pharmaceutical, biochemical) (L)* *Thermodynamic models for liquid-liquid and solid-solid separations (L)*	*Inadequate/expensive sensing technologies exist at the online level (H)* *Equipment design and engineering understanding for new streams are poorly developed (M)* *Lack of methods to combine separative technologies in novel ways (L)*	*Lack of wide range material types (H)* *Membranes* *Extractants* *Chromatographic* *Absorbents* *Inadequate material performance characteristics (H)* *Thermodynamic limitation* *Customizing selectivity* *Mimicking biology* *Extractants* *Isomer separations* *"Easy on-off"*	*Companies tend to focus on short-term goals rather than long-term goals (H)* *Knowledge management; companies have difficulty retaining 'intellectual capital' (L)* *Lack of communication between industry and academia (L)* *Lack of complete economic assessment tools for competing separations technologies (L)* *No easy way to understand lifetime cost/ benefit analysis (L)*

APPENDIX C: Table C.I.4. Research Needs for Separations from Dilute Solutions: Ionic Species from Aqueous Streams

(H = High Priority, M = Medium Priority, L = Low Priority)

Time-Frame	Chemistry and Data	Design, Modeling, and Control	Materials and Equipment	Processing
Near-Term (0–3 years)	*Compilation of improved databases (H)* *Gather speciation data* *Real-world, multi-component mixtures* *Develop new ways to gather experimental data, etc.* *Develop new approaches to share data*	*Develop improved computer models (H)* *Predictive solution behavior* *Speciation* *Fluid mechanics (transport phenomena)* *Design of extractants* *Precipitation kinetics* *Design of systems* *Measure of confidence*		
Mid-Term (3–10 years)	*Develop complexation chemistry (H)* *For selectivity* *To reduce neutralization requirements* *Develop fast ion phase transfer chemistry (M)*	*Develop clear design evaluation methodology (M)* *Reliable control strategy for reversible reactions* *Hybrid systems* *Develop robust instrumentation for specific species (L)* *Real-time, on-line control of chemical ratios* *One-line analytical*	*Develop improved materials (H)* *Selectivity* *Operational conditions* *Robust catalysts* *Increased lifetime* *Materials that stay in one phase* *Establish dedicated pilot-plant facilities, particularly for nontraditional processing (H)* *- User facilities* *- Mobile units* *Develop readily scalable equipment design (L)*	*Develop nontraditional field-based separations (H)* *Electric* *Sonic* *Microwave* *Switchable ligands* *Increase testing of nontraditional processes in plants (M)* *Develop better recovery technology of entrained extractant phase (L)* *Develop contaminant removal techniques without affecting the product stream (L)* *Develop techniques for processing with unwanted phases (solids, gels, emulsions) (L)* *Processes that deal with various phases* *Processes that eliminate different phases*

APPENDIX C: Table C.I.5. Research and Development Needs for Separations from Dilute Solutions: Organics from Aqueous Streams

(H = High Priority, M = Medium Priority, L = Low Priority)

Time-Frame	Chemistry and Data	Design and Modeling	Materials and Equipment	Processing
Near-term (0–3 years)	*Understand computational chemistry better (H)* *Molecular interaction studies* *Extend models to strong interactions*	*Develop computational fluid dynamic models (L)* *Develop experimental screening techniques (L)* *Combinatorial chemistry* *Develop quick screening tools*	*Immobilize separating agents (H)*	*Develop hybrid processes (H)* *Complexation filtration* *Magnetic filtration* *Field-induced filtration* *Reactive extraction*

APPENDIX C: Table C.I.6 Research Needs for Separations from Dilute Solutions: Contaminants from Organic Streams

(H = High Priority, M = Medium Priority, L = Low Priority)

Time-Frame	Chemistry and Data	Design and Modeling	Materials and Equipment	Processing
Near-Term (0-3 years)	*Understand interaction of physics of separations and equipment (H)* *Understand what happens at the surface of membranes to reduce fouling (M)*	*Develop models of separations processes, particularly for hybrid systems (L)* *Integrate total cost assessment with process simulation (L)*	*Develop robust ion exchange resins for organic streams (M)* *Develop tailored adsorbents for multi-component systems (L)* *Develop sensing technologies for organic phases (L)*	*Develop hybrid systems for dilute solutions (M)*
Mid-Term (3-10 years)	*Develop better under-standing of intermolecular interactions (H)* *Develop validated, accessible property and performance databases (H)* *- Near-critical fluids* *- Alternative solvents* *- Solutes*		*Develop multi-functional materials for separation and reaction (M)*	*Develop thermodynamically efficient energy transfer (L)*
Long-Term (10+ years)	*Understand interfacial phenomena for membrane absorbents (M)*			

APPENDIX D. WORKSHOP I MONOGRAPH OUTLINE

The monograph can be ordered from CWRT by contacting:

Contact:	**Joseph E.L. Rogers**
Address:	**3 Park Avenue** **New York, NY 10016-5991**
Phone:	**212-591-7727**
Fax:	**212-591-8895**
E-mail:	**jorogers@aiche.org**

Emerging Separation and Separative Reaction Technologies for Pollution Prevention

- ADSORPTION AND MEMBRANE SYSTEMS -

A Technology Review Project

of the

Center for Waste Reduction Technologies

in collaboration with

The National Center for Clean Industrial and Treatment Technologies

and

The U.S. Department of Energy Office of Industrial Technology

Chapter 1. Adsorption, Membrane, and Separative Reactor Processes— New Developments Offer Opportunities for Pollution Prevention

Chapter 1 provides characterizations of adsorption, membrane, and separative reactor processes with respect to their applications for pollution prevention. It includes descriptions of factors which affect efficiency, covers technology status and new directions, and identifies research needs. Chapter 1 is divided up into the following subsections:

- Summary—A summary section is included in Chapter 1 giving an overview of the following topics:
  - ♦ Process Modifications to Produce Less Pollution
  - ♦ Recovery and Recycle of Potential Contaminants for Reuse within Production Unit Boundaries
  - ♦ Research Needs
- Adsorption Processes—The section on adsorption processes briefly describes the fundamentals of adsorption and adsorption processes. It includes sections on:
  - ♦ Adsorbents
  - ♦ Regeneration Cycles
  - ♦ Process Configurations
  - ♦ Advantages and Disadvantages of Adsorption Processes
  - ♦ Factors Favoring Adsorption
  - ♦ Applications Utilizing Adsorption Processes for Pollution Prevention
  - ♦ Economics of Adsorption Versus Competing Processes for Clean Air Applications
  - ♦ Future Directions
- Membrane Processes – The sections of Chapter 1 dealing with membrane processes briefly describe the fundamentals of membrane separation processes. It includes subsections on:
  - ♦ Membrane Materials
  - ♦ Membrane Modules
  - ♦ Advantages and Disadvantages of Membrane Processes
  - ♦ Factors Favoring Membrane Processes
  - ♦ Applications Utilizing Membranes for Pollution Prevention
  - ♦ Membrane Phase Contactors in Pollution Prevention
  - ♦ Future Directions

- Separative Reactor Processes – This section of Chapter 1 briefly introduces the concept of separative reactors. It includes sections on:
  - ♦ Factors Favoring Separative Reactor Processes
  - ♦ Reactive Distillation
  - ♦ Absorption Reactors
  - ♦ Adsorption Reactors
  - ♦ Membrane Reactors
  - ♦ Future Directions

Chapter 2. Adsorption Technologies

Chapter 2 provides discussion on adsorption technologies at a higher level of detail than in Chapter 1. It is designed to provide enough fundamentals to give one an application-oriented understanding of adsorption processes. The chapter is arranged as follows:

- General Overview
- Current Adsorption Processes—Discussion is given regarding current adsorption processes and how they may be classified according to application, process equipment features, or adsorbent characteristics.
- Basic Adsorbent Properties—This section discusses some of the fundamentals upon which adsorptive separations are based. The fundamental forces of adsorption which are responsible for the separation of different mixtures are presented. Several of the most commonly used adsorption equilibrium descriptions are also included.
- Molecular Simulation of Adsorption—This section discusses the state of the art in molecular simulation of adsorption, a rapidly developing field. Advances in computers and application of the methods is making it more important for adsorbent characterization and adsorption process design.
- Temperature Dependence of Adsorption—Explains the effect of temperature changes on adsorptive separations.
- Heat of Adsorption—Discusses the importance of accounting for the heat of adsorption in adsorption processes.
- Types of Adsorptive Separations—The different driving forces for adsorptive separations are presented in this section.
- Introduction to Different Adsorbents and Their Usage—There are many adsorbents available that may be categorized into different classes. This section explains the general structure and strengths of each category of adsorbents.
- Selection of an Adsorbent—Some basic guidelines are given for choosing a suitable adsorbent for a desired separation.
- Need for Equilibrium and Mass Transfer Parameters—This section describes the information that is needed to design adsorption processes.
- Industrial Implementation Considerations
- Process Configuration—This section describes several of the different process configurations that are currently available for adsorption units. This section is subdivided further into the following categories:
- Regenerative vs. Non-Regenerative Adsorption Processes
- Pressure Drop/Cost Issues
- Parallel Passage/Monolith Contactors
- Fixed Bed Systems—Explanation is given for inert purge processes, displacement purge processes, thermal swing processes, and pressure swing processes.
- Moving Bed Adsorbers—Explanation is provided for “staged” fluidized beds, rotary wheel adsorbers, and “simulated counter-current” adsorbers.
- Economic Viability of Adsorptive Separations—Discussion is presented with respect to the estimation of capital and operating costs for adsorption processes.
- Environmental Benefits and Challenges—This section provides discussion on the environmental considerations that must be accounted for with adsorption processes.

- Progress Towards Implementation, Research Needs—This section primarily discusses the research needs in adsorption technology. The research needs are broadly categorized in the following three areas:
  - Adsorbent Material Development
  - Adsorption Process Improvements
  - Advances in Engineering Design Information
- Selected Emerging and Proven Non-Reactive Uses of Adsorption—This section provides introduction of many current and emerging applications for adsorption for purification and bulk separation.
- Suppliers of Adsorbents and Adsorption Processes—A listing is included of many suppliers of adsorbents and adsorption processes.

Adsorptive Chemical Reactors

- Introduction—This section provides an introduction to adsorptive chemical reactors. It explains the rationale for adsorptive chemical reactors and their possible advantages in chemical processing. Several different classes of chemical reactors are introduced and are discussed more thoroughly in the following sections.
  - Rotating Cylindrical Annulus Chromatographic Reactor
  - Countercurrent Moving Bed Chromatographic Reactor
  - Simulated Countercurrent Moving Bed Chromatographic Reactor (SCMCR)—The SCMCR is of greater interest for practical processes and is explained in further detail in the following sections:
    - Equilibrium Stage Model—Results from an equilibrium stage model for SCMCR are presented to illustrate the possible advantages of the reactor for equilibrium limited reactions.
    - Multiple Column Configuration—A multiple column configuration version of a SCMCR is presented for the hydrogenation of mesitylene. The multiple column configuration is important from a practical standpoint.
    - Esterification of Acetic Acid—Results are discussed for a study successfully using a SCMCR for a condensed phase reaction system.
    - Reactor Dynamics—Discussion on the reactor dynamics that occur in SCMCR processes.
    - Natural Gas Utilization—Results are discussed for the oxidative coupling of methane and the partial oxidation of methane using a SCMCR.
    - Methanol Production from Synthesis Gas—The application of a SCMCR to production of methanol from synthesis gas is discussed.
  - Pressure Swing Reactor—An up to date review is provided for pressure swing reactor technology. Several applications are discussed for the chemical process industry.
  - Gas Solid Solid Trickle Flow Reactor (GSSTFR)—The three-phase GSSTFR is discussed for application to methanol production from synthesis gas.
  - Temperature Swing Reactor—The temperature swing reactor is explained and its application to the water gas shift reaction and steam methane reforming process is discussed.

Chapter 3. Membrane Technologies

Chapter 3 provides discussion on membrane separation technologies at a higher level of detail than in Chapter 1. It is designed to provide enough fundamentals to give one an application-oriented understanding of membrane processes. The chapter is arranged as follows.

- Membrane Technology Overview—The first part of this section provides a general overview in terms of the existing membrane separation processes, commonly employed membrane materials, membrane module types, and membrane selection guidelines. The second part will discuss a variety of engineering, economic, environmental and energy considerations intrinsic to the introduction of membrane separation technologies into chemical processes and systems.
  - General Overview—Discussion is provided in this section regarding the fundamental mechanisms for membrane separations. The importance of membrane flux and permeability is explained.
  - Existing Membrane Separation Processes—This section provides a brief introduction to different membrane separation processes employed in industrial practice. The following membrane separation processes are discussed in more detail:

- Reverse Osmosis
- Nanofiltration
- Ultrafiltration
- Microfiltration
- Dialysis
- Electrodialysis
- Emulsion Liquid Membranes
- Pervaporation
- Membrane-Based Stripping
- Membrane Gas Permeation
- Vapor Permeation
- Membrane-Based Gas Absorption

♦ Membrane Materials—There are many membranes available that may be categorized into different classes. This section explains the general structure and strengths of each category of adsorbents.

♦ Membrane Modules—The important features of different membrane module designs are discussed. The following module designs are investigated in more detail:
- Flat Membrane Modules
- Hollow Fiber Modules
- Tubular Membrane Modules

♦ Membrane Systems—The important features of incorporating membrane modules into a membrane system are discussed in this section. Several different operating schemes for membrane systems are discussed.

■ Selected Emerging Non-Reactive In-Process Waste Reduction Membrane Applications—This section introduces several applications for membranes to reduce process waste.

♦ Membrane Gas Separation Opportunities in the Control of Greenhouse Effect—Membranes hold potential as a low cost carbon dioxide mitigation path to reduce carbon dioxide emissions in flue gases. They may also be used to remove carbon dioxide from low grade natural gas and from synthesis gases. The possible application of membranes for these processes is discussed in detail. Recovery of carbon dioxide using selective gas separation membranes (polymeric and ceramic) is discussed. Membrane Gas-Liquid Contactors are introduced for removing carbon dioxide.

♦ Solvent Vapor Recovery from Gas Streams—Membranes are capable of solvent vapor recovery in many instances. This section describes the latest technologies for recovering solvent vapors with membranes. The different membranes and modules available for this task are explained in detail. Applications are presented for solvent recovery from polyolefin polymerization vents and distillation vents.

♦ Metal Ion Recovery from Aqueous Waste Streams—Many different selective separations involving metal recovery and water reuse are examined. Guidelines are presented for selecting membranes capable of metal recovery. Module design is discussed since it is very important for metal recovery from complex waste streams. Advanced processes for metal removal including ligand enhanced membrane processing and functionalized microfiltration are discussed. Membrane contactors are introduced for use in metal separation. Also, a set of guidelines for choosing an appropriate membrane system for metals separation is included.

♦ Pervaporation/Aqueous Streams—Application of pervaporation for removal of VOCs from aqueous streams is discussed in this section. The different aspects of pervaporation system design are discussed. The competitive position of pervaporation with other technologies is presented.

Membrane Reactors

■ Overview—This section provides an introduction to membrane reactors. It explains the rationale for membrane reactors and their possible advantages in chemical processing. The different types of membrane reactors that exist are explained. The different types of reactions amenable to improvement with membrane reactors are also presented in this section. The issues critical in determining the suitability of combining reaction and separation in a membrane reactor are discussed. Membrane materials suitable for including in a membrane reactor are also included.

■ Hydrocarbon Selective Oxidation—Membrane reactors are discussed as a means to increase per pass yields and selectivities for hydrocarbon partial oxidation reactions. An example of this technology is presented for an oxidative coupling reaction. Synthesis gas production is also discussed using ionic conducting dense membranes.

Practical considerations such as scale-up, heat removal, design for membrane failure, fouling issues, and regeneration methods are included.

- Dehydrogenation Reactions—The use of membrane reactors for improving the equilibrium conversion and selectivity of dehydrogenation reactions is discussed. The membrane materials investigated for use in this type of reactor are presented and the economics of the membrane reactor process are examined.

Chapter 4. Results of February 1998 Separations Workshop

Chapter 4 documents the February 1998 Separations Workshop held in New Orleans, LA. The chapter includes summaries of the plenary lectures at the workshop, panel discussions, and breakout sessions.