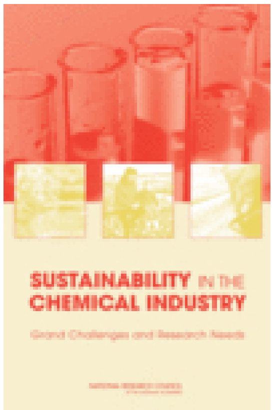

Sustainability in the Chemical Industry: Grand Challenges and Research Needs - A Workshop Report

Committee on Grand Challenges for Sustainability in the Chemical Industry, National Research Council

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SUSTAINABILITY IN THE CHEMICAL INDUSTRY

Grand Challenges and Research Needs

Committee on Grand Challenges for Sustainability in the Chemical Industry

Board on Chemical Sciences and Technology

Division on Earth and Life Studies

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Preface

Key players in chemistry and chemical engineering sectors believe that generating economically viable alternatives to current reliance on fossil fuels and business practices that degrade the regenerative capabilities of natural systems—sustainability—are critical to global leadership by the U.S. chemical industry. Government interest in sustainability revolves around assuring the future environmental and economic integrity of the nation, while industrial interest usually arises from a concern for the long-term viability of a company or an entire industry.

An interagency group has been meeting informally on the topic of science for sustainability for several years. Membership in this group includes officials from the Environmental Protection Agency (EPA), National Institute of Standards and Technology (NIST), National Science Foundation (NSF), the Department of Energy (DOE), the National Institutes of Health (NIH), the Department of Agriculture (USDA), and the Food and Drug Administration (FDA). Members of this group have been meeting with representatives from organizations such as the American Chemical Society (ACS), the American Institute of Chemical Engineers (AIChE), the American Chemistry Council, and the Council for Chemical Research to focus on the goal of achieving a "sustainable chemical enterprise". This subgroup wants to increase the application of the principles of sustainability to decision-making in the chemical industry by improving the science and technology base that can inform such decisions.

The Committee on Grand Challenges for Sustainability in the Chemical Industry, established by the National Academies, through its Board on Chemical Sciences and Technology (BCST), was asked to assist this group of government and non-governmental representatives in defining a path forward for the chemical industry in this area. The committee was composed of 10 experts in the areas of: chemistry, chemical synthesis and process engineering, green chemistry and engineering approaches and education, biotechnology, agricultural chemicals, petrochemicals, pharmaceuticals, industrial research management, business strategy and innovation, toxicology, and environmental health and safety. The group met nine times via teleconference to plan the workshop held February 7-8, 2005 in Washington, DC. The full committee met for the first time in a face-to-face meeting held in conjunction with the workshop. The fundamental premise of the committee's efforts throughout this study was to focus attention on those areas posing the greatest science and technical challenges for addressing sustainability in the chemical industry. The committee would like to thank all the organizations funding the study for recognizing the need to provide leadership and help stimulate work to address sustainability in the chemical industry. Major sponsors include the American Chemical Society, the U.S. Environmental Protection Agency, Los Alamos National Laboratory (U.S. Department of Energy), and the National Science Foundation, with additional sponsorship from the National Institute of Standards and Technology, and the American Institute of Chemical Engineering.

Jim Trainham,
Chair

Acknowledgment of Reviewers

This workshop report has been reviewed in draft form by persons chosen for their diverse perspectives and technical expertise in accordance with procedures approved by the National Research Council's Report Review Committee. The purpose of this independent review is to provide candid and critical comments that will assist the institution in making the published report as sound as possible and to ensure that it meets institutional standards of objectivity, evidence, and responsiveness to the study charge. The review comments and draft manuscript remain confidential to protect the integrity of the deliberative process. We wish to thank the following individuals for their review of this report:

Dr. R. Stephen Berry, University of Chicago, Chicago, IL
Dr. William L. Chameides, Environmental Defense, New York, NY
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Mr. Sam Smolik, Shell Chemical, Houston, TX
Dr. Jack Solomon, Praxair, Inc., Danbury, CT
Dr. John C. Warner, University of Massachusetts, Lowell, MA

Although the reviewers listed above have provided many constructive comments and suggestions, they did not see the final draft of the workshop report before its release. The review was overseen by Dr. W.

Carl Lineberger, University of Colorado, Boulder, CO, appointed by the National Research Council and Dr. David C. Bonner, Intellectual Property Business International, LLC, Houston, TX, appointed by the Division on Earth and Life Studies, who were responsible for making certain that an independent examination of this report was carried out in accordance with institutional procedures and that all review comments were carefully considered. Responsibility for the final content of this report rests entirely with the authors and the institution.

Contents

Executive Summary

The purpose of this study was to assist the chemical "industry"[1] in defining the necessary research objectives to enable the ongoing transition towards chemical products, processes, and systems that will help achieve the broader goals of sustainability. Based largely on the results of a workshop held February 7-8, 2005, and the knowledge and experience of organizing committee members, this report identifies a set of overarching Grand Challenges for Sustainability in chemistry and chemical engineering, and makes recommendations about areas of research needed to address those Grand Challenges. At the same time, this report is not inclusive of every research topic of relevance to sustainability, and it does not provide an in-depth economic analysis or policy assessment of all that is needed to achieve sustainability in the chemical industry—such as regulation and other government policies that have been historically critical in driving needed changes. The report is meant as a starting point for further analysis, with a focus on those areas that present unique challenges and opportunities where the chemical industry and

[1]Throughout this report the committee uses the term "chemical industry" in its broadest sense—which encompasses allied industries such as pharmaceuticals and agricultural chemicals as well as educational practices that ultimately feed into the industry—that is, all those entities involved in the lifecycle of chemicals. Sometimes this broad definition of the chemical industry is referred to elsewhere as the "chemical enterprise," or "chemical and allied industries." Use of the term "chemical processing industry" specifies only that part of the industry involved in the actual manufacturing of chemicals.

government research and development funding efforts can help address larger sustainability goals.

In the context of this report, "sustainability" is a path forward that allows humanity to meet current environmental and human health, economic, and societal needs without compromising the progress and success of future generations.[2,3] Sustainable practices refer to products, processes, and systems that support this path. For example, such processes might involve developing new energy resources to meet societal needs; but to be sustainable they must also be economically competitive and not cause harm to the environment or human health. The Grand Challenges and research needs identified in this report warrant further attention (largely through research investment) because one or more of the three criteria of sustainability is lacking. Working toward such sustainability goals is thus both wide in scope and deep in complexity. Addressing sustainability necessarily cuts across all disciplinary boundaries and requires a broad system view to integrate the different and competing factors involved. This includes "strategic connections between scientific research, technological development, and societies' efforts to achieve environmentally sustainable improvements in human well-being,"[4] and involves the creative "design of products, processes, systems, and organizations, and the implementation of smart management strategies that effectively harness technology and ideas to avoid environmental problems before they arise."[5] In this report, progress in the chemical industry is considered within these broader efforts to address sustainability.

There are more than 80,000 chemicals registered for use in the United States, and an estimated 2,000 new ones introduced each year.[6] Modern society depends on, and greatly benefits from having most of these chemicals in the market place. According to the American Chemistry Council,[7] "the business of chemistry [in the United States] is a $460 billion enterprise[8] and is a key element of the nation's economy . . . Chemistry compa-

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[2]World Commission on Environment and Development. 1987. *Our Common Future* (The "Brundtland" Report). Oxford: Oxford University Press. National Research Council. 1999. *Our Common Journey: A Transition Toward Sustainability*. Washington, D.C.: National Academy Press.

[3]Graedel, T. E., and B. R. Allenby. 1995. *Industrial Ecology*. New Jersey: Prentice Hall.

[4]National Research Council. 1999. *Our Common Journey: A Transition Toward Sustainability.* Washington, D.C.: National Academy Press.

[5]National Academy of Engineering. 1997. *The Industrial Green Game: Implications for Environmental Design and Management*. Washington, D.C.: National Academy Press.

[6]National Toxicology Program:*http://ntp-server.niehs.nih.gov/*

[7]*www.americanchemistry.com*

[8]This is about 26 percent of the global chemical production.

nies invest more in research and development than any other business sector." However, the effects of many chemicals on human health and the environment are far from benign, and are often largely unknown. Monitoring and controlling chemicals in the environment is also costly; each year more than $1 billion is spent just on cleaning up hazardous waste Superfund sites.[9]

Trends in fossil fuel consumption as well as compliance with regulatory policies have led to a significant evolution of the chemical processing industry (CPI) over the past 50 years. These forces, combined with transparency requirements, liability risks, and health indicators make sustainability goals, along with innovation, increasingly integral components of a company's ability to compete in the marketplace. These goals in the business world are now often referred to as the "triple bottom line."[10] At the same time, the trend toward decreasing,[11] or at least flat research and development spending in industry as a whole makes it difficult to advance the scientific knowledge to support these goals.

Going forward, the chemical industry is faced with a major conundrum—the need to be sustainable (balanced economically, environmentally, and socially in order to not undermine the natural systems on which it depends)—and a lack of a more coordinated effort to generate the science and technology to make it all possible. As the feedstock industry for modern society, the chemical industry thus plays a major role in the sustainability effort—to advance the science and technology to support the design, creation, processing, use, and disposal of chemical substances that provide a foundation for sustainability.

The set of Grand Challenges and accompanying research needs to move towards chemical products, processes, and systems that will help achieve the broader goals of sustainability are summarized below. Although the Grand Challenges are numbered, they are all important in the context of this report and to the triple bottom line of the chemical industry now and in the future. However, Figure ES-1 illustrates how the different Grand Challenges (ovals) address the sustainability transition (large arrows) from the current paradigm to the ideal vision over the course of two critical time frames:

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[9]Government Accountability Office. June 30, 2005. *Hazardous Waste Programs: Information on Appropriations and Expenditures for Superfund, Brownfields, and Related Programs*. GAO-05-746R.

[10]Elkington, J. 1997. in *Cannibals with Forks: The Triple Bottom Line of 21st Century Business.* Oxford: Capstone Publishing.

[11]NSF (National Science Foundation) *InfoBrief* (NSF 04-320). May, 2004. Largest Single-Year Decline in U.S. Industrial R&D Expenditures Reported for 2002.

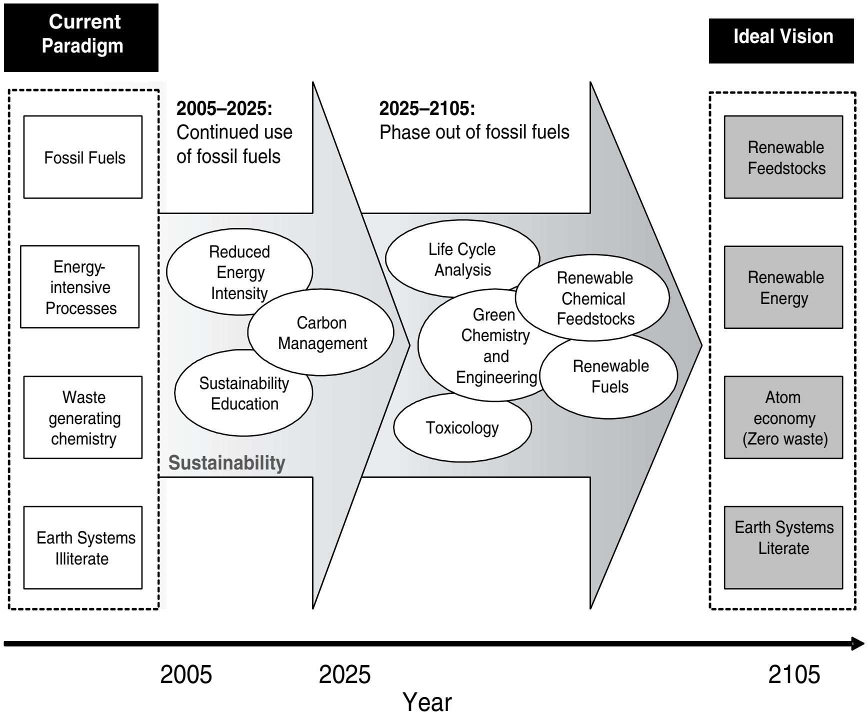

FIGURE ES-1 The Grand Challenges (ovals) for Sustainability (large arrows) that address the transition from current thinking to the ideal vision for the chemical industry over the next 100 years. See text for a more detailed description of figure and the Grand Challenges.

1. The next 20 years (2005–2025) of continued use of fossil fuels (especially oil) as the predominant source of energy and chemical feedstocks, where managing carbon, reducing the intense use of energy resources, and educational efforts to promote sustainability thinking will be critical; and

2. The next 20–100 years (2025–2105) in which the use of fossil fuels will be phased out, and where the ability to carry out green chemistry and engineering (built on fundamental understanding of the full life cycle impacts and toxicology of chemicals), and having access to alternative renewable sources of fuels and feedstocks will be critical.

GRAND CHALLENGES

The eight Grand Challenges below were chosen because they were considered to pose the greatest science and technical challenges for addressing sustainability—balanced economic, environmental, and societal progress—in the chemical industry over the next 100 years.

1. Green and Sustainable Chemistry and Engineering

Grand Challenge: Discover ways to carry out fundamentally new chemical transformations utilizing green and sustainable chemistry and engineering, based on the ultimate premise that *it is better to prevent waste than to clean it up after it is formed.*[12,13] Over the next twenty years this will involve replacing harmful solvents or improving catalytic selectivity and efficiency in chemical reactions that also provides cost savings. This area will grow in importance as fossil fuels are phased out of use and alternative and innovative approaches are required.

Research Needed:

- Identify appropriate solvents, control thermal conditions, and purify, recover, and formulate products that prevent waste and that are environmentally benign, economically viable, and generally support a better societal quality of life.

2. Life Cycle Analysis

Grand Challenge: Develop life cycle tools to compare the total environmental impact of products generated from different processing routes and under different operating conditions through the full life cycle. This is another area that is already being explored, but will play an increasingly significant role in the chemical industry in the longer term as fossil fuels are phased out of use and application of green chemistry and engineering practices become critical.

Research Needed:

- Improvements are needed in the quantity and quality of data required for such comparisons and in the approach used to evaluate life cycle metrics. There needs to be an appropriate understanding of the methodology of life cycle analysis, the influence of the life cycle inventory

[12]Anastas, P. T., and J. Warner. 1998. *Green Chemistry Theory and Practice*. Oxford: Oxford University Press.

[13]Poliakoff, M., J. M. Fitzpatrick, T. R. Farren, and P. T. Anastas. 2002. Green Chemistry: Science and Politics of Change. *Science* 297:807–810.

data on the analysis results, the interpretation of the results, and how the results will be used.

3. Toxicology

Grand Challenge: Understand the toxicological fate and effect of all chemical inputs and outputs of chemical bond forming steps and processes. This is already an area of concern for the chemical industry, and will be increasingly important as fossil fuels are phased out of use and application of green chemistry and engineering practices become critical.

Research Needed:

- Development of critical tools for improved understanding of structure-function relationships for chemicals and chemical mixtures in humans and the environment. This includes computational and genomic approaches.
- Development of methods to communicate this information to effectively move it from science disciplines and bench research to application in product designs.

4. Renewable Chemical Feedstocks

Grand Challenge: Derive chemicals from biomass—including any plant derived organic matter available on a renewable basis, dedicated energy crops and trees, agricultural food and feed crops, agricultural crop wastes and residues, wood wastes and residues, aquatic plants, animal wastes, municipal wastes, and other waste materials.[14] This is a long term challenge that will become increasingly important as fossil fuels are phased out over the next 100 years.

Research Needed:

- Development of a catalog of biomass derived chemicals, building on what DOE has already begun,[15] to provide the research community with starting points in the development of alternative pathways to achieve the desired end materials.
- Explore obtaining current basic chemicals such as simple aliphatics and aromatics, as well as fundamentally new compounds from platforms such as lignin, sugar, or cellulose.
- Improve biomass processing—including pretreatment as well as

[14] U.S. Department of Energy definition.

[15] U.S. DOE Biomass Program. August 2004. *Top Value Added Chemicals from Biomass, Volume 1: Results from Screening for Potential Candidates from Sugars and Synthesis Gas*. Report #35523.

the breakdown processes for transforming biomass material into chemicals. This requires a better understanding of the basic chemical pathways involved in biomass conversion processes as well as separation or extraction processes to isolate the basic chemicals from biomass.

5. Renewable Fuels

Grand Challenge: Lead the way in the development of future fuel alternatives derived from renewable sources such as biomass as well as landfill gas, wind, solar heating, and photovoltaic technology.[16] This is another long term challenge that will become increasingly important as fossil fuels are phased out over the next 100 years.

Research Needed:

- In the area of solar energy technology:
  — reduce the cost and environmental impact of producing photovoltaic systems;
  — directly use solar energy for cost-effective splitting of water to produce hydrogen;
  — improve heat transfer fluids that enable direct use of solar energy for meeting some of the heating requirements of the CPI; and
  — advance storage systems for solar generated electric power.
- Simultaneously develop biomass derived fuels together with chemical feedstocks (Grand Challenge 4), while addressing the energy intensity of chemical processing (Grand Challenge 6). While the growing need for sustainable energy can be met by improvements in capturing and utilizing renewable resources such as solar, wind, and geothermal, and biomass, biomass is the only renewable resource that produces carbon-based fuels and chemicals.

6. Energy Intensity of Chemical Processing

Grand Challenge: Continue to develop more energy efficient technologies for current and future sources of energy used in chemical processing. Addressing this challenge will be critical during the continued use of fos-

[16] It should be noted that nuclear energy is often mentioned as a potential long-term source of energy as an alternative to fossil fuels. As pointed out in the workshop and elsewhere, current (fission based) nuclear reactor technology does provide electricity without carbon dioxide emissions. However, it also generates highly toxic wastes, presents safety and security concerns for centuries (half life of plutonium is 24,100 years), and utilizes limited uranium resources; thus it is not a sustainable energy option. At the same time, nuclear technology based on the energy released by the fusion of deuterium and tritium is a promising long-term energy source (greater than 30 years) without the negative attributes of nuclear fission, but it still requires significant research advances to make it a viable option.

sil fuels as the predominant source of energy and chemical feedstocks over the next 20 years, and will continue to be important even when renewable energy resources are predominant.

Research Needed:

- Develop more energy and cost efficient chemical separations, especially effective alternatives to distillation.
- Explore biotechnology and other emerging technological solutions. Research and development needs in these areas include reducing production costs, increasing stability, and discovering catalysts with greater specificity.
- Better understand the mechanisms of friction, lubrication, and wear of interacting surfaces (tribology)—which leads to *one third* of the loss of the world's energy resources in present use. [17]

7. Separation, Sequestration, and Utilization of Carbon Dioxide

Grand Challenge: Develop more effective technology and strategies to manage the resulting carbon dioxide (CO_2) from current and future human activity. Addressing this challenge will also be critical during the continued use of fossil fuels as the predominant source of energy and chemical feedstocks over the next 20 years, and will continue to be important as long as carbon based fuels are in use.

Research Needed:

- Develop energy and cost efficient technologies (Grand Challenge 6) for CO_2 separation from flue gas and the atmosphere.
- Develop technologies for CO_2 sequestration that will address the technical feasibility of making and storing compressed forms of CO_2 in geological formations and elsewhere.
- Explore utilizing low cost, nontoxic, and renewable CO_2 as a feedstock for entirely new materials and for new routes to existing chemicals such as urea, salicylic acid, cyclic carbonates, and polycarbonates.[18]

8. Sustainability Education

Grand Challenge: Improve sustainability science literacy at every level of society—from informal education of consumers, citizens and future scientists, to the practitioners of the field, and the businesses that use and sell these products. Advances in chemistry and engineering must be ac-

[17] Bhushan, B., ed. 1996. *Handbook of Micro/Nano Tribology*. Boca Raton, Florida: CRC Press.

[18] Marks, T. J. et al., 2001. Catalysis Research of Relevance to Carbon Management. *Chemical Reviews* 101(4):973–975.

companied by cross-disciplinary education in sustainability science and its application to the business community. This includes greater understanding of earth systems science and engineering, ecology, green chemistry, biogeochemistry, life cycle analysis, toxicology. Addressing this challenge will be critical over the next 20 years as changes in thinking are needed to make the transition to more sustainable processes, products, and systems.

Research Needed:

- Provide professional development opportunities for educators to learn more about sustainability and how it can be advantageously incorporated into their research and teaching. This includes providing incentives for faculty to change curricula while addressing the needs of graduate students entering this complex field.
- Persuade professional societies to integrate sustainability and green chemistry and engineering concepts into standardized testing, accreditation, and certification programs such as those developed by the ACS Committee on Professional Training or ABET (Accreditation Board for Engineering and Technology). This also includes developing educational materials such as lab modules, LCA modules, and new textbooks that infuse sustainability and green chemistry concepts into the core material.
- Incorporate sustainability concepts across secondary and tertiary education curricula. This includes chemistry and chemical engineering as well as the educational practices in professional schools such as medicine, law, and business, with particular emphasis on management education and schools that educate buyers, advertisers, and designers of consumer goods.
- Provide professional development for current and future managers and executives. Equally important is the communication of sustainability thinking to middle and upper level managers and executives in business management and incorporation of sustainability objectives in annual performance goals as well as corporate strategy.

1

Introduction

Nearly 150 years ago, English chemist William Perkin set out to synthesize the alkaloid quinine from coal tar in an attempt to help treat malaria. He did not succeed in synthesizing quinine, but what he did do was create the beautiful purple dye—mauve—which would forever change everything from fundamental chemical synthesis and the design of the latest fashions, to the state of the physical environment and human health. It was the beginnings of using fossil fuel-derived hydrocarbons as the foundation of the twentieth century industrial revolution.

Today, modern society continues to depend on fossil fuel based hydrocarbons to make dyes and develop almost every chemical or material in the market place. Fossil fuels also serve as the main source of energy. But it is not clear this dependence can continue long into the future. One of the main issues with this dependence is that the combustion of fossil fuels produces carbon dioxide (CO_2) and other waste products such as particulate matter, which end up in the atmosphere and have significant consequences for human health and the environment. It is generally accepted that the rise in concentrations in CO_2 is causing global climate change[1]—warming the atmosphere, which in turn is causing sea level to rise. The CO_2 absorbed by the oceans is in turn acidifying the water. Another significant issue involves reliability of global fossil fuel supplies.

There is a need to examine this situation and attempt to map a path

[1]"Joint science academies' statement: Global response to climate change," *http://nationalacademies.org/onpi/06072005.pdf*

forward that is sustainable—which allows humanity to meet current environmental, economic, and societal needs without compromising the progress and success of future generations.[2] As the feedstock industry for modern economies, the chemical industry plays a major role in advancing the sciences and applications to support this—to work toward the design, creation, processing, use, and disposal of substances that better support the goals of sustainability.

SUSTAINABILITY AND CHEMICALS

According to the American Chemistry Council,[3] "the business of chemistry [in the United States] is a $450 billion enterprise [about 26 percent of the global chemical production] and is a key element of the nation's economy. It is the nation's largest exporter, accounting for ten cents out of every dollar in U.S. exports. Chemistry companies invest more in research and development than any other business sector." As a result of trends in fossil fuel supplies, as well as compliance with chemical regulatory policies, business drivers for the chemical industry have evolved significantly over the past 50 years. There is an increasingly competitive landscape. Once a major net exporter, the U.S. chemical industry is now essentially a net importer (trade went negative in 2000–2001).[4] These forces combined with transparency requirements, liability risks, and health indicators make sustainability goals, along with innovation, increasingly integral components of a company's ability to compete in the marketplace.[5] Go to the web site of any global top 50 chemical companies[6]—from the top three, Dow Chemical, BASF, and DuPont who each have 2004 sales in the $30-40 billion range, to number 45 on the list Lyondell Chemical with 2004 sales of about $6 billion—and there will be a statement of commitment to achieving sustainability goals. For example, the following statement appears on the Lyondell web site:

> We aim to achieve excellence in every aspect of our economic, social, and environmental performance. We are committed to operating our world-

[2]World Commission on Environment and Development. 1987. *Our Common Future* (The "Brundtland" Report). Oxford: Oxford University Press. National Research Council. 1999. *Our Common Journey: A Transition Toward Sustainability*. Washington, D.C.: National Academy Press.

[3]*www.americanchemistry.com*

[4]Storck, W. J. 2005. "UNITED STATES: Last Year Was Kind to the U.S. Chemical Industry; 2005 Should Provide Further Growth." *Chemical and Engineering News* 83(2):16–18.

[5]Bakshi, B. R., and J. Fiksel. 2003. The Quest for Sustainability: Challenges for Process Systems Engineering. *AIChE Journal* 49(6):1350–1358.

[6]Short, P. L. 2005. Global Top 50. *Chemical and Engineering News* 83(29):20-23.

wide business in a way that brings the greatest benefit to all of our stakeholders (employees, customers, investors, communities) and builds a sustainable future for generations to come,

One of the ways in which Lyondell says they work toward achieving these goals is by: "Investing in product and service innovations that use natural resources, as well as social and financial resources, in an efficient, effective, and economic manner over the long-term." Achieving such goals in the business world, including the chemical industry, is often referred to as the "triple bottom line."[7] Many chemical companies are now even part of investment indexes such as FTSE4Good and the Dow Jones sustainability indexes that seek to raise business standards and investor awareness by tracking the financial performance of leading sustainability-driven companies.

However, the trend toward decreasing or at least flat research and development spending by the top 50 chemical companies and in industry as a whole[8] (Figure 1.1) makes it difficult to advance the science and technology needed to support such sustainability goals. Going forward, the chemical industry is faced with a major conundrum—the need to be sustainable, a desire to support science and technological innovation, and a lacking investment in fundamental research and development to make it all possible.

Despite these overall conditions, many companies are making the extra effort to advance sustainability goals. Pharmaceutical companies in particular have been quite successful. In 2002, prescription and over the counter drug companies invested more than $32 billion in discovering and developing new medicines, marking the thirty-second straight year the industry has increased its investment in R&D.[9] As part of this effort, many companies are turning to green chemistry—"the design, development, and implementation of chemical processes and manufactured products to reduce or eliminate substances hazardous to human health and the environment"[10]—and applying the twelve principles[11] (Box 1.1) to redesign their active pharmaceutical ingredient (API) manufacturing processes. In this way, they have been able to dramatically reduce wastes generated. This success is highlight by the fact that five of the 52 winners

[7]Elkington, J. 1997. In *Cannibals with Forks: The Triple Bottom Line of 21st Century Business.* Oxford: Capstone Publishing.

[8]NSF (National Science Foundation) *InfoBrief* (NSF 04-320). May, 2004. Largest Single-Year Decline in U.S. Industrial R&D Expenditures. Reported for 2002.

[9]See the Pharmaceutical Research and Manufacturers of America web site: *www.phrma.org*

[10]Anastas, P. T., and J. Warner. 1998. *Green Chemistry Theory and Practice*. Oxford: Oxford University Press.

[11]Poliakoff, M., J. M. Fitzpatrick, T. R. Farren, and P. T. Anastas. 2002. Green Chemistry: Science and Politics of Change. *Science* 297:807–810.

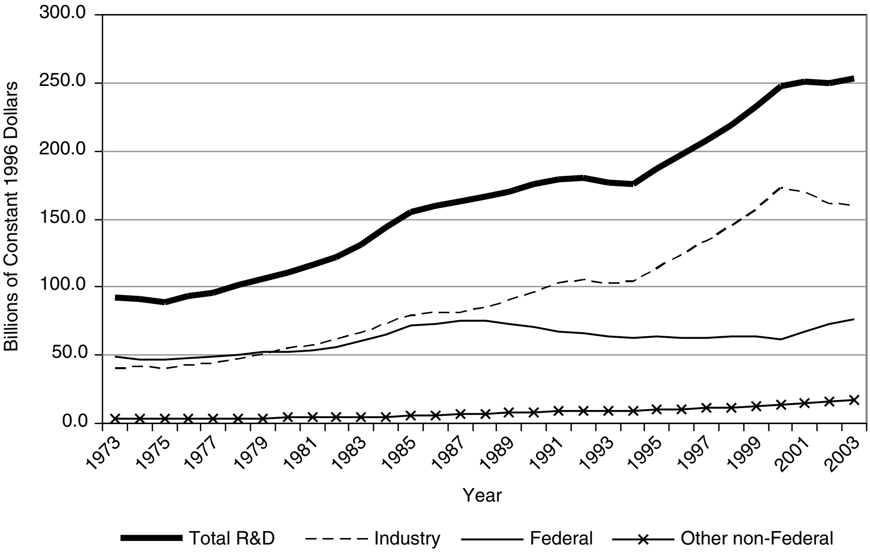

FIGURE 1.1 U.S. research and development funding, by source of funds: 1973–2003. SOURCE: National Science Foundation, Division of Science Resources Statistics, National Patterns of R&D Resources, annual series, appendix tables B-2 and B-22.

of a U.S. EPA Presidential Green Chemistry Award[12] are members of the pharmaceutical industry: Lilly (1999), Roche (2000), Pfizer (2002), Bristol Meyers Squibb (2004), and Merck (2005), which have all reported such kinds of improvements when green chemistry principles are applied.

Green chemistry thus offers a viable path for achieving sustainability goals across the chemical industry. That is, there is the potential to develop industrial technologies that could provide goods, products, and services in a way that does not reduce the supply chain of resources, harm the environment and human health, or limit the opportunities and choices for future generations.

More recently, a complimentary set of green engineering principles was developed (Box 1.2).[13] Together with green chemistry, the application of these principles ideally provide one or more of the following benefits:

- Lower costs of chemical processing
- Require less energy

[12]See EPA Presidental Green Chemistry Challenge web site: *http://www.epa.gov/greenchemistry/presgcc.html*

[13]Ritter, S. K. 2003. A Green Agenda for Engineering. *Chemical and Engineering News*. 81(29):30–32.

BOX 1.1 The Twelve Principles of Green Chemistry

1. **Prevent waste:** Design chemical syntheses to prevent waste, leaving no waste to treat or clean up.
2. **Design safer chemicals and products:** Design chemical products to be fully effective, yet have little or no toxicity.
3. **Design less hazardous chemical syntheses:** Design syntheses to use and generate substances with little or no toxicity to humans and the environment.
4. **Use renewable feedstocks:** Use raw materials and feedstocks that are renewable rather than depleting. Renewable feedstocks are often made from agricultural products or are the wastes of other processes; depleting feedstocks are made from fossil fuels (petroleum, natural gas, or coal) or are mined.
5. **Use catalysts, not stoichiometric reagents:** Minimize waste by using catalytic reactions. Catalysts are used in small amounts and can carry out a single reaction many times. They are preferable to stoichiometric reagents, which are used in excess and work only once.
6. **Avoid chemical derivatives:** Avoid using blocking or protecting groups or any temporary modifications if possible. Derivatives use additional reagents and generate waste.
7. **Maximize atom economy:** Design syntheses so that the final product contains the maximum proportion of the starting materials. There should be few, if any, wasted atoms.
8. **Use safer solvents and reaction conditions:** Avoid using solvents, separation agents, or other auxiliary chemicals. If these chemicals are necessary, use innocuous chemicals.
9. **Increase energy efficiency:** Run chemical reactions at ambient temperature and pressure whenever possible.
10. **Design chemicals and products to degrade after use:** Design chemical products to break down to innocuous substances after use so that they do not accumulate in the environment.
11. **Analyze in real time to prevent pollution:** Include in-process real-time monitoring and control during syntheses to minimize or eliminate the formation of byproducts.
12. **Minimize the potential for accidents:** Design chemicals and their forms (solid, liquid, or gas) to minimize the potential for chemical accidents including explosions, fires, and releases to the environment.

BOX 1.2 Green Engineering Principles

1. Engineer processes and products holistically, use systems analysis, and integrate environmental impact assessment tools.
2. Conserve and improve natural ecosystems while protecting human health and well-being.
3. Use life-cycle thinking in all engineering activities.
4. Ensure that all material and energy inputs and outputs are as inherently safe and benign as possible.
5. Minimize depletion of natural resources.
6. Strive to prevent waste.
7. Develop and apply engineering solutions, while being cognizant of local geography, aspirations, and cultures.
8. Create engineering solutions beyond current or dominant technologies; improve, innovate, and invent (technologies) to achieve sustainability.
9. Actively engage communities and stakeholders in development of engineering solutions.
10. There is a duty to inform society of the practice of green engineering.

- Produce both basic and fine chemicals in a way that is less hazardous to both humans and ecosystems.
- Be a source of chemical substitutes that improve quality of life.
- Provide a way of ensuring prosperity and social wealth.

At the same time, there are barriers that exist in developing and implementing these green chemistry and engineering principles. A study by RAND[14] identified a set of barriers which fall into four main areas:

1. Lack of research, technology development, and new process engineering;
2. Industrial infrastructure problems and integration barriers;
3. Up-front investments required; and
4. Lack of coordinated actions by means of regulations, incentives, and government purchasing.

[14]Lempert, R. J., P. Norling, C. Pernin, S. Resetar, and S. Mahnovski. 2003. *Next Generation Environmental Technologies: Benefits and Barriers*. Arlington, VA: RAND.

Complementary barriers have been identified elsewhere,[15,16] such as inadequacy of education and training of chemists and chemical engineers as well as managers who direct them, the difficultly with measuring progress in green chemistry, and the lack of tools for effectively comparing green chemistry with conventional approaches.[17]

Overcoming such barriers requires defining a "green" or "sustainable" agenda for the chemical industry. For example, the WTEC (World Technology Evaluation Center) Panel Report on Environmentally Benign Manufacturing[18] identified the environmental research challenges facing the polymer processing industry, and the Vision2020 roadmap[19] discusses environmental considerations for the CPI as a whole. In 2003, the UK Royal Society of Chemistry released the report *Benign and Sustainable Chemical Technologies,* which identified research opportunities to support sustainability in several areas, including: raw materials, agriculture and chemistry; new chemical routes (solvents and chemicals); catalysis, biocatalysis, and materials; new processes and process strategies; and environmental biotechnology.

STUDY AND REPORT

The purpose of this study was to assist the chemical industry in defining this sustainability agenda—that is, the necessary Grand Challenges and research objectives to enable the ongoing transition towards chemical products, processes, and systems that will help achieve the broader goals of sustainability. As a first step toward defining these objectives, a workshop was convened on February 7-8, 2005 that brought together a broad cross section of disciplines and organizations that make up the chemical industry (see Appendix C for the workshop agenda).

A detailed summary of the presentations and discussion from the workshop, a summary of the break-out sessions, and a list of participants appear in Appendixes D-G, respectively. Briefly, the workshop sessions are summarized below:

In the opening session, on **Sustainability Science Literacy and Education to Enable the Adoption of More Sustainable Practice**s, speakers

[15]Woodhouse, Edward. 2004. In *Congressional Report*.
[16]Adler, Robinson, and Rogers. 2002. In *Sustainability Workshop AIChE Center for Waste Reduction Technologies.*
[17]See presentation comments of Berkeley W. Cue in Appendix D, p. 116.
[18]International Technology Research Institute. 2001. Baltimore, MD.
[19]Vision2020 Technology Partnership. 1996. *Technology Vision 2020—The U.S. Chemical Industry*.

Braden R. Allenby, Lauren Heine, and Mary Kirchhoff discussed opportunities to improve education at every level—from education of consumers and citizens, young people, scientists in government and business, to the employees of businesses that use and sell products. They addressed how to promote incorporation of sustainability concepts into educational curricula; develop educational materials, which include sustainability concepts as part of standardized testing programs; and provide professional development opportunities for faculty to learn about sustainability and advantageously incorporate it into research and educational efforts.

Next, speakers Berkeley W. Cue Jr., Richard Helling, and Robert J. Kavlock, talked about **Enabling Technologies that Drive the Application of Green Chemistry and Engineering**. They discussed the need for dedicated tools to evaluate and appreciate the numerous benefits, and potential impacts and consequences of sustainability efforts. The basic requirements, research tools, and enabling technologies needed to drive the application of green chemistry and engineering for sustainability in the chemical industry were provided.

In the third session, on **New Chemistries and Processes that Lead to Commercially Viable Alternative Feedstocks to Fossil Fuels,** speakers Stanley R. Bull, Mark T. Holtzapple, and Douglas C. Cameron highlighted the utilization of biomass, and other renewable and recyclable feedstocks for the production of current and future commodity chemicals. Consideration was also given to the impact of resources, materials used in the processing such as catalysts, recycling, water use, and waste generated.

Finally, Jeffrey J. Siirola, Glenn E. Nedwin, William J. Koros, and Klaus S. Lackner presented in the session on **Reducing the Energy Intensity of the Chemical Process Industry**, which focused on the high energy usage (intensity) of the chemical and allied industry, and the need for pursuing energy efficiency and renewable energy resources. They discussed improvements in energy efficient separation processes; utilization of enzyme catalysts for energy reduction and selectivity increases; improvements in energy efficiency for the production of biofuels and biofeedstocks; development of more effective lubricants; step change improvements in the use of solar energy and other renewable energy sources; and technological breakthroughs in CO_2 separation, sequestration and use, were all addressed.

Based largely on the results of the two-day workshop, and the knowledge and experience of organizing committee members, this report identifies a set of overarching **Grand Challenges** for achieving sustainability in the chemistry industry, and makes recommendations about areas of research required to address those challenges. At the same time, this report is not inclusive of every research topic of relevance to sustainability, and it does not provide an in-depth analysis or an assessment of all that is needed to achieve sustainability in the chemical industry. This report is meant as a starting point for further analysis, with a focus on those areas that present unique challenges and opportunities for the chemical industry that can also help address larger sustainability goals. Chapters 2-5 of the report provide more focused discussion on aspects of the four areas covered in the workshop. Based on these discussions, the set of recommended Grand Challenges and related research needs are provided in Chapter 6.

2

Enabling Science and Technology That Drives the Application of Sustainable Chemistry

Today, chemists can make virtually any molecule, no matter how structurally complex, using the synthetic methods available to them. On the other hand, only a very small percentage of the chemical products are made following the principles of green chemistry—which is based on the ultimate premise that it is better to prevent waste than to clean it up after it is formed.[1,2]

Building this capacity to carry out what often needs to be fundamentally new chemical transformations requires a global view as well as a strong tie between academe and industry. Because the design of the chemical synthesis occurs too often without engineering input in the early stages of research and development (R&D) when it can be the most valuable, more collaboration and dialog between chemists and engineers is essential. Overall, approaches are needed to create more cross-talk between all members of the chemical enterprise. Ideally, the science and technology carried out by chemists and chemical engineers will be identical to the practices of green chemistry and engineering[3] and the overarching sustainability goals they support.

[1]Anastas, P. T., and J. Warner. 1998. *Green Chemistry Theory and Practice*. Oxford: Oxford University Press.

[2]Poliakoff, M., J. M. Fitzpatrick, T. R. Farren, and P. T. Anastas. 2002. Green Chemistry: Science and Politics of Change. *Science* 297:807–810.

[3]Green chemistry and engineering is additionally discussed in Chapter 1. Many good web sites also exist at: the EPA (*www.epa.gov/greenchemistry/*), the Royal Society of Chemistry (*www.chemsoc.org/networks/gcn/*), and the American Chemical Society's Green Chemistry Institute (*www.chemistry.org*).

> Chemists need to understand that adding an environmental or sustainability layer over research is not a constraint on creativity but rather is a challenge to creativity . . . Forward-thinking companies are beginning to realize this point. The economic advantages need to be understood.
>
> *John B. Carberry, E.I. du Pont de Nemours and Company*

GREEN CHEMISTRY AND ENGINEERING

Important green chemistry and engineering needs and capabilities are provided below.[4] In some cases the status of these capabilities may be closer to the ideal state than indicated. For these situations, the most important task is educating chemists and engineers to inform them about the availability and utility of these tools. In order to design the least wasteful process possible, it is essential that the chemist and chemical engineers know the fates and effects of all chemical inputs in the bond forming steps. This will require that they be informed by adequate life cycle analysis and toxicological data, which are discussed later in this chapter.

Efficient Chemical Bonding

Too often, a large excess of the nonlimiting reagent is used to convert the limiting reactant to product in the highest yield possible. The concept that the limiting reagent defines chemical yield encourages waste in chemical processing by focusing more attention on the end product than on how it is produced. One principle of green chemistry is that catalytic processes are preferred to stoichiometric ones. Catalysis is often used in petrochemical and bulk chemical industries where semicontinuous and continuous processing is commonplace, but less so in the fine chemical and pharmaceutical industries where batch processing is the rule. A rapidly growing area of catalysis use for these latter industries is in the area of biotransformations. This is driven, in part, by the need for chiral molecules as building blocks for drugs which have very specific stereochemical (or three-dimensional spatial) relationships with the enzymes and re-

[4]It should also be noted that there are many excellent examples of green chemistry and engineering successes in industry and academe that could not be highlighted in this report. The U.S. EPA Presidential Green Chemistry Challenge web site is an excellent source for such examples: *http://www.epa.gov/greenchemistry/presgcc.html*.

ceptors they influence. The emergence of directed enzyme evolution[5] to modify natural microorganisms in order to carry out transformations with higher chemo and stereochemical selectivity has helped fuel this growth. Asymetric chiral catalysis is an alternate route.

As pointed out by Glenn Nedwin during the workshop,[6] the production of textile derivatives synthesized by means of an enzymatic based process instead of a traditional multi-step chemical synthesis can lead to significant environmental benefits. It was found that utilizing enzymes can (1) reduce aquatic pollution by limiting the utilization of solvents, acids, chlorine derivates, oxidizing agents, sulphides, and other chemicals; (2) save energy by reducing process temperature; and (3) avoid having to resort to useful agricultural raw materials needed for other applications.

There are many other approaches to catalytic bond formation that still need to be explored, such as those being carried out at the Center for Environmentally Beneficial Catalysis (CEBC). CEBC is a multi-university NSF Engineering Research Center, headquartered at the University of Kansas with core partners at the University of Iowa, Washington University in St. Louis, and Prairie View A&M University. The center was created with a mandate to make "sustainable" manufacturing processes available to industry—that is, improved processes that minimize their "environmental footprint" while remaining profitable. CEBC's approach to doing this is by reducing or eliminating the use of hazardous materials in manufacturing (including the catalysts themselves or hazardous solvents), minimizing the formation of wasteful byproducts, and by improving energy efficiency. In pursuit of its vision and research goals, CEBC is guided by the principles of "Green Engineering" and "Green Chemistry".

Safer Solvent Selection

Another important green chemistry principle is to use safer solvents and reaction conditions by avoiding use of organic solvents, separation agents, or other auxiliary chemicals. When these chemicals are necessary, innocuous chemicals should then be used to the greatest extent possible.

Manufacturing chemicals can generate significant amounts of waste by-products and pollutants, such as halogenated or toxic organic solvents, volatile toxic or ozone-depleting organic compounds, hazardous air pollutants such as NO_x, CO_x, SO_x, and aqueous wastes. Roger Sheldon devel-

[5]For a review of this topic see: Farinas, E. T., T. Butler, and F. H. Arnold. 2001. Directed Enzyme Evolution. *Current Opinion in Biotechnology* 12:545–551.

[6]See comments by Glenn Nedwin, Workshop Summary in Appendix D, p. 143.

TABLE 2.1 Sectors of the Chemical Industry by Quantity of Byproduct per kilogram (kg) of Product Generated.

Industry Sector	Product tonnage	E-factor (kg byproducts/kg product)
Oil refining	10^6-10^8	ca 0.1
Bulk Chemicals	10^4-10^6	<1-5
Fine Chemicals	10^2-10^4	5-50
Pharmaceuticals	10-10^3	25-100+

SOURCE: Sheldon, R. A. 2000. Atom Efficiency and Catalysis in Organic Synthesis, *Pure Appl. Chem.*, 72(7):1233–1246.

oped the E-factor as a measure of the efficiency of the chemical industry, and this formula is expressed mathematically as: E = amount of waste (kg)/ amount of product (kg) for an overall process (Table 2.1). According to Sheldon,[7] "Waste is defined as everything produced in the [chemical] process except the desired product. It consists primarily of inorganic salts (e.g., sodium chloride, sodium sulfate, ammonium sulfate), formed in the reaction or subsequent neutralization steps, or derived from stoichiometric inorganic reagents (e.g., a stoichiometric metal oxidant). The E factor increases dramatically on going downstream from bulk to fine chemicals and specialties such as pharmaceuticals. This is partly owing to the fact that the production of fine chemicals involves multi-step syntheses but is also a reflection of the use of stoichiometric reagents rather than catalytic methodologies."

Recently scientists at GSK reported[8] that in a life cycle study for waste produced from pharmaceutical manufacturing facilities, approximately 80 percent of the waste is solvent-related with the remaining 20 percent being solid-related waste. Therefore, dealing with solvent waste and using green solvents in the process has become very important. Solvents can often be recovered and recycled, but recovery efficiencies typically range from 50-60 percent .[9]

[7]Sheldon, R. A. 2000. Atom Efficiency and Catalysis in Organic Synthesis. *Pure Appl. Chem.*, 72(7):1233–1246. (originally published in: Sheldon, R. A. March, 1994. CHEMTECH 38–47.)
[8]Gonzalez, Curzons, Constable, and Cunningham. 2004. *Int. J. LCA* 9(2):114.
[9]Mojica, C. June 28-30, 2004. 8th Annual Green Chemistry & Engineering Conference, Washington, D.C.

Process Analytical Technologies

The use of real time, inline, and online analysis for pollution prevention is another principle of green chemistry that relates to solvent selection. Once the desired product has reached its maximum yield in the reaction, further reaction time can lead to yield loss due to degradation to one or more side products. Moreover, traditional analytical methods that require removing a sample for analysis can expose the worker and work environment to chemical hazards. Process Analytical Technologies (PAT) tools are an important emerging technology for cleaner chemical manufacturing. PAT tools include analytical systems for the analysis and control of manufacturing processes based on timely measurements during processing. They also include measurements of critical quality parameters and performance attributes of raw and in-process materials and processes to ensure acceptable end product quality at the completion of the process. The use of inline and online PAT tools to monitor solvent distillation during recovery operations should improve the recovery efficiency. Also, improved technologies for recovering solvents, now typically achieved via distillation, may improve recovery yields. More extensive use of PAT tools in the R&D and manufacturing phases will contribute to lowering the environmental burden of chemical manufacturing.

It is well accepted within chemical processing that the development of green process chemistries to fully utilize green solvents improves product selectivity and conversion as well as reduces aqueous wastes.[10] The pharmaceutical industry's current work with global regulatory agencies to create a harmonized approach to residual solvents may be a useful tool for the rest of the chemical enterprise.

Selection Tools

Synthetic chemists expend much intellectual energy trying to answer the question, "How do I select a green solvent for the process?" This task is difficult because most of them have received little training in green chemistry, either in their academic or industrial experience. Fortunately, there are resources becoming available from a variety of sources. For example, in their guidance document on impurities and residual solvents, the U.S. Food and Drug Administration (FDA) provides information on classes of solvents based on patient safety and environmental considerations (reference: *http://www.fda.gov/cder/guidance/Q3Cfinal.htm*). In addi-

[10]Anderson, N. G. 2000. *Practical Process Research & Development.* Academic Press. Pp. 81–108; Nelson, W. M. 2003. *Green Solvents for Chemistry: Perspectives and Practice*. Oxford University Press.

tion, the EPA Office of Pollution Prevention and Toxics (OPPT) has also produced the Green Chemistry Expert System (GCES)—which is readily available from their web site at *http://www.epa.gov/greenchemistry/tools/html*. GCES allows users to build a green chemical process, design a green chemical, or survey the field of green chemistry. It includes a green solvents/reaction condition module which compares information on green solvent alternatives to traditional choices based on physiochemical properties. The system is equally useful for new and existing chemicals and their synthetic processes, and includes extensive documentation.

Elsewhere, in a recent publication[11] of the American Institute of Chemical Engineers (AIChE), the Center for Waste Reduction Technologies and Center for Chemical Process Safety has reported such a useful tool for selecting solvents—MERITT—which stands for Maximizing EHS (Environmental Health and Safety) Returns by Integrating Tools and Talents. This tool encompasses input regarding pollution prevention, inherent safety, green chemistry, and related topics. MERITT outlines a way to integrate these considerations for a chemist when designing a manufacturing process and includes a solvent selection tool.[12] This guide ranks solvent choices according to required waste treatment, impact on health, and safety. The reader is encouraged to study these references for a more comprehensive understanding.

Several other resources exist for selecting green solvents. A spreadsheet tool for solvent selection in chemical processing called CAPEC/CAMD (*http://www.capec.kt.dtu.dk*) is gaining popularity. There is an excellent tutorial program on solvent selection available at *http://www.chemsoc.org/pdf/gcn/solventsystem.ppt*. The SAGE alternative solvent guide, which was developed collaboratively by the U.S. EPA Air Pollution Prevention and Control Division (APPCD) and the Research Triangle Institute, is available at *http://www.clean.rti.org/index.cfm.*

Finally, no matter what scale is employed, chemists should at the very least always consult the material safety data sheet (MSDS) for any solvent they plan to use in a synthesis.

Controlling Thermal Conditions

Photochemistry, microwave chemistry, and ultrasonic chemistry that involve control of thermal reaction conditions offer new or expanded opportunities for greener transformation tools. Long used at laboratory scale, these technologies have not seen a commensurate use at commercial scale

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[11]See: *www.aiche.org/cwrt/projects/inherentsafety.htm*

[12]Bendixen, L., *www.CEPmagazine.org,* February 2002.

due to the perception of many chemists that these technologies are difficult to use commercially. Consequently, chemists redesign processes, often creating ones that generate more waste, in order to avoid using these tools. Hence, more development is needed to make these thermal control technologies for chemical processes commercially viable at larger scales.

Purification and Recovery

Once a molecule of interest has been created it must be separated and isolated from the reaction at a desired state of purity consistent with product specifications. As reported by Sheldon, and amplified by Constable and coworkers at GSK,[12] solvents are a major component of chemical manufacturing waste. Continuing investment in the development of separations tools such as commercial scale chromatography and membranes can play an important role in limiting the formation of waste solvents.

Crystal Engineering

For solid state chemical products, the crystalline form is critical to product performance. Traditional crystallization methods use large amounts of solvent. Once crystals are formed, they must be removed quickly in order to avoid continued growth beyond the specified size. Otherwise, energy intensive and potentially hazardous particle size reduction using high energy grinding must be used to restore the desired size range.

The emergence of crystal engineering as an important tool in the chemist's toolbox should continue to be encouraged and financially supported. Novel tools such as impinging jet crystallization (IJC) offer a unique opportunity for collaboration between chemists and chemical engineers. There are basically two types of IJC: counter-solvent and reactive crystallization that are used to produce crystals with very narrowly defined particle size distribution. Such size limitations are mandatory for optimum performance of many chemical products. In some parts of the chemical enterprise this tool is well established, while in others it is just emerging.

Equipment Cleaning

The involvement of equipment cleaning in purification and product recovery is another area that would benefit from new technologies, particularly in the batch manufacturing chemical industries represented by the Pharmaceutical Research and Manufacturers of America (PhRMA) and Synthetic Organic Chemical Manufacturers Association (SOCMA).

The traditional way to clean manufacturing equipment is to fill, boil, drain, sample, and assay (usually using an organic solvent). This cycle is repeated until the equipment is clean according to some predetermined specification. Spray balls, which use less solvent, are being used with increasing frequency but for the most part only in non aqueous systems. Ultrasonic cleaning has been studied; however, the common cleaning agents used with aqueous solutions have been found to be abrasive to glass lined equipment. Combing water-based technology (or organics as a last resort) and the use of PAT represents an opportunity for improving the cleaning process.

Formulation

Site-Specific Delivery

In the pharmaceutical industry, research into drug delivery technology offers a great opportunity to reduce its overall environmental impact. This is because for many drugs less than 50 percent is actually used in the body, with the rest being emitted from the body unused. Improved bioavailability by overcoming solubility and permeability limitations can reduce the overall amount of drug a patient consumes. The biggest payoff could come from targeted drug delivery, which is defined as a system to direct the flow of a drug to the target organ, tissue, or synthetic medical structure such as a graft. Site-specific delivery enables a therapeutic concentration of a drug to be administered to the desired target without exposing the entire body to a similar dose. When one considers that a typical daily dose of a pharmaceutical can contain a billion-fold more molecules than are needed to occupy every disease related receptor, the potential benefits of site-specific delivery technology are obvious.

Design for Degradation

Design for degradation is another principle of green chemistry. Chemical products should be designed to break down into innocuous substances after use so that they do not accumulate in the environment. Products need to be stable for their intended use lifetime before being rapidly degraded once they enter the environment. Intended lifetime includes the time to incorporate the drug into the dosage form (tablet, capsule, injectable, etc.) as well as time to produce therapeutic effects within the patient. To address the growing issue of chemicals in the environment, research is needed to study molecular triggers or chemical switches to activate degradation of active pharmaceutical ingredients (API's) following excretion into the environment after use.

> In order to change something, you have to be able to measure it, and you have to be able to do it quantitatively, and life cycle analysis gives us one way of doing that.
>
> *Richard Helling, Dow Chemical Company*

LIFE CYCLE ANALYSIS

As discussed, achieving sustainability requires a broad system view that integrates the multiple factors of social responsibility, environmental stewardship, and economical success. This involves having a keen understanding of the metabolism of chemical products—that is, their industrial ecology[13]—from the extraction of raw materials and creation of products, to their use and management of any resulting wastes. Life cycle analysis or assessment (LCA) and life cycle inventory (LCI) are tools that provide a means for systematic evaluation of the largest number of issues related to these impacts of the manufacturing of products through their full life cycle.

LCA is sometimes viewed as more comparative than absolute, and is found most useful for internal assessment and process development.[14] Some differences exist between the two approaches: LCI is a data intensive method (with quantitative figures, databases, and subsequent analysis), while LCA incorporates damage metrics and consequences through approaches of sometimes questionable subjectivity.

The need for effective LCA is illustrated by the example of chlorofluorocarbons (CFCs), which were developed as safer alternatives to the sulfur dioxide and ammonia refrigerants in the late 1920s and early 1930s. Applying the metrics of what is often considered green—low in toxicity, safe to use (nonflammable, noncorrosive, and nonreactive with other chemical species), and having other superior properties (desirable thermal-conductivity and boiling-point characteristics)—CFCs to a large extent fit the bill. Unfortunately, as pointed out by Brad Allenby during the workshop, what made CFCs desirable on one scale—their stability and safety to humans—made them highly undesirable when they managed to enter the upper atmosphere and destroy ozone. CFCs were found to be present in only trace quantities in the atmosphere and yet, because of the

[13]Frosch, R. A. 1995. The Industrial Ecology of the 21st Century. *Scientific American* 273(3):178–181.

[14]See comments by Richard Helling in the Workshop Summary, Appendix D, p. 120.

dynamics of the system, they turned out to be extremely critical. Today, there continues to be these same gaps in the way that chemistry and its impact on global systems is thought about.

Thus, the challenge going forward is to be able to foresee such unintended consequences by accounting for such properties as stability within a large complex systems analysis. The major areas in which LCI/LCA tools require improvement are:

- Economics (based on an appropriate standardized matrix such as total cost analysis—TCA)
- Social issues (for which many options and matrices have been proposed)
- Management of energy and process-related resources (water, temperature, pressure, etc.)
- Emissions of pollutants in the different ecosystems (solid waste, aqueous effluents, air, etc.)
- Availability, accessibility (extraction and related impacts), quality, and supply chain of raw and platform chemicals (including the management of their toxicity—MSDS contents need to be completed and verified for numerous products)
- Optimization of the chemical processing industry (CPI): solvents, separation chemistry, etc.
- Replacement of multi-step, wasteful chemistry by more selective and innovative biologically driven procedures
- Reduction in environmental impacts for workers (occupational regulation, collective and personal protection) and local residents (dispersion and eventual transformation of pollutants)
- Establishment of routes and yields of formation of waste and byproducts, management, and recycling when initiating projects: The end-of-life disposition or recovery of chemical products (especially those generated in large quantities and which present potential long term toxicity) constitutes a strategic element which is now largely used on the commercial side (percentage of recycling materials; set up of a recovery channel; injection of the excess of electric energy into the local network, etc.)
- Interpretation, utilization, and dissemination of the study results (data sharing with other companies)

Some of these items are priority elements that will be emphasized in the forthcoming European REACH (Registration, Evaluation and Authorisation of Chemicals)[15] program and regulations. They are also

[15]European Commission. 2001. *White Paper on the Strategy for a Future Chemicals Policy* (COM(2001)88); available at: *europa.eu.int/comm/environment/chemicals/whitepaper.htm*

incorporated in the principles of green chemistry and green engineering discussed earlier in this chapter.

Despite the fact that there is no systematic, comprehensive method for analyzing opportunities for chemical processing improvement, LCA (now an ISO-standardized methodology of the 14040-14043 series) has expanded the traditional process boundary, considering up and downstream processes in terms of energy and materials use, waste generation, and business value creation.[16] Some of these items require further technological developments and other related sustainability research programs in order to provide adequate answers and solutions.

According to Warner and coworkers,[17] LCA should function as a strategic link between green chemistry and Environmental Impact Assessment (EIA). As pointed out by Helling during the workshop, many commercial and publicly released software and data that could assist chemists and chemical engineers in this way already exist, such as: Ganzheitliche Bilanzierung, version 4 (GaBi IV, found at *www.gabisoftware.de*), and Tool for Reduction & Assessment of Chemical & other Environmental Impacts (TRACI) from the U.S. Environmental Protection Agency (EPA). However, use and interpretation of such LCA software largely remains a job for specialists because most chemists and chemical engineers do not have the training to interpret the results they obtain.

Going forward, many scientists believe that more emphasis should be placed on understanding the toxicity of chemicals and on increasing the capacity of chemical sciences and toxicology to provide this necessary basic information. The current unavailability of reliable toxicity data and corresponding uncertainties (discussed in more detail later in this report) constitute major hurdles that hamper the application of efficient LCA studies and hinder progress in sustainability. There is also a need to understand the long-term impacts of chemicals in the environment—such as persistence, bioaccumulation, global warming potential, or ozone depletion—and be able to evaluate within LCA as discussed earlier. However, it is clear that present state-of-the-art LCA methodologies such as GaBi IV and TRACI are very useful for internal comparative assessments of environmental and societal impacts for those who know how to use them. The need for more effective and easier to use tools to guide sustainable chemical process development is essential to the future of the chemical industry.

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[16]Consoli et al. 1993. *Guidelines for Life Cycle Assessment: A Code of Practice*. Society for Environmental Toxicology and Chemistry.

[17]Warner, J. C., A. S. Cannon, and K. M. Dye. 2004. Green Chemistry. *Environmental Impact Assessment Review* 24:775–799.

TOXICOLOGY

Many data related to human and environmental toxicology of chemicals are either questionable or missing, which has significant implications for advancing the application of green chemistry and engineering and overall sustainability goals. For example, ionic liquids,[18] which provide both superior properties and environmental benefits, are promising replacements for volatile organic solvents currently used by industry. However, as it has been recently pointed out,[19] "Despite the potential for ionic liquids to reduce [volatile organic compound] emissions. . . . Little is known about the toxicity or mobility of ionic liquids in the environment."

Thus, there is clearly a role for all involved in the chemical industry to assist in funding and otherwise supporting the collection of critical data related to the most pervasive—and the most potentially useful—chemicals in the industrial environment.

Such a resource is essential for more effective LCA, which requires a large volume of data input in order to produce reliable final figures to support decision making. Current data sources for LCA are derived from MSDS and other technical fact sheets, but numerous others have to come from separate sources that must often be identified, retrieved, and correctly handled by the user on a case-by-case basis. Other information is either inconsistent or not thorough in terms of relevant environmental data.

Human Toxicity Data

In order to increase basic knowledge of the biological impacts of chemicals on human health, and to generate the experimental and/or theoretical values needed for a quantitative toxicological assessment of a larger number of products (all major elements qualified to justify the forthcoming European REACH program), priority should be given to research in the topics discussed in this section.

In Vitro Biological Assays

In vitro biological models (see Figure 2.1) are of primary importance in providing the numerous data needed in LCA studies. This is because management of toxicity pathways plays a key role in LCA. Measurements

[18]For a recent review, see: Welton, T. 1999. Room-Temperature Ionic Liquids. Solvents for Synthesis and Catalysis. *Chem. Rev.* 99(8):2071–2084.

[19]Gorman-Lewis, D. J., and J. B. Fein. 2004. Experimental Study of the Adsorption of an Ionic Liquid onto Bacterial and Mineral Surfaces. *Environ. Sci. Technol.* 38(8):2491–2495.

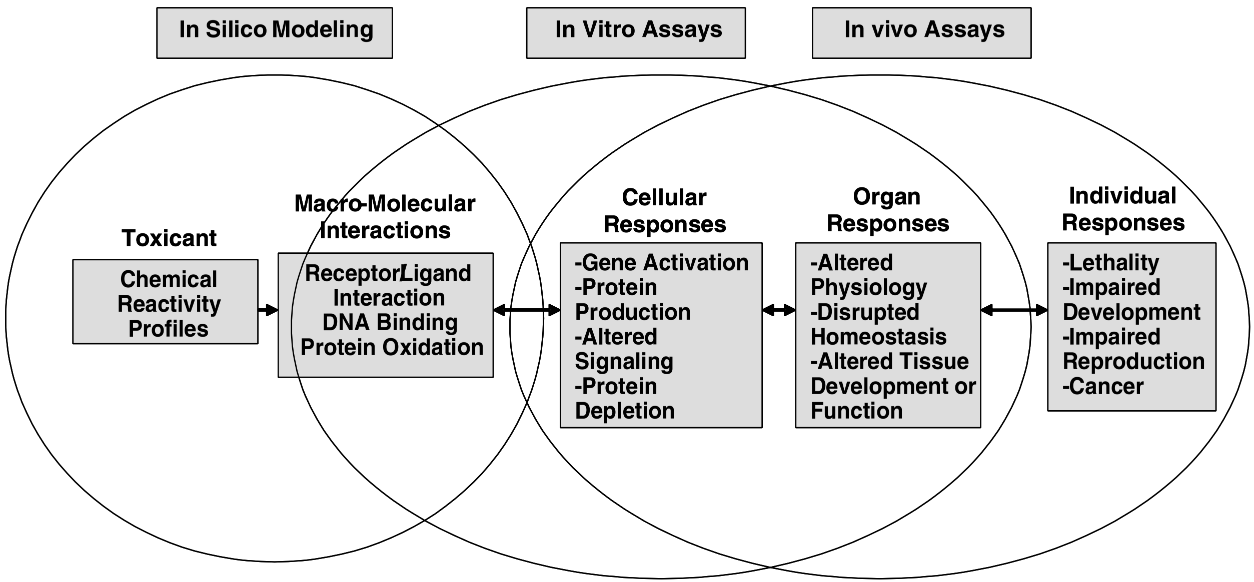

FIGURE 2.1 Example of a toxicity pathway.
SOURCE: *A Framework for a Computational Toxicology Research Program* U.S. Environmental Protection Agency, 15, *http://www.epa.gov/comptox/publications/comptoxframework06_02_04.pdf.*

performed on human and animal cells, subcellular fractions, or specific biological receptors or biomolecules have the potential to provide an efficient alternative to tedious, labor intensive, and costly standard toxicity test methods based on *in vivo* experimentation. Only a small number of chemicals can be processed by animal based toxicological assays. In some industrial countries, green politicians and parties are lobbying to lower the number of animals incorporated into toxicity tests, and regulations in this direction become more stringent each year. At the same time, it is crucial for scientists and toxicologists to generate reliable quantitative information on individual chemicals according to their respective biological effects (from identification of discrete molecular initiating events to adverse outcomes to molecular alterations and linkages across biological levels of organization).

There is pressure to develop sensitive new assay methods for measuring those biological effects that are most likely to cause dramatic human health impacts. These impacts include: reproductive and developmental impacts, neurotoxicity, carcinogenicity and cancer hazard, and endocrine disruption and fertility.

The views presented for *in vitro* testing above are complementary to those presented by Robert Kavlock during the workshop,[20] and several FDA[21] and other[22] scientific and technical reports. There is agreement that intensive research should be conducted in order to increase the number of toxicological tools and reliable data needed to verify and validate theoretically generated figures (see discussion later in this chapter).

Efforts need to be made to better understand chemical mixtures. New experimental biological assays based on precise study protocols are necessary to approach the impacts of binary and tertiary chemical mixtures. Enzymatic induction, inhibition, or any other mechanisms of interaction with fundamental and critical metabolic pathways related to important endogenous compounds such as thyroidal and steroid hormones should be thoroughly investigated. Identification of synergistic, promoting, inhibitory, and antagonistic effects would be a great benefit to increasing understanding in toxicology. Management of waste, which involves treating complex matrices containing trace amounts of pharmaceuticals or endocrine disrupting chemicals (EDCs), would largely benefit from these

[20]See comments by Robert Kavlock, Workshop Summary in Appendix D, p. 124.

[21]See the FDA Office of *In Vitro* Diagnostics (OIVD), *www.fda.gov/cdrh/oivd/*

[22]Sam Brauer (Business Communications Company Inc.), June 2003, *The Market for In Vitro Toxicology Testing* (B110R report); and ECVAM (European Center for the Validation of Alternative Methods) reports: Workshop Report 45: *Novel Advances in Vitro Methods for Long Term Toxicity Testing* (2001).

such advances. Data metrics would also be required to set a priority list of potentially active compounds that could be detrimental to human health.

These experimental data would be integrated into dose-response relationships that are generally used to establish dose of exposure values. This would be accomplished by performing calculations on appropriate models, such as those proposed by implementation of a threshold level to the biologically measured effect. Whenever possible, more sophisticated mathematical models should be promoted, such as the Physiologically Based Pharmacokinetic (PBPK) model, which measures time of exposure to a target dose, and the Biologically Based Dose-Response (BBDR) model, which identifies target organ dose to early biological effects. These models require larger sets of data which could be supplied by experiments. The selectivity and sensitivity of newer assay methods would have a positive impact on the accuracy and overall quality of the data, which in turn would affect the evaluation of uncertainty values that accompany published reference dose or concentration figures. Data issued from complementary toxicity studies (animal *in vivo* assays, epidemiological studies, computational toxicology, etc.) would complete those databases that provide validated bio-statistical analysis.

Metabolic and Degradation Pathways

The characterization of the various toxicity properties of chemicals requires additional information such as the identification of their metabolic pathways in humans and the (bio)degradation routes of compounds in various environmental ecosystems.

Modern analytical instrumentation based on combined HPLC–mass spectrometry technique offer many opportunities to perform these experiments on biological models, ranging from simplified *in vitro* tests to *in vivo* studies on animals. High-throughput, sensitive assays can now be performed at reduced cost. Metabolic and transformation patterns of chemicals would also be useful for generating valuable kinetic information. These patterns could be used to set up priorities in lists of compounds that require additional testing. This type of prioritization would be necessary because such compounds are widely spread into the environment and could enter the food chain as a result of their long life in ecosystems. For example, the part of the food industry that prepares flour-based foodstuff uses nutrients recycled from materials of different origins, and this is a source of great concern in various western European countries. Biotransformation studies will also identify enzymatic reactions related to well known genetic polymorphism. Specific tests are now available to identify individual metabolic deficiencies such as those related to the P-450's isoenzyme activities or to phase II metabolic pathways like those regulated by

N-acetyltransferase. These data also have positive impacts for the uncertainty linked to heterogeneity in different populations.

Computational Approaches

The gap of missing toxicity data is so large that it will be impossible to perform the complete battery of tests required to fill up databanks. Toxicologists need additional data on numerous chemicals. Agencies such as the EPA, which are charged with protecting human health and the environment from exposure to potentially harmful compounds in water, food, air, and soil, are interested in assessing—by alternative, non invasive methods—possible hazardous effects for tens of thousands of compounds. Such information would allow for prioritization of additional data requirements and accurate risk assessments.

Over the last ten years, advances in theoretical, computational chemistry, and molecular biology have led to generation of data related to potential biological activity and toxicity. The pharmaceutical companies largely rely on these new tools to design drugs. This new area, known as "computational toxicology," may be able to predict the potential effects of compounds from their chemical (sub)structures if substantial developments, validation steps, and budgets are created to achieve the objectives and validate these computer tools. Understanding how structures are correlated and transformed to chemical functions and biological activities (including deleterious toxic effects), requires additional and sustainable efforts. In 2003, the Office of Research and Development (ORD) of the EPA launched an ambitious research program leading to the installation of a Framework for Computational Toxicology.[23] This program already involves the collaboration of several partners: NIEHS, DOE, NERL, NCER, NCEA, NRMRL and NHEERL.

Computational toxicology is designed to address the questions of "when" and "how" to test chemicals because they could be hazardous, improving the prioritization of data requirements, and risk assessment. This multidisciplinary project of the EPA has been peer reviewed and evaluated by the experts in toxicology. Computational toxicology establishes the links with the other resources needed to reach the goals and objectives of sustainability in the chemical industry. The main objectives of the framework are to:

[23]See more details in R. J. Kavlock's presentation in the Appendix D, p. 124, and on the EPA Web sites: *www.epa.gov/comptox/* (a general survey of the project) and *www.epa.gov/comptox/comptox_framework.html* (the entire text of the proposal).

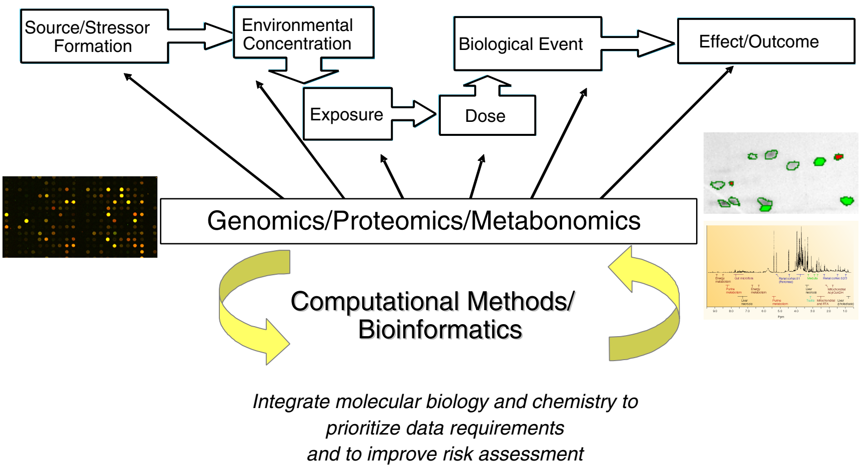

FIGURE 2.2 Source to outcome continuum—Development of Sound Structure-Activity Tools to Predict Health and Environmental Impact of Specific Chemicals. SOURCE: Robert Kavlock, U.S. EPA.

- Improve linkage across the source-to-outcome continuum (Figure 2.2)—from adding the chemical into the environment to the eventual biological effects
- Develop approaches for prioritizing chemicals for subsequent screening, testing, and data generation in order to enhance the predictive understanding of toxicity pathways
- Produce faster accurate assay methods (e.g. using systems biology to understand cells and organ's mode of functioning) and provide predictive models for a secure hazard identification and enhancement of reliable quantitative risk assessment. This would permit the classification of chemicals by their potential to influence molecular and biochemical pathways of concern. The program could also integrate developments in cross species extrapolation and in the mixtures issues.

Quantitative Structure Activity Relationship (QSAR) development (see the DSSTox program of the EPA at *www.epa.gov/NHEERL/dsstox/About.html*) will also be considered by the Europeans in their REACH program as a bearing tool to supply more toxicity data without resorting to complex and costly *in vivo* experimentation. It is important that there be some collaboration on both sides of the Atlantic Ocean (and elsewhere) to validate harmonized approaches of these computerized tools in order to avoid future controversial discussions and conflicts.

Toxicity studies are ideally focused on the applications of chemicals; a component present in various products at different concentration levels likely has diverse toxicity profiles that should be addressed as well. This is a very challenging issue as is the question of the toxicity of isomers. The scientific literature has reported well-known examples of different dramatic toxic effects observed between isomeric forms. In such cases, experimentation is the only solution to solve this question.

Boundaries of assessment should be delimited in these topics; the main objective is to deliver indicative, pertinent, and relevant sources of information. The proposed solution should not transform scientific consideration into pure speculation that leads to questionable or subjective conclusions. Heuristic tools are also needed to fix boundaries and limitations to the implementation of such computerized solutions in LCA studies.

A strategic approach is recommended in order to provide the most appropriate toxicity data. To set up priorities and risk, computational toxicology should be the first line of investigation. *In vitro* testing should be carried out for a large number of compounds to provide preliminary dose-response data (and establish temporary Reference Doses (RfDs) or Reference Concentrations (RfCs). Then, *in vivo* experimentation could take place for a limited number of very hazardous chemicals present in measurable quantities in materials issued from any sources (including environmental ecosystems) and which come in contact with human beings.

How do we get into that list of 850 pesticidal inerts and tell the agency, these 63 are the ones you should worry about; and you should worry about 21 of them for birth defects and 32 of them for cancer effects; and be able to put some kind of a priori knowledge in the system?

Robert Kavlock, U.S. Environmental Protection Agency

Ecotoxicity Data

Environmental metrics often expressed as "Eco-Efficiency" do not exist under global standard protocols. Instead, most approaches involve energy intensity and consumption, mass intensities (including fossil resources and water), and pollutant emissions (limited to the major compounds released in the air, water, and soil). However, numerous factors can influence the fate and dispersion of chemicals into the different environmental compartments and ecosystems. Persistence, (bio)degradation, and mobility represent key elements that exert direct threats on surface, ground water, and soil with consequences for the food supply chain (according to the importance of the enrichment factors associated to each trophic level). The establishment of physico-chemical parameters related to environmental fate, transport, and bioconcentration effects can be regarded as cost-effective surrogates for data generated from more complex laboratory experimentations.

For specific classes of compounds (i.e. endocrine disrupting products and carcinogens), the EPA has launched a series of databases (such as ECOTOX at: *www.epa.gov/ecotox/*), which contain comprehensive figures on the ecotoxicity of chemicals towards aquatic and terrestrial organisms, including plants. This internationally recognized source of information is also linked to predictive models for ecotoxicity endpoints and physico-chemical properties in the absence of empirical data. Similar trends concern other priority pollutants like pesticides, pesticidal inerts (constituents added to the active ingredients of a registered pesticide), heavy metals, and small particulate matters with high uptake coefficients (e.g. diesel exhaust).

Additional basic research is needed to better screen and identify persistent chemicals that would play an active role in the adverse health effects stressed by eco-toxicologists. Application of emerging technologies into new assay methods should be encouraged to generate complementary robust data sets relative to impacts resulting from the biology of chemicals in various environmental compartments. The development of a new discipline to better understand these issues would be very useful. It should incorporate and integrate basic concepts taken from geology, hydrogeology, agronomy, chemistry, and biology, particularly when it is related to soil and water dispersion.

The feasibility of a separate "Environmental Fact Sheet" assembling the items that should be integrated into LCA studies should be envisioned. Its content should be defined, evaluated, and thoroughly reviewed. There must be guidelines and standardized techniques for supplying such information.

CENTRALIZED DATA COMPILATION AND MANAGEMENT, AND INCREASED COLLABORATION

Many companies are building internal capacity to address sustainability parameters into their daily operations. One excellent example can be found at GlaxoSmithKline (GSK). Part of GSK's Eco-Design Tool Kit includes a *Green Chemistry Guide* that offers guidance to GSK scientists and engineers on applying green chemistry concepts. This would allow them to enable more efficient use of resources, reduce environmental, health and safety impacts, and minimize costs. It includes:

- A ranking and summary of the most used chemistries and 'best-in-class' examples from well-developed GSK processes.
- A ranking and review of issues encountered during process design and development.
- A ranking and summary of common technology alternatives for chemical processing.
- Guidance on materials, process alternatives, synthetic route strategies, and metrics for evaluating chemistries, technologies, and processes.

A larger wide-scale effort is needed to compile such information from across industrial and academic R&D institutions, as well as other high-tech industries (e.g. defense-related). Such an effort would help identify technologies that have been developed by one member of the enterprise that can be useful, but are unknown, to the other.

The EPA's Green Chemistry Program is currently compiling and organizing journal articles into specific sub-topics for a literature database on the subject. Topic areas include alternative synthesis methods, catalysis, reaction conditions, and alternative solvents. The goal of this project is to have a database compilation of green chemistry literature which is publicly accessible that will enable researchers across the chemical industry to identify the new approaches to chemical synthesis. In addition to compiling such information, it will be important that greenness parameters such as E-factors[24] and atom economy[25] be supplied (or even required) for all chemical synthetic routes published in the scientific literature.

There is also a need to expand the availability of sound LCI data and methods. Future LCA studies and risk assessments would largely benefit from additional experimental and computer-generated (eco)toxicological data. In order to facilitate their utilization and incorporation into studies, some complementary practical measures should be taken. Verification and validation operations should be performed by agency senior staff, and centralization on a dedicated site should be made accessible to all (free of charge or at affordable cost) while being duly managed and maintained. This centralized and standardized repository of information, which requires coordinated efforts, must be adequately organized and presented in inventory matrices to provide easy pattern recognition and transfer to LCA platform and templates. Lauren Heine has proposed[26] a toxicology

[24]E stands for efficiency, and is the amount of waste (kg) generated per amount of product (kg) for an overall process. This is discussed more later in this chapter under Solvent Selection in the section on Chemistry Tools.

[25]Atom economy is the ability to avoid loss of atoms in a chemical synthesis—and is one of the 12 principles of green chemistry discussed in the Introduction.

[26]See Lauren Heine's comments, Workshop Summary in Appendix D, p. 112.

and exposure summary table. Improvements and complimentary figures should be incorporated into this model (i.e. the introduction of quantified parameters).

Chemistry is a complex discipline. Providing ways to deal with this complexity and determining where decisions should be made is not an easy task. Therefore, the organization and classification of data should be associated with a quantification process (scoring methods, weighing factors, and heuristics) that will allow for prioritization of hazard and risk and for further multi-criteria based analysis. These metrics should be evaluated extensively in order to reach a balanced agreement, since no validated equation to accurately evaluate "sustainability" has been presented thus far. Communicating the results of a complex analysis into a single figure, or into a simple and readily understood form that does not oversimplify the analysis conclusions, is an additional challenge that needs to be addressed.

CONCLUSIONS AND RECOMMENDATIONS

New scientific developments and more efficient tools to evaluate them are needed to enable the chemical industry to more effectively incorporate sustainability into general practices. Such an effort will require science, technology, and harmonized strategic approaches across disciplines, industries, and geographic boundaries:

Green Chemistry and Engineering. While chemists can currently make virtually any molecule using synthetic methods available to them, much more effort is needed in the development of green chemistry and engineering capabilities. These include the ability to:

- efficiently form chemical bonds,
- select solvents,
- control thermal conditions,
- purify and recover chemical products,
- develop analytical methods,
- formulate products,
- model chemical reactions, and
- perform all these tasks in an environmentally benign manner

These are essential for the development of industrial technologies that support sustainability.

Life Cycle Analysis. Life cycle assessment (LCA) is considered to be a powerful tool for comparing the environmental performance of products generated under different operating conditions. In order to effectively implement LCA, there is a need to be more systematic about the generation and handling of data inputs and models. Improvement in the quantity and quality of data being used is necessary, and agreement on the approach used to evaluate LCA metrics (environmental indicators, impact factors, etc.) is crucial. LCA metrics should be easy to calculate with available data, useful for decision-making, reproducible, scientifically rigorous, usable at multiple scales of analysis, and extendable with improved understanding.[27]

Toxicology. At the foundation of improved life cycle and chemistry tools is the development of methods to supply toxicity data on chemicals and chemical mixtures. Computational toxicology and QSAR (Quantitative Structure Activity Relationship) analysis will be significantly involved in generating such data, which will also need to be compiled in centralized and accessible databases.

Data Compilation, Management, and Collaboration. There is a need to create a network system of all upstream, lateral, and downstream channels that will enable exchanges between different companies and different countries. Ideally, one end-of-line material will serve as a feedstock supply to another activity to create a chain of supply. Close partnership and collaboration between subcontractors of services, suppliers of materials, clients, and authorities should be identified, encouraged, and demonstrated with concrete actions such as sharing of databases and related scientific resources. It is crucial that closely related aspects of chemical safety and environmental impacts are approached more consistently and managed in all developed countries.

[27]Schwarz et al. 2002. Use of Sustainability Metrics to Guide Decision-Making. *Chem. Eng. Prog.* 98(7):58.

3

New Chemistries and Processes That Lead to Commercially Viable Alternative Feedstocks to Fossil Fuels

Since 1850, there has been an evolution of both energy resources (Figure 3.1) as well as the source of feedstocks for the commodity chemical industry. In 1850, the predominant fuels were wood or other biomass depending upon location. During this time period, the chemical enterprise was relatively small. However, as the industrial revolution gained momentum, the need for new chemicals and new materials to meet the growing demands of industry and consumers increased. At the turn of the twentieth century, carbon-based chemical feedstocks were already primarily derived from coal. Over the course of the twentieth century, global political and economic forces initiated significant change. During that time, the United States, and subsequently the global chemical enterprise, moved farther away from renewable sources of carbon-based feedstock and became heavily dependent on fossil fuels—crude oil and natural gas—both as a feedstock for commodity chemicals and as a primary energy source.

As concerns about the fundamental nature of the crude oil supply and concerns about impacts on the environment and human health arose, there was a shift from crude oil (as a fundamental energy source) to natural gas (and to a limited extent, non-fossil sources such as nuclear, wind, solar, and biomass). Thus, today there is a multitude of fossil based fuels—coal, oil, and natural gas—used for energy, but overall energy consumption has also increased (Figure 3.2). There are also simultaneous demands on fossil fuels as energy resources and feedstock for the commodity based chemicals.

Thus, the chemical enterprise is faced with two fundamental ques-

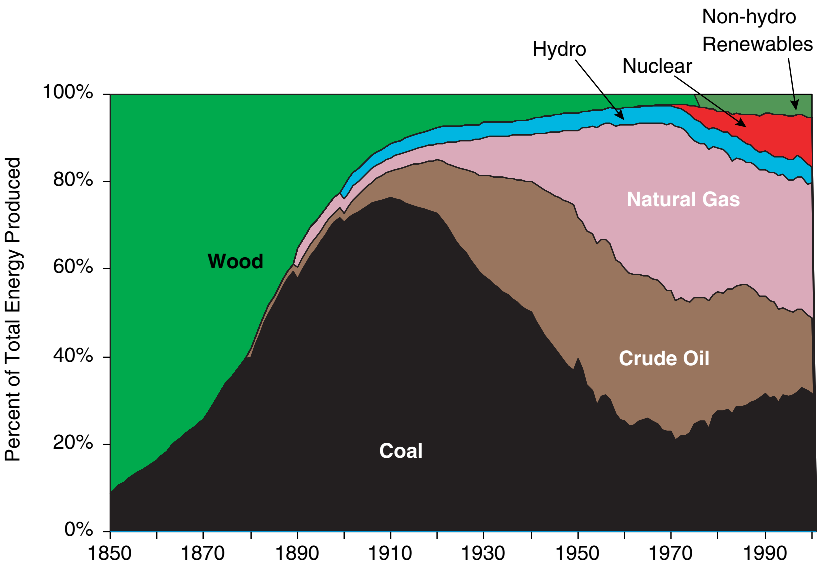

FIGURE 3.1 U.S. energy production by source—1850–2000.
SOURCE: U.S. Department of the Interior. 1975. 1850–1949, Energy Perspectives: A Presentation of Major Energy and Energy-Related Data; 1950–2000, *Annual Energy Review 2000*, Table 1.2.

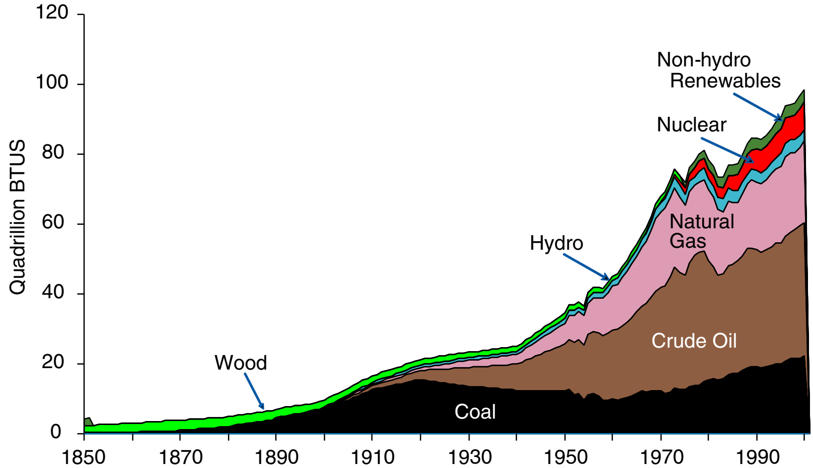

FIGURE 3.2 U.S. Energy consumption by source—1850–2000.
SOURCE: U.S. Department of the Interior. 1975. 1850–1949, Energy Perspectives: A Presentation of Major Energy and Energy-Related Data; 1950–2000, *Annual Energy Review 2000*, Table 1.3.

tions that drive the need for the development of the new chemistries and processes for a sustainable future:

1. Where is the fuel needed to support the energy demands of the economy and quality of life that the developed world currently enjoys (and the developing world—especially rapidly developing China and India[1] —is striving for) going to come from?
2. What feedstock sources are going to be used in the future to produce the basic chemical building blocks of the chemical enterprise (which are required for the production of materials and products consumers demand)?

Drivers for Change

The current prognosis for the fossil fuel economy in terms of global supply over the next 20 years is good. According to a recent analysis[2] by the U.S. Energy Information Administration, "For the forecast period out to 2025, there is sufficient oil to meet worldwide demand. Peaking of world oil production is not anticipated until after 2030." The EIA also estimates adequate supplies of natural gas over the next 60 years, and coal supplies for 100 years or more. However, this is an optimist picture, because it largely assumes a business-as-usual market environment, with no disruptions to these supplies from geopolitics, weather, or regulatory controls on using fossil fuels. The current challenge is about the amount of hydrocarbon that will be available over the next 20 years, and the sustainability of producing and transforming that hydrocarbon into useful feedstocks.

Fossil Fuel Quality and Security

Crude oil quality[3] is changing significantly as is the political stability of the areas that have oil versus those who use oil (Table 3.1), presenting considerable challenges for U.S. national security. For example, the United States currently depends heavily on Middle Eastern nations for oil sup-

[1]According to the U.S. Energy Information Administration, China is world's second largest energy consumer (after the United States), and India is the world's sixth.

[2]Energy Information Administration, *International Energy Outlook 2005*, DOE/EIA-0484(2005), p. 29 *http://www.eia.doe.gov/oiaf/ieo/index.html*.

[3]High quality (light sweet) crude oil is low in hydrogen sulfide and carbon dioxide and easier to refine, and provides high yields of high-value products such as gasoline, diesel fuel, heating oil, and jet fuel.

TABLE 3.1 U.S. Dependence on Foreign Oil

Have Oil	Percent	Use Oil	Percent
Saudi Arabia	26	U.S.	26
Iraq	11	Japan	7
Kuwait	10	China	6
Iran	9	Germany	4
UAE	8	Canada	4
Venezuela	6	Russia	3
Russia	5	Brazil	3
Libya	3	S. Korea	3
Mexico	3	France	3
China	3	India	3
Nigeria	2	Mexico	3
U.S.	2	Italy	2

SOURCE: Energy Information Administration. 2001. International Energy Annual, Tables 11.4 and 11.10.

plies, but crude oils from these areas tend be lower quality than from North and South America or West Africa.[4] Thus, one driver for change is to reduce the dependency on foreign sources of oil and ensure that there will not be a disruption in the energy supply.

Problems also arise from the basic economics and reliability of transforming fossil fuels into useable materials. As the quality of crude oil declines, and there is a shift from one fossil fuel to another—the regulatory and technical requirements for processing such as coking, hydrocracking, and sulfur removal increase and hence the cost associated with processing increases. This is then transferred throughout the economy to increased feedstock costs for commodity chemicals and an increase in transportation fuel costs. At some point, these resulting economic factors become the ultimate driver for change to alternative feedstocks. Although it is anticipated that the total amount of fossil fuels (coal, natural gas, and oil) available can support current and future needs for at least another hundred years (Chapter 4, Table 4.1), at some point there must be a shift from nonrenewable fossil fuels to renewable sources.

Resource Demands and Impacts

However, achieving sustainability is not just about addressing the supply of fossil fuels; it is also a matter of addressing the demand for their

[4]For more information see the Energy Information Administration at: *www.eia.doe.gov*

use and their full life cycle of impacts. Taking a look at the concept of the demise or "tragedy" of the commons,[5] another fundamental driver for change emerges—reaching the production capacity of the planet because of the consequences of population growth. That is, given the current demands of 6 billion people on the planet, and a projected population of 9 billion in 2050 with its increased demands for consumer goods, the impacts of fossil fuels (mainly due to the combustion of hydrocarbons) on the environment and human health cannot continue regardless of there being adequate supplies.

In the past, the demand and use of fossil fuels were limited and the impact on the environment was not seen or detected. As the use increased, or the concentration of the use increased, there were significant impacts on the environment. Examples include smog, coal dust, and widespread environmental blight in cities and other congested areas that persisted until about 1970 with the passage and enforcement of legislation to protect the environment. Other impacts such as how wildlife became harmed by pesticide use, led Rachel Carson to write the book *Silent Spring*, which awakened the general public to the underlying issue of sustainability later articulated by Hardin. That is, how can resources (even renewable ones) continue to be utilized without fundamentally "trashing" the commons? This becomes a significant driver for the need to look for alternative sources of feedstocks and fuels.

OPPORTUNITIES FOR RESEARCH AND DEVELOPEMENT

Exploring alternative, sustainable feedstocks requires simultaneous consideration with development of alternative energy sources and future fuels, as well as continued improvements in the efficient use of current resources (see Chapter 4 for more detailed discussion of energy). As alternative, sustainable feedstocks and fuels are explored and new processes or technologies are developed, the impact on resources must be considered. First, from the perspective of the base materials used in the process—the alternative feedstock. Secondly, from the materials use of the process itself, such as what type of catalyst does this process require? What type of recycling is employed? What materials are needed, particularly if the process utilizes water? What is the impact on the recycled material? What wastes are generated from these processes? Are these wastes better or worse than the current processes? How are the wastes managed?

These considerations lead to a level of understanding that is essential for the future development of the chemical enterprise. The enterprise

[5]Hardin, Garrett. 1968. The Tragedy of the Commons. *Science* 162(3859):1243–1248.

needs to have tools and guidelines for the consideration of the risks and rewards. It needs to be able to adequately assess the various alternatives being proposed. There needs to be a means of providing a value assessment associated with the alternatives. Hence, the physical science professional is going to have to take a multi-disciplined approach in the evaluation of the potential gains or risks associated with the technology (see Chapter 5 for discussion of education needed to support sustainability goals).

Alternative Energy Sources

Energy is a key need in the development of future growth. This particular area and potential research applications have been previously addressed by others,[6] and will also be addressed in Chapter 4; therefore it will not be discussed in much detail here. However, it is important to note that the chemical process industry (CPI) consumes about 7.7 percent of all the energy (fossil fuels, electricity, etc.) resources used in the United States.[7] Of this, about 50 percent of the energy resources are used as chemical feedstocks, rather than consumed as energy. Because of the competing needs for feedstocks and fuels, it is thus a grand challenge for the chemical enterprise to lead the way in the development of future fuel alternatives. These alternatives could be in the development of hydrogen, landfill gas, and biomass[8] fuel sources utilizing fuel cell, wind, solar heating, and photovoltaic technology.

Biomass is an especially promising avenue to pursue for the chemical industry. According to the U.S. DOE, biomass recently surpassed hydropower as the largest domestic source of renewable energy and currently provides over 3 percent of the total energy consumption of the United States. Current efforts to integrate production of fuels and feedstocks from biomass—biorefineries—show great promise for developing future fuels. This has been demonstrated by efforts of the DuPont-DOE Integrated Corn Biorefinery project, which not only uses the starch, but also the cellulose, the corn, and the corn stover to produce chemicals, bioethanol and power, and to feed the production of Dupont's Sorona® polyester.

In addition to specific future fuel alternatives, the chemical enterprise should accelerate its efforts to examine the technologies needed to fully

[6]Hoffert, M. I., et al. 2002. Advanced Technology Paths to Global Climate Stability: Energy for a Greenhouse Planet. *Science* 298:981–987.

[7]*http://www.eere.energy.gov/industry/about/pdfs/chemicals_fy2004.pdf*

[8]Any plant derived organic matter available on a renewable basis, including dedicated energy crops and trees, agricultural food and feed crops, agricultural crop wastes and residues, wood wastes and residues, aquatic plants, animal wastes, municipal wastes, and other waste materials.

integrate, or close the loop on, production activities— such as in the pulp and paper industry where waste products are utilized as fuel for the process—and thereby reducing current energy needs. These applications could be expanded and potentially integrated into additional processes.

Finally, the chemical enterprise should be a significant player in the development of enabling energy technologies. These include:

- Energy storage materials and devices
- Materials that improve energy efficiency
- Biomass pretreatment processes
- Fermentation processes
- Separation processes
- Water treatment processes

All of these enabling technologies are going to be required to bring the innovative technologies from the laboratory to a commercially viable alternative.

Alternative Feedstocks

Today's economy relies on inexpensive access to chemicals and related materials—from basic and fine commodity chemical building blocks to finished products such as textiles, pharmaceuticals, and agricultural chemicals—which are largely derived from a fossil fuel based feedstock. It is thus essential that commercially viable alternative feedstocks and processes be developed.

Biologically Derived Basic Chemical Building Blocks

As pointed out by Stanley Bull in the workshop, and discussed briefly in the previously section, the growing need for sustainable energy can be met by improvements in capturing and utilizing renewable resources such as solar, wind, and geothermal, and biomass; however, biomass is the only renewable resource that produces carbon-based fuels and chemicals. It is important to note that biomass is not just derived from agricultural food and feed crops, it includes any plant-derived organic matter available on a renewable basis, including dedicated energy crops and trees, agricultural crop wastes and residues, wood wastes and residues, aquatic plants, animal wastes, municipal wastes, and other waste materials. According to a recent DOE-USDA analysis, by 2030,[9] combined forest and

[9]U.S. DOE and USDA Report. April 2005. *Biomass as a Feedstock for a Bioenergy and Bioproducts Industry: The Technical Feasibility of a Billion-Ton Annual Supply.*

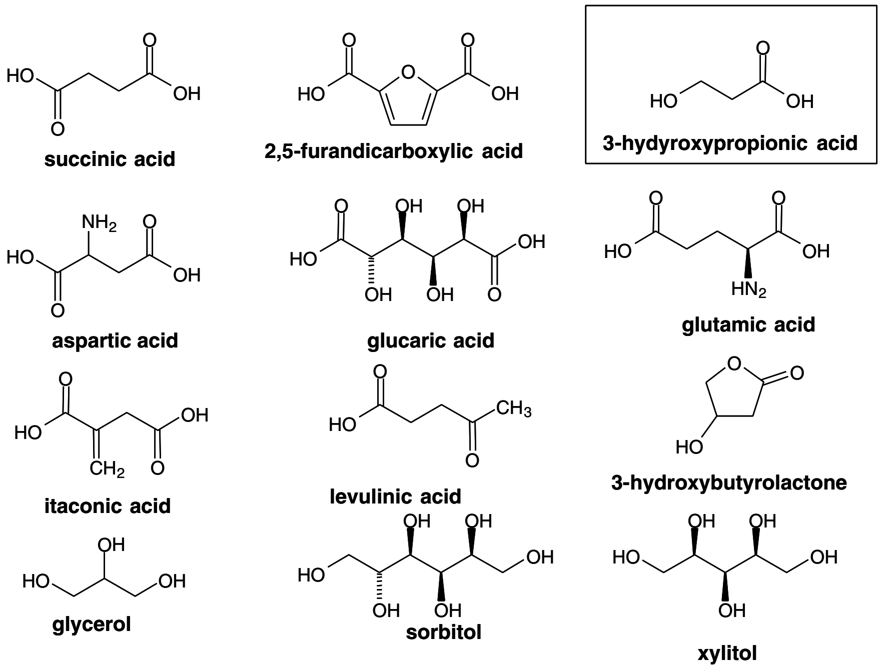

FIGURE 3.3 DOE biomass program "Top 12" sugar-based building block chemicals.

agriculture land resources alone have the potential of providing a sustainable supply of more than one-third of the nation's current petroleum consumption. In addition, the U.S. Department of Energy (DOE) has identified twelve sugar-based chemical building blocks via biochemical or chemical conversion (Figure 3.3) as a starting point for the development of biomass as a feedstock for commodity chemicals.[10] Such chemicals are seen as essential in the development of a commercially viable biomass generated feedstock. Much research is still needed to determine the means of producing these materials.

However, questions remain. What building block chemicals are currently available? Are these chemicals the right ones? Do they lead to what the chemical enterprise currently obtains from fossil fuel sources—basic aliphatic and aromatic building blocks—which feed into the products that consumers demand? A fundamental challenge for the sustainability effort

[10]U.S. DOE Biomass Program. August 2004. *Top Value Added Chemicals from Biomass, Volume 1: Results from Screening for Potential Candidates from Sugars and Synthesis Gas, Report #35523.*

is the development of a catalog of biomass derived chemicals, which DOE has already begun to work on. Fundamental studies on biomass could provide such building blocks—lignin chemistries, a re-examination of cellulose chemistries, or other biomass-based chemistries that were historically viewed as uneconomic or difficult. This "catalog" of potential starting chemicals would provide the research community with starting points in the development of alternative pathways to achieve the desired end materials.

> We [in biomass] need to be doing the same thing [as] the petroleum folks, and that is, get every value . . . of every product possible out of it.
>
> *Stanley Bull, National Renewable Energy Laboratory*

Technologies for Converting Biomass into Chemical Feedstocks

While the "catalog" of potential starting chemicals is extremely important, the development of technologies to produce these chemicals is equally important. The chemical enterprise is going to have to address the pretreatment as well as the "breakdown" processes to take the starting biomass material (this could be switch grass, corn, grains, energy cane, water hyacinth, etc.) to the potential building blocks to develop the platform chemicals.

A common method of initial "breakdown" is a fermentation process. The development of specific organisms for the express purpose of producing a specific compound from the biomass is a viable avenue of research. The development of the specific organism—whether by directed evolution, gene splicing, or a traditional selective isolation—is a significant need to enable the technology. At the same time, the development of such organisms leads to a number of ethical and social issues surrounding the genetic modification. This is another area where the chemical enterprise is going to have to develop tools to deal with the potential risks associated with genetic modification and examine the social implications of the technology.

Fermentation processes are but one potential initial step. There could be other potential pathways to the building block chemicals; there could be direct extraction from the plant or biomass material, enzymatic reactions, etc. These other pathways also need directed research in order to achieve the platform chemicals.

Once the base chemicals have been obtained via what ever selected pathway, the chemical will then have to be separated from the complex mixture. This identifies the need for better separation chemistries that will be required—particularly aqueous separations as well as concentrating techniques as it is anticipated that many of these platform chemicals will be produced in very dilute mixtures. The dilute mixtures also point to another significant research need—understanding of water chemistries. Water will be of significant concern in the production of platform chemicals from biomass—identification of sources, water quality, and the water treatment.

Fermentation processes imply the production of biomass as a waste product. Waste treatment, handling, and disposal are also going to be issues associated with the bio-production of platform chemicals. Hence, research opportunities abound related to the basic chemistries associated with fermentation, separations, water treatment, water chemistries, waste management, etc.

From this brief discussion of the various process chemistries, it should become evident that a life cycle analysis of the process from biomass through use and disposal is essential. The complex chemistries and potential side products of production need to be analyzed and considered as potential feedstocks for alternative processes. The fermentation liquor is going to be a complex mixture with potential chemistries that are not currently well understood by chemists.

The development of the building block chemical assumes that chemistries exist for such transformations to the ultimate production chemical. Since the fundamental platform chemicals may be significantly different than those obtained from the fossil fuel based starting materials, there needs to be a firm understanding of the steps to take the platform chemical to the production chemical. Thus, research in the areas of basic chemical transformations—such as oxidation, hydrogenation, and Fischer-Tropsch synthesis—is essential. Figure 3.4 illustrates how 3-hydroxypropionic acid (3-HP) derived from sugar (Figure 3.3) can be transformed into more useful chemicals with varying moieties.

Finally, since the handling of biomass materials is different than that of handling fossil fuels, one would anticipate that materials handling issues would also be a fruitful area of research. Mixing, solid handling, and heat transfer are areas where it is anticipated that new process chemistry and engineering technologies will have to be developed.

CONCLUSIONS AND RECOMMENDATIONS

In order to develop the required new commercially viable alternatives to fossil fuel feedstocks, attention must be given to a number of critical research areas. Many of these are already being addressed through increased federal funding or collaborative efforts between industry and

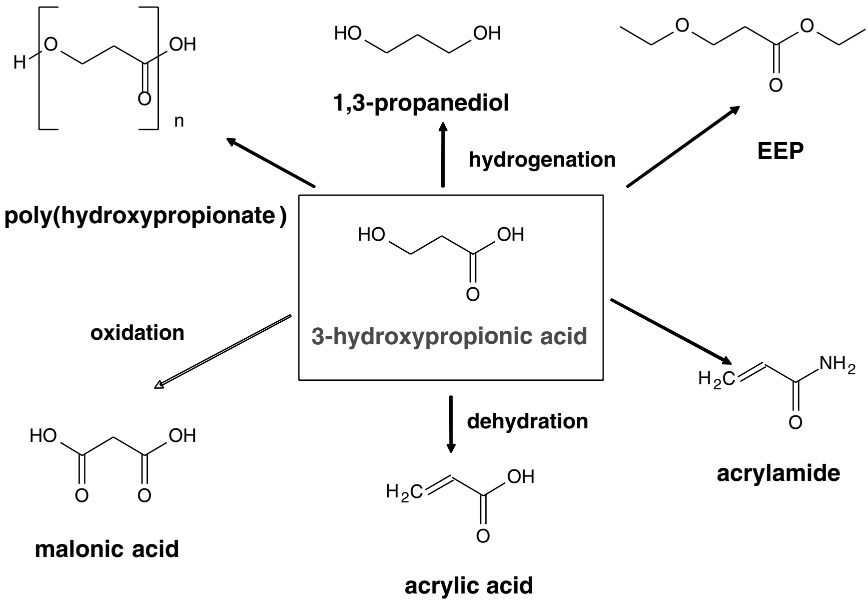

FIGURE 3.4 3-HP from sugar platform as a chemical building block.

government. All of these issues need to be tempered through the lens of life cycle analyzes as well as the ethical and social risk assessments. This is a new lens for the chemical enterprise, which means that there needs to be a fundamental change in thinking regarding how one approaches research—a need for sustainability literacy (see Chapter 5 for more discussion). Issues surrounding the biomass life cycle need to be considered—the seasonality of the growth cycle, the land nutrient cycle, and biomass waste (see Chapter 2). Taking such a holistic approach to the problem is a different viewpoint for the chemical enterprise.

Fundamentally, the underlying issue surrounding all of these research topics is that of functionality. At the consumer level, the fundamental need is functionality—transportation from point A to B, a pharmaceutical that treats a specific illness or pain, a material with specific properties, etc. The ultimate grand challenge is how to change the approach to research to provide for the desired functionality in a way that is sustainable.

The need for a "catalog" of biomass derived materials. A fundamental challenge for the sustainability effort is the development of a catalog of biomass derived chemicals, which DOE has already begun to work on. This would mean fundamental studies on biomass could provide such building blocks—lignin chemistry, a re-examination of cellulose chemistries, or other biomass-based chemistries that were historically viewed as uneconomic or difficult. This "catalog" of potential starting chemicals would provide the research community with starting points in the development of alternative pathways to achieve the desired end materials.

Future fuel alternatives. Because of the competing needs for feedstocks and fuels, clearly, it is a grand challenge for the chemical enterprise to lead the way in the development of future fuel alternatives. These alternatives could be in the development of hydrogen, landfill gas, and biomass fuel sources utilizing fuel cell, wind, solar heating, and photovoltaic technology. A great example of such efforts includes the integration of producing fuels and feedstocks from biomass via biorefineries, such as the DuPont-DOE Integrated Corn Biorefinery project. Such efforts need to be emulated and expanded.

Integration of process chemistries. In addition to developing future fuel alternatives, the chemical enterprise should accelerate its efforts to examine the technologies needed to fully integrate production activities—thereby reducing current energy needs. Examples of where this is already taking place include smaller niche operations such as the pulp and paper industry where waste products are utilized as fuel for the process. These applications could be expanded and potentially integrated into additional processes.

Development of platform chemicals (sugar, lignin, etc.) from biomass that lead to basic building block chemicals. There needs to be an alternative means of producing the basic commodity chemicals such as simple aliphatics and aromatics since the chemistry will be quite different from transforming fossil fuel hydrocarbons. Much research is still needed to determine the means of producing these materials from sugars, starch, lignin, and cellulose. An example includes the efforts by the DOE, which identified sugar-based chemical building blocks via biochemical or chemical conversion as a starting point for the development of biomass as a feedstock for commodity chemicals. Such building block chemicals are seen as essential in the development of a commercially viable biomass generated feedstock.

Understanding of the basic chemical processes to transform the platform chemicals to the final production processes. While the "catalog" of potential starting chemicals is extremely important, the development of technologies to produce these chemicals is just as important. The chemical enterprise is going to have to address the pretreatment as well as the "breakdown" processes to take the starting biomass material (this could be switch grass, corn, grains, energy cane, water hyacinth, etc.) to the potential building blocks to develop the platform chemicals.

Understanding the basic separation or extraction processes need to isolate the building block chemicals from biomass. Once the platform chemicals have been obtained via whatever selected pathway, the chemical will then have to be separated from the complex mixture. This identifies the need for better separation chemistries that will be required—particularly aqueous separations as well as concentrating techniques as it is anticipated that many of these platform chemicals will be produced in very dilute mixtures. The dilute mixtures also point to another significant research need—understanding of water chemistries. Water will be of significant concern in the production of platform chemicals from biomass—identification of sources, water quality, and the water treatment.

4

Addressing Energy Intensity of the Chemical and Allied Process Industry

The high standard of living accorded by the availability of food, water, clothing, shelter, transportation, and recreation, are the result of great advances in chemical and biological sciences and technology. However, the chemical products resulting from these advances require considerable energy input or intensity.[1] The U.S. energy use constitutes about 24 percent of the global consumption of energy, 88 percent of which is derived from fossil fuels (petroleum, coal, and natural gas combined).[2] Industrial activity accounts for 33 percent of all the energy (fossil fuels, electricity, etc.) used in the U.S. The U.S. chemical process industry (CPI) consumes nearly 25 percent of this,[3,4] or about 7.7 percent of all the energy resources used in the United States. In short, energy use in the CPI is significant. The readily available and relatively inexpensive sources of fossil fuels that the chemical industry has enjoyed for the last century are in part responsible for the present situation.

The implications for sustainability of the high energy use in the CPI are well documented. Similar to the discussion in Chapter 3, these include business risks associated with the:

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[1]Energy consumption relative to total output (gross domestic product or gross national product).

[2]U.S. Department of Energy, Energy Information Administration. 2003. Annual Energy Review.

[3]*http://www.eere.energy.gov/industry/chemicals/pdfs/annual03_chemical.pdf*

[4]Schwarz, J. M., B. R. Beloff, E. R. Beaver, and D. Tanzil. Winter 2001. Practical Minimum Energy Requirements for Chemical Product Manufacturing: A Management Tool for Achieving Sustainable Products. *Environmental Quality Management* 75–89.

- Increasingly higher cost of energy which is reflected in the increasing production cost of chemical products;
- Uncertainties in the reliability of supply;
- Impacts on global climate change from emissions of greenhouse gases (CO_2, etc.) as well as ones causing acid rain and ground-level ozone pollution (NO_x, etc.)
- Competition with other industries (transportation, domestic, etc) for fossil fuel resources.

Global events in the last three decades, however, have brought the realization that fundamental changes in energy use are necessary for continued sustainability of the chemical and allied industries. Recently, the price of a barrel of oil reached more than $60, and is likely to continue to fluctuate, with the mean value staying substantially above the price over the last 20 years. The price of natural gas is at an all time high in the United States, which is the highest price in the world. This places the U.S. chemical industry at an economic competitive disadvantage. The fourfold increase in oil prices since the mid-1990s has driven the CPI to discover energy efficient technologies that have contributed to more useful products, reduced emissions, and improved productivity. Indeed, there are numerous examples of real gains made by the chemical industry in addressing the high energy intensity. One company has publicly reported[5] achievements of more than 20 percent improvement in energy efficiency in a ten year period from 1994 to 2004. However the exploration, discovery and implementation of innovative and more energy efficient technology are, and must remain, ongoing pursuits.[6]

The goal of these pursuits is for the chemical industry to continue to deliver products essential to improved living conditions of the current generation and still be able to meet the needs of future generations. As pointed out by Jeff Siirola during the workshop, it is expected that in the near term the chemical industries will continue to rely on fossils fuels, eventually converting from oil and natural gas to coal, as dictated by price. However, it is anticipated that carbon (i.e., CO_2) management—closing the carbon cycle—will become vital prior to the depletion of fossil fuel reserves (Table 4.1).[7] Eventually, the use of renewable energy sources will be required. The following innovative strategies and technologies are necessary for success:

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[5] *http://www.dow.com/commitments/stewardship/increase.htm*

[6] Hoffert, M. I., et al. 2002. Advanced Technology Paths to Global Climate Stability: Energy for a Greenhouse Planet. *Science* 298:981–987.

[7] See comments by Jeff Siirola and Klaus Lackner, Workshop Summary, Appendix D, p. 139 and p. 151, respectively.

TABLE 4.1 Fossil Fuel Reserves

	Recoverable Reserves (Gigaton Carbon)[a]	Reserve life at current consumption rate (years)[b]	Reserve life at projected GDP growth (years)[c]
Oil	120	35	25
Natural Gas	75	60	45
Coal	925	400	100

[a]SOURCE: Energy Information Administration website (*www.eia.doe.gov*).
[b]Estimated reserves divided by current consumption
[c]SOURCE: Population trends for each geographic sector of the world were taken from the Population Reference Bureau website (*www.prb.org*) and GDP per Capita for every country were taken from a table at *www.photius.com/wfb1999/rankings/gdp_per_capita_0.html*. Estimates were made for how fast GDP/Capita (in constant dollars) might grow in each country, and were then multiplied by the expected population growth in each country and summed for the whole world to get a ratio for how energy demand will grow (energy demand grows historically at half the rate of GDP growth). Provided courtesy of Jeffrey Siirola.

- Continually reduce the energy intensity of the CPI towards practical minimum levels, with the obvious benefit of reducing the cost to manufacture
- Reduce dependence on the increasingly costly and unreliable supply of fossil fuels
- Allow the greater use of renewable energy resources, including solar energy and biomass-derived energy
- Reduce the environmental impact by decreasing carbon emissions

OPPORTUNITIES FOR R&D

One area of opportunity for research and development in sustainability for the chemical industry has to do with improving energy efficiency and reducing the energy intensity of the CPI. Well known endeavors towards reduction of energy intensity involve continuous improvements and optimization of existing processes and operating practices, heat recovery and heat integration methods (including co-generation of electric power and steam), selection and use of equipment with enhanced mechanical and electrical efficiencies. Greater investments are being made to capture and use currently wasted natural gas in the form of liquefied natural gas (LNG). At the workshop, several other ideas for reducing the energy intensity of the chemical and allied process industry were suggested. Several of these ideas are already in use at some level but require further research and development to achieve breakthrough inno-

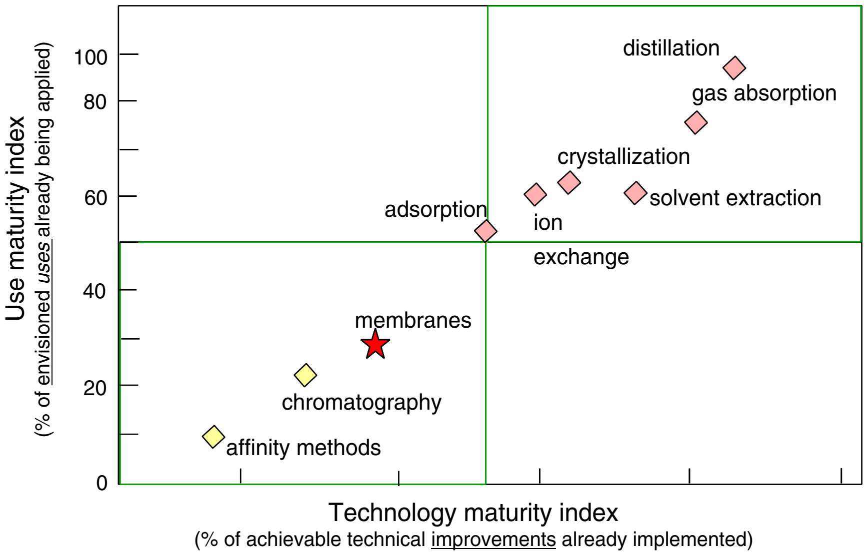

FIGURE 4.1 Maturity of separation technologies.
SOURCE: William Koros, adapted from Humphrey, J. L. and Keller, G. E., II, 1997, *Separation Process Technology*, McGraw-Hill.

vations. A few of these ideas are presented below, and note the research challenges to be addressed.

Energy Efficient Separations

Chemical processes typically include one or more energy intensive separation steps. Distillation is by far the most common separation method, and this one unit operation consumes 35-40 percent of the all the fuel used for energy by the CPI (dominated by petroleum refining), amounting to roughly 3 percent of all the energy needs of the entire United States.[8] At the same time, as shown in Figure 4-1, distillation is quite a mature technology that is becoming increasingly difficult to improve upon.[9] A large percentage of achievable technical improvements have been made and a large percentage of envisioned uses have already been

[8]U.S. Department of Energy (Energy Information Administration). 2004. Country Analysis Brief, USA. *www.eia.doe.gov/emeu/cabs/usa.html*

[9]Humphrey, J. L., and G. E. Keller, II. 1997. *Separation Process Technology*. McGraw-Hill, and comments by William Koros during workshop, p. 147.

applied to distillation. In contrast, less mature technologies such as membrane separations, adsorption, and extractions usually occur at lower temperatures and consequently tend to be lower energy intensive processes. However, there are significant technical challenges that currently limit the use of these alternative separation processes and that must be overcome to realize significant reductions in the energy intensity of the CPI.

Membrane Separations

Membranes are increasingly being used in separation processes and novel synthetic processes.[10] As pointed out by William Koros during the workshop,[11] membranes have the greatest potential for low energy intensity processing, but they are the least technologically mature of large scale separations. Further growth in membrane applications will require research and development effort that includes the following:

- Development of advanced membrane materials with well-characterized physical and performance (selectivity and permeability) properties as well as appropriate selection and applications guidelines
- Development of quantitative predictive models that relate membrane structure to the performance characteristics for separating complex mixtures
- Development of catalytic membrane reactors
- Manufacturing technology for cost effective assembly of reliable membrane separation modules for both liquid and gas phase separations
- Fouling: understanding the mechanisms for fouling and ways to reduce or prevent it.

> [Membrane separation] technology is about where I would say aqueous reverse osmosis was in the late 1960's. It was clear that it worked, but it didn't work very well, and there still has to be a significant investment made. We are making a decision. We are either going to invest in something that has this ability to cause an order of magnitude reduction [in cost], or we won't.
>
> *William Koros, Georgia Institute of Technology*

[10] Koros, W. J. 2004. Evolving Beyond the Thermal Age of Separation Processes: Membranes Can Lead the Way. *AIChE J.* 50(10):2326–2334.

[11] See comments by William Koros in the Workshop Summary, Appendix D, p. 147.

Adsorption

The design of novel materials provides the opportunity for highly selective adsorption separations. Research challenges associated with adsorption include the following:

- Finding adsorbents with appropriate selectivity for specific separations and that retain their integrity through many adsorption-desorption cycles
- Energy efficient and cost effective desorption strategies
- Improving the science and technology of simulating moving beds technology to make adsorption technology effective for essentially continuous operations.

Extraction

While not new technology, liquid-liquid extraction needs to be more fully exploited in the CPI. The primary limitations have been selectivity, cross-contamination, and the toxicity of the solvents. Thus, the primary research challenges that exist are:

- Developing and identifying solvents that give the appropriate selectivity and partition coefficients, without significant loss of the solvent to the raffinate[12]
- Developing and identifying solvents with lower toxicity

Separation and Recovery of Components from Dilute Aqueous Solutions

Separation of valuable components and waste products from dilute solutions is a particularly challenging separations problem that warrants special attention. Removing contaminants from wastewaters is vitally important, as is the recovery of products from fermentation broths. Evaporation of large amounts of water is usually a poor choice from an energy standpoint due to the large heat of vaporization of water. Thus, strategies for removal of components from dilute aqueous solutions constitute a particularly urgent research challenge.

[12]This is portion of an original liquid that remains after other components have been dissolved by a solvent.

Novel and Effective Catalysts

As pointed out in a recent special issue of *Science* magazine on catalysts,[13] "Industrial catalysis will continue to require chemical engineers to take the work of chemists, and increasingly biologists, and run it efficiently on a grand scale." Improvements in chemical and biological catalytic selectivity and activity under varying conditions has the potential to substantially reduce the energy intensity of the CPI, in addition to other aspects of achieving sustainability discussed elsewhere in the report (e.g., managing carbon dioxide, producing feedstocks from biomass, developing green chemistry and engineering, etc.). Recent advances in nanoscience[14,15] are now contributing to a greater understanding of how particle size, structure, and composition affect catalyst performance, which should lead to greater opportunities for reducing the energy intensity of the CPI.

Biocatalysis[16] through use of enzymes was highlighted in the workshop as a promising approach to reducing the energy intensity of the CPI, and as a way of creating innovative solutions to fuel growth for future generations without the environmental insult (also see discussion in Chapter 3 on "Technologies for Converting Biomass into Chemical Feedstocks"). Glen Nedwin pointed out how the use of enzymes exploits their key properties, which include: specificity of catalytic activity; effectiveness at low temperature and concentrations; ability to biodegrade; and availability from renewable resources.

Nedwin suggested several areas of research and development that need to be explored to reduce the manufacturing cost of enzymes, and increase the enzyme specific activity per gram. Many of these advances will involved improvements in overall genetic engineering capabilities to support enzyme production, and include:

- Finding less costly feedstocks for the manufacture of enzymes
- Enhancing enzyme recovery and separation methods to make them less costly
- Ways to increase fermentation yields for enzyme production
- Developing process technologies for on-site or in-situ production
- Finding more stable enzymes or develop methods to enhance their stability

[13]Coontz, R., J. Fahrenkamp-Uppenbrink, and F. Szuromi. 2003. Introduction to special issue: Speeding Chemistry Along. *Science* 299(5613):1683.

[14]Bell, A. T. 2003. The Impact of Nanoscience on Heterogeneous Catalysis. *Science* 299(5613):1688–1691.

[15]Rolison, D. R. 2003. Catalytic Nanoarchitectures—The Importance of Nothing and the Unimportance of Periodicity. *Science* 299(5613):1698–1701.

[16]Thomas, S. M., R. DiCosimo, V. Nagarajan. 2002. Biocatalysis: Applications and Potentials for the Chemical Industry. *Trends in Biotechnology* 20(6):238–242.

- Discovering enzymes with greater specificity
- Optimization of cellulase enzyme mix

Alternative Fuels

Reducing the energy intensity of biofuel[17] and biofeedstock production (see Chapter 3 of this report) is another important research area. A major challenge associated with biomass utilization for both fuels and feedstocks is developing technologies for carrying out separations, especially separation of relatively dilute chemicals from aqueous solutions (e.g., fermentation broths), as mentioned in Chapter 3. According to Stanley Bull, only recently has even ethanol production from corn sugars (which has been invested in heavily) become efficient enough that it is a net energy producer.[18]

There is also a continued need for technologies for cogeneration of high value chemical building blocks and power starting with fossil fuel feedstocks, such as coal and lignite as oil supplies dwindle in the short term and renewables become more viable sources of fuel in the long term. The chemical industry has steadily increased its cogeneration capacity over the years, more than doubling between 1985 and 1998—providing about 20 percent of the net demand for electricity in for the CPI in 1998.[19] Optimization of production of chemical feedstocks, power production and efficient heat recovery will continue to be needed regardless of the sources of energy.

Lubrication

A vast amount of the energy used by modern societies is wasted as a result of unproductive friction in internal combustion and aircraft engines, gears, cams, seals and bearings. According to some estimates,[20] *one third* of the world's energy resources in present use disappear as friction in one form or another. Typical automobile engines convert only 20-35 percent of the chemical energy of combustion to useful mechanical work. The rest is lost due to frictional losses and heat via engine cooling and exhaust. Jost has estimated[21] that the United States could save in excess of $16 billion

[17]This includes fuel such as methane produced from renewable resources, especially plant biomass and treated municipal and industrial wastes.

[18]See comments by Bull in the Workshop Summary, Appendix D, p. 128.

[19]Energy Information Administration. 2001. *Manufacturing Energy Consumption Survey.*

[20]Bhushan, B., ed. 1996. *Handbook of Micro/Nano Tribology*. Boca Raton, Florida: CRC Press.

[21]Jost, P. 1976. Economic Impact of Tribology. *Proc. Mechanical Failures Prevention Group.* NBS Spec. Pub. 423. Gaithersburg, MD.

per year from better tribological practices. Advances in nanoscience have led to new understanding of adhesion, friction, wear, and thin-flm lubrication at sliding surfaces taking place from the atomic and molecular scales to microscales.[22] Further developments in **micro/nanotribology** have the potential to provide breakthrough technology for reducing the energy intensity of the CPI. Major research challenges include:

- Development of a fundamental understanding of how lubrication works to allow design and selection of compounds and mixtures with the appropriate properties
- Development of more stable, higher temperature lubricants

Solar and Other Non-Fossil Fuel Sources of Energy

While reduction in energy intensity and improvements in energy efficiency of using fossil fuels in the short term are absolutely vital for the sustainability of the CPI, eventually the CPI must look to alternative and renewable feedstocks and energy sources. These may include landfill gas, wind, and solar energy. Renewable sources are a vital component of any effort to be less dependent on conventional feedstocks and fuels, to reduce manufacturing costs, and to decrease the impact of the CPI on the environment.

Among the options that exist, solar energy is the only truly sustainable energy solution. Obviously the sun is the primary source of energy on earth. Solar energy is abundant, clean, and renewable, but unfortunately it is intermittent and diffuse. To realize its potential, it must be captured, concentrated and stored or converted to other useful forms. The research challenges include:

- Advances in technologies that will reduce the cost and the environmental impact of producing photovoltaic systems.
- Advances in technologies that allow the direct use of solar energy for cost-effective splitting of water to produce hydrogen
- Improvements in heat transfer fluids that enable direct use of solar energy for meeting some of the heating requirements of the CPI
- Advances in storage systems for electric power generated from solar energy.

[22]Bharat, B. 1999. *Handbook of Micro/Nano Tribology*, Second edition. Boca Raton, Florida: CRC Press.

It should be noted that nuclear energy is often mentioned as a potential long-term source of energy as an alternative to fossil fuels. As pointed out in the workshop and elsewhere,[6,23] current (fission based) nuclear reactor technology does provide electricity without carbon dioxide emissions. However, it also generates highly toxic wastes, presents safety and security concerns for centuries [half life of plutonium is 24,100 years], and utilizes limited uranium resources; thus it is not a sustainable energy option. At the same time, nuclear technology based on the energy released by the fusion of deuterium and tritium is a promising long-term energy source [greater than 30 years] without the negative attributes of nuclear fission, but it still requires significant research advances to make it a viable option.[6]

Carbon Management

Since fossil fuels are significantly less expensive than alternative energy sources (due to the many research challenges; see section on "Solar and Other Non-Fossil Fuel Sources of Energy" above), it is anticipated that the CPI will continue to use fossil fuels for energy for many decades into the foreseeable future. In addition, there is significant capital investment that would be required to convert from fossil fuels to renewable sources. When the price of oil and natural gas becomes prohibitively high due to dwindling supplies or other factors, the CPI will convert to relatively abundant coal. Even with steady growth in GDP, it is anticipated that coal reserves will last for at least another century (Table 4.1).[24] There is general agreement among the scientific community that there is a link between atmospheric CO_2 concentrations and global temperature increases.[25] Moreover, as atmospheric CO_2 concentration increases, it is projected that the associated global climate change will reach a critical stage by mid century, well before the depletion of all fossil fuel reserves. Thus, developing technology and strategies for effective carbon management is a key to sustainability of not just the CPI, but life on earth in general.

Current estimates for the energy required for CO_2 recovery from flue gas by amine scrubbing, pressurization, and re-injection into geological formations varies from about 13-25 percent of the energy value of the

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[23]Pacalal, S. and R. Socolow. 2004. Stabilization Wedges: Solving the Climate Problem for the Next 50 Years with Current Technologies. *Science* 305(5686):968–972.

[24]See Workshop Summary: comments by Siirola on p. 139; Lackner on p. 151.

[25]National Research Council. 2005. *Radiative Forcing of Climate Change: Expanding the Concept and Addressing Uncertainties.* Washington, D.C.:The National Academies Press.

original fuel that produced the CO_2 (natural gas vs. pulverized coal).[26] This is a very significant burden that needs to be reduced if effective CO_2 management is to be employed on a widespread basis. In addition, there are issues with regard to leakage from geological formations that have not been fully resolved.

Thus, the research and development challenges for carbon management include:

- Development of energy efficient technologies for CO_2 separation, not just from flue gas, but also from the atmosphere
- Development of technologies for CO_2 sequestration. Questions that need to be addressed include:
  - —Is it technically feasible to make carbonates from CO_2 without excessive energy use and with a viable carbonate disposal plan?
  - —Is it possible to effectively utilize CO_2 in the production of cement?
  - —Can CO_2 hydrates be made a practical solution?
  - —What are the issues (e.g., leakage) associated with storage of compressed CO_2 in geological formations?

Development of technologies for CO_2 utilization is needed. CO_2 is considered to be a cheap, nontoxic, and renewable feedstock that is currently being used to produce entirely new materials and for new routes to existing chemicals such as urea, salicylic acid, cyclic carbonates, and polycarbonates.[27] With further progress, utilizing CO_2 for synthesis of chemicals could play a more significant role in managing global carbon emissions.

CONCLUSIONS AND RECOMMENDATIONS

Reducing the energy intensity of the CPI is an absolutely vital component in ensuring the sustainability of the chemical and allied industries. Continued reliance on fossil fuels can be anticipated, with eventual conversion from less abundant oil and natural gas to more abundant coal. This makes the issue of carbon management extremely important. The CPI will eventually need to look to renewable energy resources. Finally, it is clear that development of more energy efficient technologies will be

[26]David, J. 2000. Economic Evaluation of Leading Technology Options for Sequestration of Carbon Dioxide. MIT Masters Thesis; Herzog, H. J., and D. Golomb. 2004. Carbon Capture and Storage from Fossil Fuel Use., in C. J. Cleveland, ed. *Encyclopedia of Energy*. New York: Elsevier Science Inc. Pp. 277–287.

[27]Marks, T. J., et al. 2001. Catalysis Research of Relevance to Carbon Management. *Chemical Reviews* 101(4):973–975.

necessary whatever the source of energy being used by the CPI, with priority given to research and development in the following areas:

More energy efficient separation processes. Chemical processes typically include one or more energy intensive separation steps. Distillation is by far the most energy intensive. In contrast, membrane separations, adsorption, and extractions tend to be lower energy intensive processes. However, there are significant technical challenges that currently limit the use of these alternative separation processes and that must be overcome to realize significant reductions in the energy intensity of the CPI.

Utilization of improved catalysts for energy reduction and selectivity increases. **Biotechnological and other emerging technological** solutions need to be explored to reduce the energy intensity of the CPI. In contrast to the typical catalysts in chemical reactions that require high temperatures and pressures while offering low selectivity, **biocatalytic approaches** and new developments in **nanoscience** have the ability to provide greater specific catalytic activity under mild reaction conditions. In the case of enzymes, such activity can be very specific under mild reaction conditions, while at the same time being biodegradable and produced from renewable resources. Such approaches present possible solutions for reducing the energy intensity of the CPI, and as a way of creating innovative solutions for future generations without harming the environment.

Improvements in energy efficiency for the production of biofuels and biofeedstocks. A major challenge for sustainability in the chemical industry is how to reduce the energy intensity of biofuel and biofeedstock production (see Chapter 3 of this report for more discussion). There is a need for an effective biomass feedstock process to recover not only hemi-cellulose and sugars for oxygenated molecular building blocks but also lignin as a source of aromatic molecules.

Development of more effective lubricants. A vast amount of the energy used by modern societies is wasted as a result of unproductive friction in internal combustion and aircraft engines, gears, cams, seals, and bearings. Fundamental understanding of how lubrication works is needed to allow design and selection of compounds and mixtures with the appropriate properties. There also needs to be development of more stable, higher temperature lubricants

Step change improvements in the use of solar energy and other renewable energy sources. While reduction in energy intensity and improvements in energy efficiency are absolutely vital for the sustainability of the

CPI, eventually, the CPI must look to alternative and renewable feedstocks and energy sources. These may include landfill gas, wind, and solar energy. Renewable sources are a vital component of any effort to be less dependent on conventional feedstocks and fuels, to reduce manufacturing costs, and to decrease the impact of the CPI on the environment.

Technological breakthroughs in CO_2 separation, sequestration, and use. It is anticipated that the CPI will continue to use fossil fuels for energy for many decades into the foreseeable future. This is mainly due to abundant supplies of coal and the significant capital investment that would be required to convert from fossil fuels to renewable sources. At the same time, there is general agreement among the scientific community that there is a link between atmospheric CO_2 concentrations and global temperature increases. As atmospheric CO_2 concentration increases, it is projected that the associated global climate change will reach a critical stage well before fossil fuel reserves run out. Thus, developing technology and strategies for effective carbon management is a key to sustainability of not just the CPI, but life on earth in general.

5

Sustainability Science Literacy and Education That Enables the Adoption of More Sustainable Practices in the Chemical Industry

Progress in all other areas discussed so far depends upon greater literacy in what is coming to be called sustainability science, which brings together "scholarship and practice, global and local perspectives from north and south, and disciplines across the natural and social sciences, engineering, and medicine."[1] Given its ubiquitous influence over economies, effective transitional steps for the chemical industry to move toward sustainability are based fundamentally upon the initial stepping stone of communicating the dispersed science knowledge that makes sustainability thinking clear. While seemingly fragmented, the fields of green chemistry, industrial ecology, and earth systems science are interconnected constituents of this knowledge. Exposure to these ideas through education and training is essential to chemical industry adoption of practices that will enhance the nation's economic strength and security, and position the industry advantageously as an innovative force for future prosperity. Engagement with sustainability principles offers the United States the opportunity to lead on the inevitable path toward more intelligent industrial activity with respect to nature's dynamics, human health, and political stability.

THE CHALLENGE OF COMMUNICATING SUSTAINABILITY

Addressing the gap between the dominant conventional understanding of the nature-human relationship on the one hand, and the different

[1]Clark, William C., and Nancy M. Dickson. 2003. Sustainability Science: The Emerging Research Program. *Proceedings of the National Academy of Sciences (USA)* 100(14):8059–8061.

mindset required for businesses to function effectively going forward on the other, is the first hurdle. The gap will be filled with state of the art knowledge about the nature-human interface, which in turn establishes the requisite mindset for innovation. At present, the knowledge base is distributed across disciplines. But the challenge can be expressed simply. The chemical industry and society at large must understand the reality and implications of the economy existing within society, which in turn is embedded within a biosphere. The biosphere has countless interdependent systems from the planet's scale to human's most recent frontier of microscopic inquiry, the nanotechnology scale. Bench level chemistry changes in material design and diffused molecular concentrations above normal background levels influence and alter the dynamics of these systems. In other words, we are now engineering—or designing—nature, and should therefore proceed with as much caution and information about consequences as possible. In this context, the government must understand and guide economic development according to its best comprehension of conditions which favor greater prosperity for more people.

> Unless we understand that something that is designed at bench scale will, in fact, in many cases, impact systems at regional and global scale, we have not yet begun to grapple with what is already occurring in our world; not what is going to occur, what is already occurring.
>
> *Brad Allenby, Arizona State University*

Understanding Earth Systems

Adoption of "sustainability practices" in any industry presupposes at the outset a clear understanding of society at multiple levels and why one would be concerned about these issues. What does it mean when the term "sustainability" is used? While the term may sound ambiguous, there is consensus on the foundational science that forms the bedrock of sustainability frameworks currently used. Accumulated data from scientific communities, ranging from earth scientists and demographers to immunologists and toxicologists, argue that humans have become a central force in nature, shaping nature through potentially irreversible modifications to its systems. The distinction between "impacting" and "shaping the dynamics" of natural systems needs emphasis. As a species, humans have moved from the assumption that relatively small activity could have no enduring influence on nature, to understanding that such impacts have occurred. In 2005, there has been sufficient evidence that the scale and character of industrial activity can and have already irreversible changed the chemical dynamics of what had once been considered "stable" systems in nature.

This reality needs to be communicated through education and training. Today, it is still relatively segregated and marginalized in the study of ecology and other environmental sciences. In management education, the actions are segregated (and therefore marginalized) in Environment Health and Safety (EH&S) offices or in debates about ethics and social responsibility. As central topics in the science communities and related to the health and stability of societies today, these issues are migrating to the core of corporate strategy, but education has not kept up. While having always influenced the physical environment, the reach of humans has been extended dramatically in the last 100 years through technology and globalization, yet we still design feedstocks and final products, and maintain industries that produce them as though we were ignorant of these changes. Anthropogenic impact fundamentally alters the chemistry, ecology, and biology of living and nonliving systems. Historically unprecedented population growth, with accompanying exponentially expanded throughput of industrial materials, has led to unavoidable pollution and health challenges. Moreover, growth demands and technological advances place ever growing requirements for natural and synthetic materials. The scale and accelerating rate of change results in activity and waste streams that disrupt and degrade natural systems worldwide (e.g. air, hydrologic, and biogeochemical cycles). Yet these same systems provide critical services on which society and the economy depend—clean water, healthy air, clean energy, productive soil, and safe food. This knowledge cannot remain marginal to the education of citizens. Not only does the knowledge base of scientists need augmenting but those working in industry, including throughout supply chains to final product users, need the systems orientation of green chemistry and sustainability science.

Recognition of this reality has spread outward from the scientific communities to governments, international and national standard setting bodies, advocacy organizations, and community- and professionally-based groups worldwide concerned with human health and environmental degradation. Greater awareness drives public policy decisions as well as corporate strategy to respond and adapt and attempt to function successfully given these changing conditions, but the knowledge of how to respond and adapt has to be communicated. In summary, population growth combined with the expanding materials intensity of economic activity and the scientific capabilities to better understand their implications presents the current generation with a simply reality: The global demand for resources and the waste generated now collide with the ability of natural systems to regenerate.

Many describe the situation as humans consciously and unconsciously designing (engineering) natural systems.[2] For example, gene manipulation is an example of conscious engineering, and ozone depletion, and dead zones in coastal areas are examples of unintended engineering. The first step in a research agenda for sustainability in the chemical industry should include how to effectively educate the people in industry to this reality.

EDUCATIONAL PRIORITIES

Enhancing the level of sustainability literacy generally and incorporating the concepts and strategies of sustainable practices in science and business education are key to attaining sustainability in the chemical enterprise. Broader implementation of sustainable practices depends both on "market pull" from consumers and "technological push" from the research and development community. Priorities for education efforts in sustainability should thus address the purchasers of innovative products, the designers, and the business practitioners. Goals for sustainability literacy and education must include:

- Supporting the research agenda put forth in the preceding sections of this report through education about underlying drivers and science
- Stimulating demand for environmentally benign technology among industrial scientists, business people, and consumers
- Advocating a better understanding of the science challenges and opportunities associated with sustainability within the chemical enterprise, and overcoming resistance within the disciplines

A number of barriers to change exist. One of these has to do with the ability of industry to adopt new practices, which can be difficult because of: (1) mature products and processes that make innovation risky, difficult, or unwarranted, (2) lack of reliable metrics to drive decision making and societal impact quantification, and (3) the perception that economic pay-offs are too distant and not well understood.

In fact, the contribution to corporate value creation is increasingly well understood. While changes in course content are relatively constant, there needs to be integration of "green" into standard course materials. Textbooks need updating. New approaches that focus more on sustainability take time and resources to develop and implement, compete with existing programs, and must overcome the inertia of well-entrenched

[2]See comments by Brad Allenby in the Workshop Summary, Appendix D, p. 103.

> Many people today distrust business. Yet younger people, idealistic and full of creative ideas, want to do meaningful work. What if research and educational funding supported clean technology innovation and a shift toward sustainability practices? Why couldn't, why shouldn't, this country lead in ideas, education, and the transformation of its economy.
>
> *Andrea Larson, Darden Graduate School of Business Administration*

teaching practices. Thus updates to core and essential course materials are essential. In addition, accreditation and standardized testing procedures favor the existing programs, contributing an additional barrier. Finally, there has been little recognition of economic opportunities for business creativity, opportunity, and innovation inherent in addressing issues of sustainability, making the field less attractive to researchers and educators and keeping the issues marginalized as "ethics" or "environmental compliance." A shared barrier in both the industrial and academic venues is a lack of clear definition of terms describing the field (e.g. "green" vs. "sustainable" vs. "green chemistry"). Again, there exists the research challenge of framing and articulating science knowledge in terms and ways that the ideas are well communicated to diverse audiences. The timing for change is now. A wide variety of factors have converged to stimulate change. Among others are shareholder petitions, Dow Jones Sustainability Indexes driving corporations to achieve sustainability goals, global full cost accounting and financial reporting standards, and leadership by firms through organizations such as the World Business Council on Sustainable Development.[3]

There is an opportunity to improve sustainability education at every level—from informal education of current and future consumers and citizens to future scientists, to the chemistry and engineering practitioners, to the business leaders who sell these products and define corporate strategy. In order to make progress toward this goal, these efforts need to be prioritized, identifying the audiences to target and what they need to learn. In the short term, efforts should be placed on educating the practitioners of the field (scientists and engineers) who are capable of discovering and developing new, more sustainable technologies and the business leaders who will decide if and how these technologies are implemented. In the longer term, educational efforts that target K-12, university students

[3]See: Willard, B. 2005. *The Next Sustainability Wave.* New Society Press; Larson, A. 2003. *Reframing Global Environmental Issues through an Innovation and Entrepreneurship Lens*. #UVA-ENT-0041. University of Virginia: Darden Business Publishing.

and teachers, consumers, and policy makers are needed now to create demand for more sustainable products and practices. Efforts by pioneering individuals and institutions are already underway. Identifying and supporting these early efforts and seeding additional initiatives are essential. As with any new area that changes how people think, and therefore act, the pioneers often work in relative isolation and even opposition. If these topics are to be taken seriously by the U.S. government, those who have laid the cornerstone to the new house need support.

EDUCATING FUTURE PRACTITIONERS—WORKFORCE AND EDUCATORS

As the source of innovative ideas and technologies for the future chemical enterprise, future practitioners are a critical audience for educational programs that promote a more sustainable industrial system. Although the details of the changes in the curriculum will depend upon the target group, in general, changes in education should: address the interdisciplinary nature of the research problems introduced earlier in this report; develop the fundamental tools for solving complex problems; give students experience assessing the relative merits of different technological solutions; and help students appreciate the relevance of their work to industry and society as a whole. At the most basic, education is needed to communicate an understanding of why the chemical industry must change and the probable consequences of maintaining the status quo. More specific needs are described below for each group.

Educators

Within the context of this report, there currently exist three broad classes of educators: a small number that are already incorporating sustainability into their courses, a growing number who would like to do so, and many who are resistant to or unaware of this type of change. Thus, there is a need for new educational materials and incentives that support those who are pioneering or are interested in change and incentives that encourage faculty to incorporate sustainability into their coursework. Examples of educational materials that are needed will be described below. Although there has been considerable progress made in developing materials,[4] there exists an appetite for new materials that span a broad range

[4]See Stuart L. Hart's work at Cornell's Johnson School of Business, Andrea Larson's work at the University of Virginia's Darden Graduate School of Business Administration for business management educational materials, and the textbooks: Allen, D. T., and D. R. Shonnard.

from introductory, stand-alone materials to fully integrated curricula across multiple disciplines. Incentives to promote adoption include:

- Resources to encourage development of new educational materials, such as the National Science Foundation (NSF) Course, Curriculum, and Laboratory Improvement (CCLI) program;
- Changes in the direction of accreditation and certification programs, such as the American Chemical Society (ACS) Committee on Professional Training, similar to what the Accreditation Board for Engineering and Technology (ABET) has put in place to catalyze engineering curriculum reform through its Engineering Criteria 2000 (EC2000);
- The inclusion of this subject matter on standardized exams (e.g., ACS subject exams); and
- Opportunities to align faculty research and education objectives, such as the NSF Faculty Early Career Development (CAREER) program, which can be powerful motivators for young faculty to pursue activities that will promote a more sustainable chemical enterprise. Interested institutions can hold forums to disseminate the research and concepts to introduce young faculty to materials and topics. Pedagogy programs to consolidate and accelerate understanding can be established to move this agenda forward more expeditiously. This acceleration is necessary because the natural course of change will be slow due to disincentives. These include promotion paths that support specialization and discourage cross-discipline and cross-field research and teaching efforts, inertia that persists without funding to direct intellectual effort toward change, and the tenure system that defends and preserves the status quo knowledge.

Chemistry and Chemical Engineering Graduate Students

In order to solve the complex research challenges described earlier in this report, chemists and chemical engineers will need a range of skills that span from fundamental chemistry to applied science that enable them to work effectively with colleagues from biology to business. In addition, they will need to acquire new skills such as life cycle assessment and toxicology that permit them to assess and develop new technologies that offer high performance and have a minimal environmental footprint. The following elements are needed to prepare students to excel in careers in this area:

2002. *Green Engineering: Environmentally Conscious Design of Chemical Processes.* Prentice Hall; Parent, K., and M. Kirchhoff., eds. 2004. *Going Green: Integrating Green Chemistry into the Curriculum.* Washington, D.C.: American Chemical Society.

1. A strong component of interdisciplinary research that helps students learn to integrate their work with other disciplines while contributing to the development of a knowledge base needed to address sustainability challenges. In particular, activities that get chemists and chemical engineers working together should be included. Also important is research and curricula that span schools and disciplines to insure chemistry and engineering concepts are integrated with professional schools: medicine, business, and law.
2. A strategic approach that encourages students to apply their basic chemistry knowledge to real problems and provide them with familiarity of business thinking and industrial practices, business opportunities, and challenges.
3. An emphasis on skills such as communication and teamwork that are needed to work effectively with a broad range of professionals.
4. A basic understanding of current science and alternative risk assessment methods associated with the biological impacts on natural systems resulting from new compositions of matter and routes of exposure.

A model similar to the NSF Integrative Graduate Education and Research Traineeship (IGERT) program—which helps establish innovative new models for graduate education and stimulates collaborative research that transcends traditional disciplinary boundaries—would seem an excellent way to provide incentives for faculty to change curricula while addressing the needs of graduate students entering this complex field. [5]

Specialized Masters Degree programs that assist students in applying the basic science they have learned during their undergraduate education toward industrially-relevant problems may be an important approach to assist students in preparing to make contributions to the challenges faced in developing a more sustainable chemical enterprise.

Chemistry and Chemical Engineering Undergraduate Students

At the undergraduate level, effort should be made to introduce students to the concepts of sustainability within the context of the core curriculum. Although there is considerable pressure to add new material to the curriculum, it is possible to incorporate green chemistry (and related topics regarding sustainability) without giving up the core learning objectives. Students are often more interested in learning these core objectives

[5] This NSF-wide endeavor was initiated in 1997, is now comprised of approximately 125 award sites, and in 2005 continues into its sixth annual competition. For more information see the NSF-IGERT web site: *http://www.nsf.gov/crssprgm/igert/intro.jsp*

when the relevance has been made clear, for example through relationship to their everyday lives or to the environment. Chemistry majors who gain exposure to these topics are better prepared to address sustainability challenges in the workforce or in their graduate work.

> . . . it is important to hold students' interest in green chemistry as early as possible, and to show them that chemistry is not the grand polluter of the planet and, instead, offers solutions to some of these environmental challenges that we face.
>
> *Mary Kirchhoff, American Chemical Society*

Research and Development Managers

As the industrial world begins to shift to the production of more and more sustainable products and services in response to a changing market place, R&D managers will have to understand and support innovations that have a reduced environmental and social impact. They will need the tools and time to be able to teach the chemists and engineers in their organizations the basic concepts of sustainability in business, and green chemistry and engineering. These tools can take many forms from external short courses certified by the ACS and AICHE to internal topical symposia to self-taught e-learning tools. To ensure this happens it is recommended that this responsibility of research management be codified in their annual performance goals. These managers will be more successful the more they understand the interrelationship between synthetic chemistry and the natural biological systems in nature. All research directors will be best served by being prepared in the biological sciences. As petroleum based raw materials become scarce and costly, renewable (biobased) sources will likely become preferred based on their life cycle and more competitive as well as benign to the biosphere and human health. With these factors in mind, science majors in their educational preparation and industrial scientists in seeking diversity in their work experience, will ultimately reshape our future.

Business Administration Education

MBA Students and Executive Education

Awareness of cost reduction, risk avoidance, market differentiation, and other benefits from sustainable business strategies is spotty at best in

MBA curricula and advanced management training. This is not to ignore the leadership role of a small number of faculty. However, these early stage efforts need resources to accelerate and deepen their influence. The contribution sustainability can provide to business practices and financial performance (as well as public health and safety) needs to be disseminated through teaching materials at both the MBA and executive levels to address deficiencies in current education and to inform working managers and executives of changing competitive conditions. Business education is key to the transformation of the chemical enterprise because most chemists and chemical engineers in firms are not business unit managers, nor are they typically on senior management teams. Yet it is these positions that determine operating and strategic policies within firms. The science and empirical evidence driving markets toward green chemistry alternatives, as well as the market shifts that create opportunities for new products and processes based on sustainability concepts, are urgently needed in management education. Programs that collect, integrate, and disseminate teaching materials are needed. Research funding that rewards research and knowledge creation is also essential to overcome obstacles to change.

General Education

In order to increase the demand for more sustainable products, education within the K-12 school systems, in introductory university courses, and of consumers will be essential. This education is necessary to allow for change within the industry as this creates the consumer pull for sustainable processes and products. Development of materials for use in K-12 settings and getting greater involvement of graduate students (such as supported by the NSF GK-12 fellowship program), ACS student affiliate groups, and others familiar with sustainability concepts in these settings can help K-12 students and teachers become more familiar with the opportunities for young scientists to craft a more sustainable future through science or citizenship. In the universities, introductory science courses that include the concepts of sustainability or multidisciplinary nonmajors courses that bring together chemistry or engineering with other disciplines such as business, public policy, or environmental science can be excellent vehicles to raise awareness among nonscientists within our universities. Universities and businesses should collaborate with nongovernmental organizations (NGOs) to educate the broader public about the choices that they make as consumers and citizens and how these choices can promote a sustainable future.

Unified Instruction of Life Cycle Analysis/Life Cycle Inventory

Across the disciplines there is the need to develop methods that facilitate comparison of alternative technologies and processes. One of the most powerful approaches to make these comparisons is through life cycle assessment (LCA). The development of effective LCA tools and inventory information that can be used in these analyses would be of considerable benefit to students in chemistry and engineering from the undergraduate to graduate level. In each venue, an appropriate treatment should address the process of life cycle analysis, the influence of the inventory data on the analysis results, the interpretation of the results, and how results will be used. Awareness of the tools, frameworks (industrial ecology and green chemistry, for example), and how their application benefits companies must be addressed in professional schools, particularly business schools.

CONCLUSIONS AND RECOMMENDATIONS

Progress in all other areas discussed so far—development of green chemistry and engineering capabilities, alternative fuels and feedstocks, and energy efficiency—depends upon greater literacy in sustainability science. Education targeted to business leaders, buyers, and product/process designers is essential. This educational agenda is the fundamental grand challenge. Chemists and chemical engineers need to have a firm grasp of their disciplines' subject matter from the theoretical to the practical, but at the same time deeply understand how their work has global and local impacts, and how they can inform and be informed by other disciplines across the natural and social sciences, engineering, and business. Business decision-makers must understand *why* these are priorities and *how* to implement change. Exposure to these sustainability ideas through education and training is essential to chemical industry adoption of practices that will enhance the nation's economic strength and security. These steps also position industry advantageously as an innovative force for national competitiveness and future prosperity. In summary, there is a need to improve sustainability education at every level—from informal education of consumers and citizens to future scientists to the practitioners of the field to the businesses that use and sell these products. In order to make progress toward this goal, attention must be given to a number of important research areas described below.

Research Needed

Promote incorporation of sustainability concepts—into curricula, particularly in chemistry and chemical engineering, but also spanning professional schools with special emphasis on management education because knowledge in this sector can significantly accelerate application and learning in the "real" world of business and markets. Without this link, certainly industry will adapt much more slowly, particularly compared with its international competition that is under pressure from the same set of changing conditions. **At a minimum**, infuse fundamental concepts of sustainability—green chemistry, industrial ecology, earth systems science, ecology, biogeochemistry, and sustainable business innovation—into core curricula as appropriate.

Develop and promote educational materials (e.g. lab modules, LCA modules, new text books that infuse sustainability and green chemistry concepts into the core material). There is a need for new educational materials and incentives that support those who are pioneering or are interested in change, and incentives that encourage faculty to incorporate sustainability into their coursework. Incentives to promote adoption include resources to encourage development of new educational materials such as the National Science Foundation (NSF) Course, Curriculum, and Laboratory Improvement (CCLI) program.

Include sustainability concepts as part of standardized testing programs. Changes are needed in the direction of accreditation and certification programs such as those developed by the ACS Committee on Professional Training or ABET, and the inclusion of this subject matter on standardized exams such as ACS subject exams.

Develop effective life cycle assessment (LCA) tools and inventory information. LCA would be of considerable benefit to students in chemistry and engineering from the undergraduate to graduate level. In each venue, an appropriate treatment should address the process of life cycle analysis, the influence of the inventory data on the analysis results, the interpretation of the results and how results will be used. LCA is also a powerful teaching tool in business education. If business students have never heard of LCA (and other sustainability approaches and tools), their understanding of how these issues integrate into corporate strategic decisions will be limited.

Provide professional development opportunities for faculty. Educators need to learn about sustainability and how it can be advantageously incorporated into their research and education. Opportunities to align faculty research and education objectives such as the NSF Faculty Early Career Development—CAREER—program can be a powerful motivator for young faculty to pursue activities that will promote a more sustainable chemical enterprise. More senior educators also need exposure and education. The problem is often lack of understanding, not opposition per se.

Provide sustainability focused NSF-IGERT-like training grants. Such programs are needed to help establish innovative new models for graduate education and stimulate collaborative research that transcends traditional disciplinary boundaries. This would be an excellent way to provide incentives for faculty to change curricula while addressing the needs of graduate students entering this complex field.

Include sustainability as part of annual performance goals for R&D managers, product development heads, and business unit managers. As the industrial world shifts to the production of more and more sustainable products and services in response to feedback from nature and the human body and a changing market place, these managers will have to first understand and then support innovations that have a reduced environmental and social impact (or, literally eliminate risk). They will also need the tools and time to be able to teach the chemists and engineers in their organizations the basic concepts behind sustainability and green chemistry and engineering.

6

Conclusions and Recommendations

Based on the discussion provided in the previous chapters of this report, a set of grand challenges and accompanying research needs were identified and are summarized below. Although the Grand Challenges are numbered, they are all important in the context of this report and to the triple bottom line of the chemical industry now and in the future. However, Figure 6-1 illustrates how the different Grand Challenges (ovals) address the sustainability transition (large arrows) from the current paradigm to the ideal vision over the course of two critical time frames:

1. The next 20 years (2005–2025) of continued use of fossil fuels (especially oil) as the predominant source of energy and chemical feedstocks, where managing carbon, reducing the intense use of energy resources, and educational efforts to promote sustainability thinking will be critical; and
2. The next 20-100 years (2025–2105) in which the use of fossil fuels will be phased out, and where the ability to carry out green chemistry and engineering (built on fundamental understanding of the full life cycle impacts and toxicology of chemicals), and having access to alternative renewable sources of fuels and feedstocks will be critical.

GRAND CHALLENGES

The eight Grand Challenges below were chosen because they were considered to pose the greatest science and technical challenges for ad-

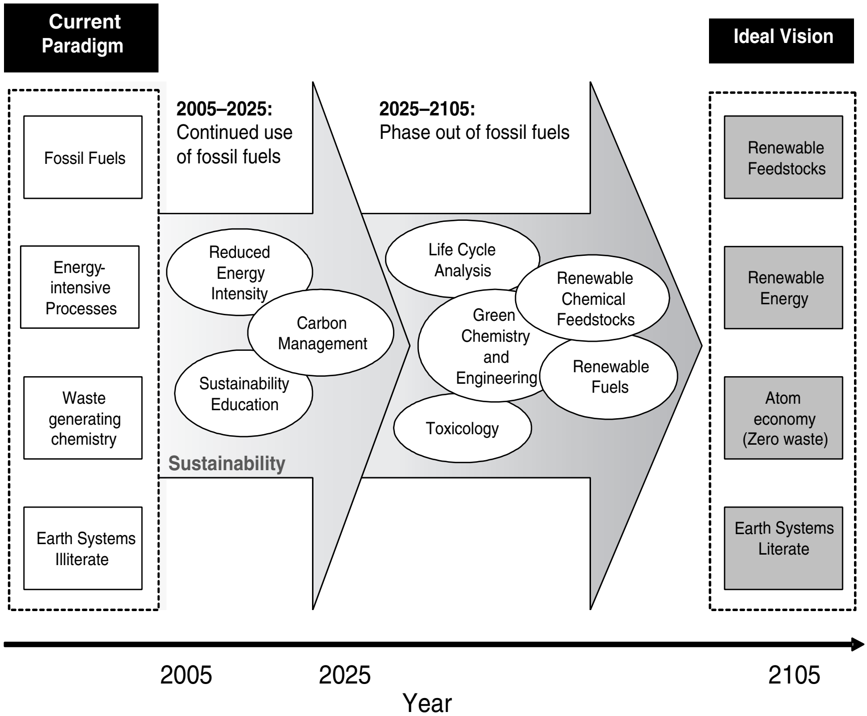

FIGURE 6-1 The Grand Challenges (ovals) for Sustainability (large arrows) address the transition from the current thinking to the ideal vision for the chemical industry over the next 100 years. See text for a more detailed description of figure and the Grand Challenges.

dressing sustainability—balanced economic, environmental, and societal progress—in the chemical industry over the next 100 years.

1. Green and Sustainable Chemistry and Engineering

It is a grand challenge for all chemists and chemical engineers to be involved in discovering ways to carry out more chemical transformations utilizing green and sustainable chemistry and engineering. This builds on the ultimate premise of green chemistry[1,2] that *it is better to prevent waste than to clean it up after it is formed*, and its integration into processing and

[1]Anastas, P. T., J. Warner. 1998. *Green Chemistry Theory and Practice*. Oxford: Oxford University Press.

[2]Poliakoff, M., J. M. Fitzpatrick, T. R. Farren, and P. T. Anastas. 2002. Green Chemistry: Science and Politics of Change. *Science* 297:807–810.

other operations through green engineering.[3] Achieving this grand challenge ideally provides production of both basic and fine chemicals in a less hazardous environment for humans and ecosystems, uses less energy, and lowers costs of production. Over the next twenty years this will involve replacing harmful solvents or improving catalytic selectivity and efficiency in chemical reactions that also provides cost savings. This area will grow in importance in the long term as fossil fuels are phased out of use and alternative and innovative approaches are required.

Research Needed:
While chemists can make most any molecule no matter how structurally complex, they need to develop with their engineering partners lower energy reaction pathways for current synthetic processes, and more environmentally benign solvent systems with higher yield efficiencies and less toxic waste.

2. Life Cycle Analysis
Today, there continue to be gaps in the way that chemistry and its impact on global systems is thought about. There is a need to understand the long-term impacts of chemicals in the environment—such as persistence, bioaccumulation, global warming potential, or ozone depletion—and to account for such properties within a large complex systems analysis. This involves having a keen understanding of the metabolism of chemical products—that is, their industrial ecology[4]—from the extraction of raw materials and creation of products, to their use and management of any resulting wastes. Life cycle analytical tools are especially needed for comparing the total environmental impact of products generated from different processing routes and under different operating conditions through the full life cycle. This is another area that is already being explored, but will play an increasingly significant role in the chemical industry in the longer term as fossil fuels are phased out of use and application of green chemistry and engineering practices become critical.

Research Needed:
Improvements are needed in the quantity and quality of data required for such comparisons and in the approach used to evaluate life cycle metrics. There needs to be an appropriate understanding of the methodology of life cycle analysis, the influence of the life cycle inventory data on the

[3] Ritter, S. K. 2003. A Green Agenda for Engineering. *Chemical and Engineering News.* 81(29):30–32.
[4] Frosch, R. A. 1995. The Industrial Ecology of the 21st Century. *Scientific American* 273(3):178–181.

analysis results, the interpretation of the results, and how the results will be used.

3. Toxicology

In order to successfully develop green and sustainable chemistry and engineering approaches, it is a grand challenge that chemists know the toxicological fate and effect of all chemical inputs and outputs of bond forming steps. Many data related to human and environmental toxicology of chemicals are either missing or questionable, which to a large extent affects the significance of some LCA studies, as well as the usefulness of material safety data sheets (MSDS) and other technical fact sheets. This is already an area of concern for the chemical industry, and will be increasingly important as fossil fuels are phased out of use and application of green chemistry and engineering practices become critical.

Research Needed:

Development of critical tools for improved understanding of structure-function relationships for chemicals and chemical mixtures in humans and the environment is needed. It would be tremendously useful to have a centralized repository for human health related data (issued from validated industrial, occupational, and community-generated resources) as well as ecotoxicity figures (for LCA studies) in the public domain at little or no cost to all interested parties. There is clearly a role for the associations within the chemical industry to assist in the funding and development of critical data related to the most pervasive and problematic chemicals in the industrial environment. Computational and genomic approaches to toxicology must be included in such efforts, such as those already underway at the U.S. Environmental Protection Agency and their partners at the National Institute of Environmental and Health Sciences and the Department of Energy.

4. Renewable Chemical Feedstocks

In order to provide desired chemical functionality in a way that is sustainable, another grand challenge for sustainability in the chemical industry is to derive chemicals from biomass**.** This includes any plant derived organic matter available on a renewable basis, including dedicated energy crops and trees, agricultural food and feed crops, agricultural crop wastes and residues, wood wastes and residues, aquatic plants, animal wastes, municipal wastes, and other waste materials.[5] This is a long term challenge that will become increasingly important as fossil fuels are phased out over the next 100 years.

[5] U.S. Department of Energy definition.

Research Needed:
There is a need to develop a catalog of biomass derived chemicals, building on what DOE has already begun.[6] This "catalog" of potential starting chemicals would provide the research community with starting points in the development of alternative pathways to achieve the desired end materials.

This effort should involve studies on biomass that can provide current basic chemicals such as simple aliphatics and aromatics as well as fundamentally new compounds from platforms such as lignin, sugar, or cellulose. This should include a review of biomass-based chemistries that were historically viewed as uneconomic or difficult. It may also mean providing support for proven chemistries that need further research on applications and commercialization.

In developing biomass as a source of chemicals, improvements in processing are critically important. Pretreatment as well as the breakdown processes for transforming biomass material into useful chemicals must be addressed. This requires a better understanding of the basic chemical pathways involved in biomass conversion processes. While the catalog of potential starting chemicals is extremely important, the development of sustainable technologies to produce these chemicals is just as important (Grand Challenge 1).

Separation or extraction processes to isolate the basic chemicals from biomass are a very important part of processing (Grand Challenge 6). In particular, aqueous separations as well as concentrating techniques require attention because many biomass platform chemicals will likely be produced in very dilute and complex mixtures. As a result, the removal of water is a significant concern in the production of chemicals from biomass; identification of sources, and water treatment must all be addressed.

Overall, issues surrounding the biomass life cycle (Grand Challenge 2) need to be considered—the seasonality of the growth, the land nutrient cycle, and waste products. It is essential that a holistic approach to developing renewable chemical feedstocks be taken.

5. Renewable Fuels

The chemical process industry (CPI) consumes about 7.7 percent of all the energy (fossil fuels, electricity, etc.) resources used in the United States.[7]

[6]U.S. DOE Biomass Program. August 2004. *Top Value Added Chemicals from Biomass, Volume 1: Results from Screening for Potential Candidates from Sugars and Synthesis Gas.* Report #35523.

[7]*http://www.eere.energy.gov/industry/about/pdfs/chemicals_fy2004.pdf*

Of this, about 50 percent of the energy resources are used as chemical feedstocks, rather than consumed as energy. Because of the competing needs for feedstocks and fuels and the substantial use of energy by the CPI, it is a grand challenge for the chemical industry to lead the way in the development of future fuel alternatives derived from renewable sources such as biomass as well as landfill gas, wind, solar heating, and photovoltaic technology. This is another long term challenge that will become increasingly important as fossil fuels are phased out over the next 100 years.

Research Needed:
The only truly global sustainable source of energy is abundant, clean, and renewable **solar energy**. Unfortunately, it is intermittent and diffuse. To realize its potential, it must be captured, concentrated and stored or converted to other useful forms, and will require significant research advances including:

- Reduction in the cost and the environmental impact of producing photovoltaic systems;
- The ability to directly use solar energy for cost-effective splitting of water to produce hydrogen;
- Improvements in heat transfer fluids that enable direct use of solar energy for meeting some of the heating requirements of the CPI; and
- Advances in storage systems for electric power generated from solar energy.

Development of biomass derived fuels is also an important area of research that is intimately connected with biomass derived chemical feedstocks (Grand Challenge 4) and the energy intensity of the chemical processing (Grand Challenge 6).

6. Energy Intensity of Chemical Processing
Reducing the energy intensity of the CPI is another grand challenge for sustainability in the chemical industry. Continued reliance on fossil fuels can be anticipated, with eventual conversion from less abundant oil and natural gas to more abundant coal over the next 100 years. This makes the issue of carbon management extremely important (Grand Challenge 7), and presents a need for the CPI to transition to renewable sources of energy (Grand Challenge 5). However, it is clear that the continued development of more energy efficient technologies will be necessary whatever the source of energy being used by the CPI. Addressing this challenge will be critical during the continued use of fossil fuels as the predominant source of energy and chemical feedstocks over the next 20 years, and will continue to be important even when renewable energy resources are predominant.

Research Needed:
The energy efficiency of chemical separations is a key research component of this grand challenge. Finding effective alternatives to distillation are especially needed. While membrane separations, adsorption, and extractions tend to be less energy intensive, significant technical challenges must be overcome in the development of these alternatives in order to realize any significant reductions in the energy intensity of the CPI.

Biotechnological and other emerging technological solutions need to be explored to reduce the energy intensity of the CPI. In contrast to the typical catalysts in chemical reactions that require high temperatures and pressures while offering low selectivity, biocatalytic approaches[8] and new developments in nanoscience have the ability to provide greater specific catalytic activity under mild reaction conditions. In the case of enzymes, such activity also occurs while being biodegradable and produced from renewable resources. These approaches present ways of creating innovative solutions to fuel growth for future generations, without harming the environment or human health. Research and development needs in these areas include reducing production costs, increasing stability, and discovering catalysts with greater specificity.

Fundamental understanding of the mechanisms of friction, lubrication, and wear of interacting surfaces—tribology—also presents a fruitful area of research for addressing energy loss in the CPI. According to some estimates,[9] *one third* of the world's energy resources are consumed due to frictional losses. It has been estimated[10] that the United States could save in excess of $16 billion per year from better tribological practices. Advances in nanoscience have led to new understanding of adhesion, friction, wear, and thin-flm lubrication at sliding surfaces taking place at the atomic and molecular scale.[11] Further developments in micro/nanotribology has the potential to provide breakthrough technology for reducing the energy intensity of the CPI .

7. Separation, Sequestration, and Utilization of Carbon Dioxide
Developing technology and strategies to manage the resulting carbon dioxide (CO_2) of current and future use of fossil fuels is a grand challenge for sustainability for not only the chemical industry but life in general. As

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[8]Thomas, S. M., R. DiCosimo, and V. Nagarajan. 2002. Biocatalysis: Applications and Potentials for the Chemical Industry. *Trends in Biotechnology* 20(6):238–242.

[9]Bhushan, B., ed. 1996. *Handbook of Micro/Nano Tribology*. Boca Raton, Florida: CRC Press.

[10]Jost, P. 1976. Economic Impact of Tribology. *Proc. Mechanical Failures Prevention Group*. NBS Spec. Pub. 423. Gaithersburg, MD.

[11]Bharat, B. 1999. *Handbook of Micro/Nano Tribology*, Second edition. Boca Raton, Florida: CRC Press.

global industrial society continues to use fossil fuels for energy, there is general agreement among the scientific community that CO_2 concentrations and global temperature will also increase.[12] At the same time, current estimates for the energy required for CO_2 recovery from flue gas by amine scrubbing, pressurization, and re-injection into geological formations varies from about 13-25 percent of the energy value of the original fuel that produced the CO_2 (natural gas vs. pulverized coal).[13] This is a very significant burden that needs to be reduced if effective CO_2 management is to be employed on a widespread basis. Addressing this challenge will also be critical during the continued use of fossil fuels as the predominant source of energy and chemical feedstocks over the next 20 years, and will continue to be important as long as carbon based fuels are in use.

Research Needed:
Energy efficient technologies (Grand Challenge 5) need to be developed for CO_2 separation from flue gas and the atmosphere.

Technologies for CO_2 sequestration will need to address the technical feasibility of making carbonates from CO_2 without excessive energy use and with a viable carbonate disposal plan; effectively utilizing CO_2 in the production of cement; storage of compressed CO_2 in geological formations; and whether or not CO_2 can be successfully stored adjacent to the ocean floor.

Ways of utilizing CO_2 as a feedstock need to continue to be explored. CO_2 is considered to be a cheap, nontoxic, and renewable feedstock that can be used to produce entirely new materials and for new routes to existing chemicals such as urea, salicylic acid, cyclic carbonates, and polycarbonates.[14] With further progress, utilizing CO_2 for synthesis of chemicals could play a more significant role in managing global carbon emissions.

8. Sustainability Education

Progress on all other grand challenge areas discussed depends upon greater literacy in the triple bottom line[15] from the perspective of business

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[12]National Research Council. 2005. *Radiative Forcing of Climate Change: Expanding the Concept and Addressing Uncertainties.* Washington, D.C.: The National Academies Press.

[13]David, J. 2000. Economic Evaluation of Leading Technology Options for Sequestration of Carbon Dioxide. MIT Masters Thesis and Herzog, H. J., and D. Golomb. 2004. Carbon Capture and Storage from Fossil Fuel Use., in C. J. Cleveland, ed. *Encyclopedia of Energy*. New York: Elsevier Science Inc. Pp. 277–287.

[14]Marks, T. J. et al. 2001. Catalysis Research of Relevance to Carbon Management. *Chemical Reviews* 101(4):973–975.

[15]Elkington, J. 1997. *Cannibals with Forks:The Triple Bottom Line of 21st Century Business.* Oxford: Capstone Publishing.

and the sciences. There is a need to improve and accelerate sustainability education at every level—from informal education of consumers and citizens, to future scientists, practitioners of the field, and businesses that use and sell these products. Advances in chemistry and engineering must be accompanied by cross-disciplinary education in sustainability science and its application to the business community. This includes greater understanding of earth systems science and engineering, ecology, green chemistry, biogeochemistry, life cycle analysis, and toxicology. Exposure to these sustainability ideas through education and training underlies chemical industry adoption of practices that will enhance the nation's economic strength and security, and position the industry advantageously as an innovative force for future prosperity. Addressing this challenge will be critical over the next 20 years as changes in thinking are needed to make the transition to more sustainable processes, products, and systems.

Research Needed:
Educators across disciplines need to be sensitized to the finite nature of the planet and its natural systems. Opportunities to align research and educational objectives such as the NSF Faculty Early Career Development (CAREER) program can be a powerful motivator for young faculty to pursue activities that promote a more sustainable chemical industry. Sustainability focused NSF IGERT-like training grants—which help establish innovative new models for graduate education and training and stimulate collaborative research that transcends traditional disciplinary boundaries—should also be encouraged. This would be an excellent way to provide incentives for faculty to change curricula while addressing the needs of graduate students entering this complex field.

Professional societies also play a significant role here by encouraging the integration of sustainability and green chemistry and engineering concepts into standardized testing, accreditation, and certification programs such as those developed by the ACS Committee on Professional Training or ABET (Accreditation Board for Engineering and Technology). Educational materials such as lab modules, LCA modules, and new textbooks that infuse sustainability and green chemistry concepts into the core material must be developed. If these efforts are not mirrored in fields that intersect with chemistry and that can amplify or discourage sustainability, the goals will be difficult to achieve. There is also a need to support pioneers who are interested in effecting change by offering incentives that encourage faculty to incorporate sustainability into their coursework and research, whether in chemistry, engineering, product development, process methods, or business education. An example of such an incentive is the National Science Foundation (NSF)—Course, Curriculum, and Laboratory Improvement (CCLI)—program.

Curricula are needed that incorporate sustainability concepts—earth systems science and engineering, ecology, green chemistry, biogeochemistry, life cycle analysis, toxicology—into secondary and tertiary education. Building on existing efforts and accelerating their delivery is needed. Although particular focus must be placed on training chemistry and chemical engineering students, sustainability concepts and practices should also be a part of the educational practices in professional schools such as medicine, law, and business. There should be special emphasis on management education where knowledge about sustainability as a design protocol and corporate strategic advantage could significantly accelerate application and knowledge of new products and technology in the business world. Sustainability concepts, science, systems analysis, new product development, emerging markets, full cost accounting, and valuation metrics need attention in business management to enable systematic implementation of sustainability practices. Ignoring management education creates a disconnection between chemistry and corporate leadership. Business managers and executives more broadly need customized curricula on sustainability ideas.

Business executives (including general managers, R&D managers, and financial managers) also need professional development in sustainability. R&D managers, in particular, need to first understand and then support innovations that avoid or reduce environmental and societal impact. Equally important is the communication of sustainability thinking to middle and upper level managers and executives in business management and incorporation of sustainability objectives in annual performance goals as well as corporate strategy.

Appendixes

A

Statement of Task

The National Research Council, through its Board on Chemical Sciences and Technology (BCST), will work with the chemistry and chemical engineering community to define the research needed to move toward green chemistry and engineering, and sustainable products, processes, and systems for the chemical industry. This project will:

1. Identify a set of Grand Challenges for sustainability research in chemistry and chemical engineering; and
2. Make specific recommendations about areas of research required to address those Grand Challenges.

B

Committee Biosketches

James A. Trainham *(Chair)* is vice president of science and technology for PPG Industries. Trainham joined PPG in 2005 from Invista, Inc., formerly DuPont Textiles and Interiors, where he was chief technology officer from 2002 until its divestiture from DuPont in 2004. After two years on the faculty at the University of South Carolina, Trainham joined DuPont as a research engineer in polymer products. His almost 25 years with DuPont included assignments in central research and development and in business units with responsibility for process and product technology. In 1987 he led the development of HFC-134a, the ozone safe replacement for Freon®12, then in 1992 he was appointed director of engineering research, and in 1996 global technology director for Dacron® polyester fibers and intermediates. In 1999 he assumed responsibility as global technology director, Lycra® synthetic fibers and Terathane® polyether glycols. He was then appointed global technology director, apparel and textile sciences, before the formation of DuPont Textiles and Interiors. Trainham earned bachelor and doctoral degrees in chemical engineering from the University of California, Berkeley, and a master's degree in chemical engineering from the University of Wisconsin, Madison. He was elected to The National Academy of Engineering in 1997, and received the Chemical Engineering Practice Award from the American Institute of Chemical Engineers in 2002.

Victor Atiemo-Obeng is a Scientist in the Engineering Science and Market Development (ESMD), a capability within the Corporate Research and

Development (CR&D) at The Dow Chemical Company (TDCC). Prior to his transfer to CR&D in 1997, Atiemo-Obeng spent 14 years in Global Process Engineering. He was lead process engineer for several multimillion-dollar capital projects that were recognized with Global Engineering Excellence Awards. He previously conducted process scale-up and modeling studies as a research engineer on various projects in the Applied Process Research and Process Development Departments in the Michigan Operations of the TDCC. Atiemo-Obeng is an active member of the American Institute of Chemical Engineers (AIChE), and currently serves as the Dow Director for the AIChE Mid-Michigan Section. He was the 2003 recipient of NOBCChE's prestigious Percy Julian Award for significant contributions in applied engineering science, the Dow Michigan Consultants Award in 1997, the 1995 Chemical Engineer of the Year for the Mid-Michigan AIChE section, and TDCC President's Community Service Award in 1993. He received a Ph.D. in Chemical Engineering from the University of Wisconsin, Madison in 1975, and a bachelor degree in Chemical Engineering from The Catholic University of America, Washington DC.

Michael D. Bertolucci is the president of Interface Research Corporation (IRC), chairman of the Envirosense® Consortium, Inc.—a not-for-profit organization concerned with Indoor Air Quality—and Senior Vice President of Interface, Inc. He serves on the board of the CEO Coalition to Advance Sustainable Technology (CAST). He spent six years as Vice President of Technology for Highland Industries, an industrial fabrics company, fifteen years in numerous research and development management posts with the General Electric Plastics Business Group, and four years in chemical research at Union Carbide Chemicals and Plastics. He received his Ph.D. in Physical Chemistry from the California Institute of Technology, and his BS degree in Chemistry from San Jose State.

Joan F. Brennecke is the Keating-Crawford Professor in the Department of Chemical and Biomolecular Engineering at the University of Notre Dame. She joined the faculty at Notre Dame after completing her Ph.D. and M.S. degrees at the University of Illinois at Urbana-Champaign and her B.S. at the University of Texas at Austin. Her research has focused on studies of supercritical fluids, including supercritical CO_2 and supercritical water. Brennecke was awarded the 2001 Ipatieff Prize from the American Chemical Society in recognition of her pioneering high-pressure studies of the local structure of supercritical fluid solutions and the effect of this local structure on the rates of homogeneous reactions. Much of her current research involves ionic liquids, which are organic salts that are liquid at temperatures around ambient. These salts have received tremendous recent attention as potential substitutes for volatile organic solvents since the ionic liquids are nonvolatile and, thus, cannot contribute to air pollution. In developing these solvents, Brennecke's primary interests are in thermodynamics, phase behavior, and separations.

Berkeley W. Cue, Jr. retired from Pfizer in April 2004 after almost 29 years. As vice president of Global Research and Development he was responsible for the six departments that comprise Pharmaceutical Sciences at Pfizer's Groton R&D site. He was a member of the Worldwide Pharmaceutical Sciences Executive Team and the Groton Laboratories Leadership Team. Cue led Pfizer's Green Chemistry initiative and has spoken extensively on this topic since 2000. He started in Pfizer in 1975 in the Animal Health Organic Chemistry Department. He transferred to the Process R&D Department of Developmental Research in 1979. He received a BA from the University of Massachusetts-Boston (1969), and his Ph.D. in Organic Chemistry from the University of Alabama (1974). Dr. Cue completed postdoctoral research at Ohio State University (1974) and was a National Cancer Institute Research Fellow at the University of Minnesota in 1975. In 2000 he was appointed to the Science Advisory Board at the University of Massachusetts-Boston. In 2003 he was appointed to the Green Chemistry Institute Board of Directors. He is a member of the Board of Directors of Bend Research, Inc. in Bend, Oregon.

Jean De Graeve is a professor of Occupational and Environmental Toxicology at the University of Liege in Belgium. His research fields include analytical chemistry (traces identification and measurements), toxicology (drugs, occupational and environmental risk evaluation), and clinical pharmacology (drug distribution, metabolic pathway, and kinetic compartmental analysis). De Graeve is also Executive Manager of Advanced Technology Corporation since 1985 and serves as a Scientific Advisor to various public and private analytical laboratories. He is member of the Scientific Council of the Hormonology division of the Centre d'Economie Rurale of Marloie, Belgium; member of the Agreement Commission for the accreditation of Hazardous Waste companies (transport, transformation, and elimination of hazardous waste); and, member of various Scientific and Technical Commissions created by the Belgian Authorities in order to control hazardous waste installations (like cement kilns, municipal incinerators, dump sites, industries, and their impact on workers and neighbor's health (Health consultation program), He received a B.S. and Ph.D. in chemistry from the University of Liege.

James E. Hutchison is an associate professor of chemistry at the University of Oregon, where he also serves as director of the Materials Science Institute. Professor Hutchison received his Ph.D. in organic chemistry from Stanford University and his B.S. from the University of Oregon. He received a NSF Postdoctoral Fellowship to work on analytical and surface chemistry at the University of North Carolina, Chapel Hill. Hutchison conducts research on gold nanoparticles and self-assembled monolayers. He is also very involved in green chemistry curriculum development and recently directed the renovation of a green chemistry organic laboratory at the University of Oregon. Professor Hutchison has received several awards and honors including the Alfred P. Sloan Research Fellow and the NSF CAREER Award.

Andrea Larson is Associate Professor of Business Administration at the Darden School teaching in the MBA program and in Executive Education in the areas of entrepreneurship, innovation, and sustainable business. Sustainable business is a "triple bottom line" approach by corporations incorporating economic, social, and environmental performance considerations into operations and strategy. Building upon earlier research in entrepreneurship, alliances, and network organizations, her current research, teaching, and curriculum development focuses on innovation by companies engaged in sustainable business as a strategic and competitive advantage. She holds a PhD from Harvard University, awarded jointly by the Harvard Business School and the Harvard Graduate School of Arts and Sciences.

Pamela G. Marrone is the Chairman and Founder of AgraQuest, Inc., a firm she founded that has a portfolio of proprietary natural-product pesticide discoveries and products. Marrone has substantial management expertise in startup and multi-international biotechnology firms. Before this endeavor, Marrone was president of Entotech, a subsidiary of Novo Nordisk, and senior group leader of insect control at Monsanto Agricultural Company. She received her PhD degree in entomology from the North Carolina State University. She served on the NRC Committee on the Future Role of Pesticides in Agriculture (study published in 2000) and her company won the Presidential Green Chemistry award in 2003.

Frankie Wood-Black is the Director, Business Services for Downstream Technology, ConocoPhillips. In this position, she has responsibility for those business functions—finance, business analysis, training, and assets for Downstream Technology. Prior to this position, Frankie was the Technology Services Marketing Manager for Phillips, and was responsible for in-sourcing research and development activities into the Bartlesville Technical Center. Before that she was Quality Assurance Team Leader at the Borger Refinery and NGL Center. Wood-Black began her career with ConocoPhillips in 1989 in Bartlesville, Oklahoma, as a research scientist for research and development. At ConocoPhillips she as held the position of environmental scientist with responsibilities for regulatory compliance for air, Community-Right-to-Know, and the Toxic Substance Control Act. She was also a member of the Corporate, Health, Environment and Safety in the Property Risk Management Group, where she was the site manager for nonoperating sites. Wood-Black received a B.S. in physics with a minor in chemistry from Central State University (now the University of Central Oklahoma), Edmond, OK in 1984, a Ph.D. in physics from Oklahoma State University in 1989, and completed her MBA in Dec. 2002. She has been active in numerous professional activities and serves as the ConocoPhillips representative on Corporation Associates of the American Chemical Society. Wood-Black is a registered environmental manager.

C

Workshop Agenda

CRITICAL BUILDING BLOCKS AND TOOLS FOR SUSTAINABILITY IN THE CHEMICAL INDUSTRY: IDENTIFYING AN AGENDA FOR NATIONAL RESEARCH

Monday, February 7, 2005

8:15 a.m.	*Welcome and Overview of Workshop* **James Trainham** PPG Industries Chair, Committee on Grand Challenges for Sustainability in the Chemical Industry
	SESSION 1: *Sustainability Science Literacy and Education that Enables the Adoption of More Sustainable Practices in the Chemical Industry* Chair: **Andrea Larson** University of Virginia
8:30 a.m.	Overview Speaker: *Current Knowledge about the Nexus of Industrial Activity and Natural Systems (Earth Systems to Infant Immune System Impacts)* **Braden R. Allenby** Arizona State University

9:30 a.m.	*Targeting and Guiding Demand for Green Chemistry in Product Design* **Lauren Heine** GreenBlue Institute
10:00 a.m.	*Is Chemistry Education Sustainable?* **Mary Kirchhoff** American Chemical Society
10:30 a.m.	Break
10:45 a.m.	Concurrent sessions (five groups)
12:30 p.m.	Lunch
	SESSION 2: *Enabling Technologies that Drive the Application of Green Chemistry and Engineering* Chair: **Michael D. Bertolucci** Interface Research Corporation
1:30 p.m.	Overview Speaker: *Enabling Technologies that Drive the Application of Green Chemistry and Engineering* **Berkeley W. Cue, Jr.** Pfizer, Inc. (retired)
2:30 p.m.	*Life Cycle Analysis—A Tool for Change* **Richard Helling** The Dow Chemical Company.
3:00 p.m.	*Development of Sound Structure/Property Relations, and Tools to Predict the Health and Environmental Impacts of Specific Chemicals* **Robert J. Kavlock** U.S. Environmental Protection Agency
3:30 p.m.	Break
3:45 p.m.	Concurrent sessions (five groups)
5:30 p.m.	Adjourn

Tuesday, February 8, 2005

	SESSION 3: *New Chemicals and Processes that Lead to Commercially Viable Alternative Feedstocks to Fossil Fuels* Chair: **Frankie Wood-Black** ConocoPhillips
8:00 a.m.	Overview Speaker: *Current Fossil Fuel Dependence and Future Alternative Feedstocks* **Stanley R. Bull** National Renewable Energy Laboratory
9:00 a.m.	*Sustainable Fuels and Chemicals* **Mark T. Holtzapple** Texas A&M
9:30 a.m.	*Specialty Intermediate and Complex Molecule Synthesis* **Douglas C. Cameron** Cargill Research
10:00 a.m.	Break
10:15 a.m.	Concurrent sessions (five groups)
12:00 p.m.	Lunch
	SESSION 4: *Reducing the Energy Intensity of the Chemical Process Industry* Chair: **Joan Brennecke** University of Notre Dame
1:00 p.m.	Overview Speaker: *Sustainability, Stoichiometry, and Process Systems Engineering* **Jeffrey J. Siirola** Eastman Chemical Company
2:00 p.m.	*Enzymes: Advances in Sustainable Industrial Processes and Bioenergy* **Glenn E. Nedwin** Novozymes Biotech, Inc.

2:30 p.m.	*Membrane Processes as Low energy-Intensive Enablers for Energy Conservation in the Chemical Industry* **William J. Koros** Georgia Institute of Technology
3:00 p.m.	*Green Chemistry for Carbon Management* **Klaus S. Lackner** Columbia University
3:30 p.m.	Break
3:45 p.m.	Concurrent Sessions (five groups)
5:30 p.m.	Adjourn

D

Workshop Summary

EDUCATION

In the first item on the agenda, participants debated the value of green chemistry on the curriculum of the future and spoke about the challenges of rooting sustainability in both the curriculum and textbooks. The need to educate faculty, industrial scientists, and the general public was also discussed. As an introductory comment, Andrea Larson stated that the challenge lay in approaching education at all levels and emphasized the difficulty in understanding the scope and scale of the challenges facing the chemistry community.

Brad Allenby described education in sustainable chemistry within the larger context of the overall changes taking place in this field. Chemistry is shifting in meaning right now, he said. "We appear to be in the period of fundamental redefinition of much of the intellectual landscape, and I think that is important to bear in mind when we think about what we know and what we don't know," Allenby said.

Allenby believes the current education system fails to equip any student for the world in which they will be working and living. In particular, the topics of ethics and systems complexity are either missing or severely de-emphasized. In his opinion, no student should be permitted to graduate from any institution of higher learning without completing a course that equips him or her to think about complexity. This should not be a technical course that teaches modeling; instead, it should be designed to teach them how to intuitively consider complex systems and the limitations when working with them.

Many American students also obtain the best education in terms of the specifics of their disciplines. However, education at all levels currently lacks conceptual insight in sustainability and green chemistry. The curricula, teaching materials, and emphasis on multi-disciplinary programs that cover not only technical competence but also the social and environmental dimensions of green chemistry are missing. Allenby stressed that there is a need for the ability to understand large-scale systems at an appropriate scale, especially since this is not something that an individual scientist or firm will do effectively. "We need an institutional basis to maintain a dialogue with these systems so that, for example, when the atmosphere begins to display strange chemistry based on a very, very small percentage of CFCs, we are able to respond," Allenby said.

There is also a need for an appropriate prioritization of values, ethics, and goals. Opinions differ on the values placed upon different aspects of green chemistry. "If I am working in a factory and you find a way to substitute for a carcinogen that I am being exposed to, then I am going to like that. I may not care too much if that has impacts down the line on ecosystems," Allenby explained. These problems are currently being solved on an individual scale. The policy structure at the moment encourages the imposition of individual values, an adversarial process. A single set of values applied to difficult questions will most likely be inadequate, which the field of chemistry needs to move beyond. To achieve this, institutional capability must exist. However, Allenby warned that there might not be any easy solutions. "I think that we need to appreciate the complexity of what we are doing and begin to develop tools that allow us to do better in the short run, while we are working on evolving the institutions we need in the longer run," he said.

Mary Kirchhoff of the American Chemical Society (ACS) looked at some trends in green chemistry education. The ACS Green Chemistry Institute is a strong advocate for green chemistry education. Other voices are also joining this call, which helps to build the case for increased education in this area. "Right now, there are a few champions who are very passionate about what they are doing, believe very strongly in green chemistry, but it is not across the board, and that is really where we have to keep working," she said.

Schools with green chemistry courses include Carnegie Mellon University, Davidson College (North Carolina), and Hendrix College. "You are not limited by the size of your institution, if you want to integrate green chemistry into the curriculum," Kirchoff said. The green chemistry lab at the University of Oregon offers the most comprehensive approach she has seen. All undergraduates who take organic chemistry are exposed to a green chemistry approach in the lab. The University of Massachusetts has instituted a Ph.D. program in green chemistry. At the University of

Scranton, Michael Cann has developed a number of online modules that are easily accessible for use in different categories, such as in physical chemistry, general chemistry, and organic chemistry. However, sustainability education must move beyond four-year-colleges. For example, community colleges tend to be overlooked in the educational picture. In a critical move, the University of Oregon has partnered with the local community college to encourage transfers from two-year to four-year colleges. When these students move to the four-year schools, educators want them to have been exposed to green chemistry and sustainability concepts.

Educational textbooks are also devoid of green chemistry, sustainability, or many of the related topics. *General Chemistry*, Brown and LeMay's most recent edition, contains five pages on green chemistry within its "chemistry and the environment" chapter. Zumdahl[1] has a sidebar on green chemistry that describes the use of CO_2 for dry cleaning. Kirchoff said that these are steps in the right direction, but educators tend to skip sidebars in an effort to get through an overly ambitious syllabus. Many interesting topics, especially the more modern research areas, tend to be in sidebars and side boxes. As a result, they do not get covered in the main body of the course. However, *Organic Chemistry* is very encouraging; Solomon's most recent edition has five different green chemistry examples embedded in the text. Overall, green chemistry is starting to creep into mainstream textbooks. "This is where I think we really need to be focusing our efforts, if we want to see a lot of students impacted by green chemistry," Kirchhoff said. In addition, the subjects of toxicity and toxicology should receive more appropriate attention. Usually, the LD50—the "lethal dose" that kills 50 percent of a group of test animals exposed to a material—is the only toxicity or toxicology topic covered. Occasionally, the textbook will refer to poisons and cover the alkaloids and poison dart frogs. There is room for improvement to incorporate these subjects into educational material.

Lab lectures should also incorporate more information on sustainability. Even in her own teaching experiences, Kirchhoff only provides technical information about chemicals, such as whether a chemical is hazardous or toxic, when to use it in a hood, or where MSDS sheets are located if students want to look at them. "We don't have a culture of emphasizing green chemistry topics or related topics like toxicology," she said.

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[1]Zumdahl, Steven S. 2003. *Introductory Chemistry: A Foundation,* Fifth Edition. Houghton-Mifflin.

In addition to the lack of educational materials and the over-crowded chemistry education curriculum, the perceived lack of rigor of green chemistry and sustainability is another barrier. It is challenging to conduct and teach green chemistry, because the easy reactions, which involve the use of hazardous materials at high temperatures and pressures, have already been identified. Inertia is also another challenge. Today's educators have not been trained in green chemistry; it was not part of the curriculum when many of today's working chemists and chemical engineers were in undergraduate and graduate school. It is a challenge to get over this mind set.

What, then, are the available resources? Paul Anastas and John Warner came out with their pivotal work, *Theory and Practice*, in 1998. Since then, other green chemistry texts have emerged. Even though Doxsee and Hutchison's lab manual[2] focuses on the organic lab, the information is widely applicable to green chemistry in general, and it forms more than just a simple collection of experiments. About a year ago, the *Journal of Chemical Education* began running a regular feature about topics in green chemistry. One can find lab experiments and different activities regarding green chemistry that can be integrated into the curriculum. In addition, Kirchoff praised the environmental chemistry text by Colin Baird and Mike Cann.[3] It provides a breakthrough in terms of integrating green chemistry into mainstream textbooks.

A number of different ACS resources also exist. *Introduction to Green Chemistry* is specifically designed for high school students and is the most popular of the green chemistry materials that ACS has. Students at the high school level and teachers appear to be very interested in this topic. In terms of general public outreach, ACS' Outreach video provides a good introduction of green chemistry. This informational video focuses on the work of three Presidential Green Chemistry Challenge award winners in a way that is accessible and understandable.

Kirchhoff and other speakers noted that chemistry should be considered in the broader context of societal issues. *Beyond the Molecular Frontier*,[4] a National Academies report, specifically emphasized the need for scientists and engineers to understand societal implications in order to enhance stewardship of the planet and recommended a greater emphasis

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[2]Doxsee, K. M., J. E. Hutchison. 2004. *Green Organic Chemistry: Strategies, Tools and Laboratory Experiments*, First Edition. Brooks/Cole. 244.

[3]Baird, C., M. Cann. 2004. *Environmental Chemistry*, Third Edition. WH. Freeman.

[4]*Beyond the Molecular Frontier.* 2003. Washington, D.C.: The National Academies Press.

on the human aspect of the scientific endeavor. ACS also has an ongoing project called Exploring the Molecular Vision, an initiative by the Society Committee on Education division to examine the reform of chemical education. Project participants have cited the need for emphasizing toxicity education, highlighting the role of chemistry in supporting the environment, and promoting high ethical standards in environmental performance.

Green chemistry, sustainability, ethics, toxicology, and safety issues are generally absent from the chemistry curriculum at this point. ACS recommends that green chemistry be taught at the high school, undergraduate, and graduate levels in terms of classroom lectures and laboratory training. The Committee on Professional Training (CPT) also stresses interdisciplinary work. CPT guidelines currently emphasize subjects such as economics, marketing, and business within an environmental context, generally pointing out connections between science and society. CPT also has an environmental chemistry option in which the ACS Committee on Environmental Improvement has recommended that green chemistry should be included.

Kirchhoff described different approaches for integrating green chemistry into existing courses and curricula. One method is to develop a whole new course around green chemistry, which has the advantage providing great depth into the subject. The disadvantage is that a new course is usually treated as an elective and therefore does not impact as many people as a required course does. Nevertheless, it is still an excellent way to introduce students to the real "nuts and bolts" of green chemistry. Another route is to integrate green chemistry into existing courses both within the classroom and the laboratory. This can be tricky, especially if educators use textbooks that do not include green chemistry, which requires them to be creative with introducing the subject into their courses.

Students should also be encouraged to explore green chemistry on their own. Kirchhoff suggested that, as an alternative to teaching research students the use of established methods, have them instead look in the literature for "greener" tools. There should be an over-arching philosophy of "what are you producing when you do this reaction, what are the by-products," Kirchhoff said. Educators should consider this even as they teach organic chemistry. Many textbooks do not include the by-products. "There are by-products, and those by-products have consequences," she said.

Conferences, symposia, and school activities provide great opportunity to educate students more about this subject. For example, ACS is organizing their third summer school on green chemistry for graduate students and postdoctoral researchers to be held at McGill University at Montreal in July. The ACS student affiliates program also recognizes green chemistry chapters at schools. Another often-overlooked opportunity is the incorporation of sustainability into campus building construction and landscaping. St. Olaf College not only received $500,000 from the Keck Foundation to integrate green chemistry into their curriculum, but they also were awarded $98,000 from the Kresge Foundation for the design of an environmentally friendly science center. "In the end, what you ideally want is a building that is green, with a program that is green. Tie these two together," Kirchhoff said.

There are several benefits in the incorporation of green chemistry into the education curriculum. One is professional preparation; as industry moves toward an increased emphasis on sustainability, they will need students who are trained in green chemistry and sustainability issues. Students themselves have an interest in environmental issues and in demonstrating that chemistry and environmental stewardship are not mutually exclusive. On a practical level, sustainability and green chemistry education can increase lab safety and decrease lab waste.

In terms of continuing education opportunities, summer workshops such as the program at the University of Oregon may help faculty members feel comfortable with introducing these topics into their teaching. Many faculty members are uncomfortable because they lack the background in sustainability or green chemistry education and practice. However, continuing education programs may enable them to teach and practice sustainability on their own campuses. Industrial chemists may need similar workshops. Many chemists who currently work in industry also do not have training in green chemistry or sustainability, so they also need to enhance their skills.

One participant pointed out that it might also be important to educate patients and doctors concerning the metabolism of drugs. There is a question of how to educate people to take 100 milligrams of a cox-2 inhibitor, instead of pressing for 400 milligrams, he said.

Mary Kirchhoff emphasized that it is important to hold students' interest in green chemistry as early as possible, and to show them that that chemistry is not the grand polluter of the planet but instead offers solutions to some of the environmental challenges that we face.

DEFINITION OF GREEN CHEMISTRY

One of the recurrent themes was the search for a term for sustainable chemistry, and discussion about the use of the label "green chemistry" or "environmental chemistry" and its definition.

Some participants thought the term "green chemistry" did not do justice to the multidisciplinary and integrative nature of the projects they are working on. Some asked if the name green chemistry is not a detriment to what they are trying to achieve. Mary Kirchhoff said it might be a question of moving "away from the model that, here is chemistry and here is everybody else." She said there is a need to see that chemistry does not operate in a vacuum, especially at the industrial level.

There was also the question that the label green sometimes doesn't just mean biologically derived; in fact, it means "stop and think about whether it really is better all the way through the life cycle." Mary Kirchhoff pointed out that the term biologically derived is not so much of the confusion as is the term environmental chemistry. She said when she sometimes receives applications to review green chemistry chapters, many of them have included monitoring the pH in a local stream or cleaning up trash as green chemistry activities. "So, they are sort of confusing care of the environment with green chemistry," Kirchhoff said.

Lauren Heine said it was a great challenge to define what is green. There is no green chemical, she pointed out. "Water, of course, you can drown in it," she pointed out. But everything is context based, and the material and the metabolism in which it flows have to be considered, she said.

According to Heine, the lack of agreement on what defines a sustainable product or sustainable chemistry makes it hard for companies to market a new product. People are often averse to taking a chance in designing a green material, if they don't know that that definition is going to hold up in the market place. "Because if somebody comes out with a different definition, they may well have invested in a green product that is not perceived of as green," she said.

Heine pointed out that companies should not focus on developing just one or two green chemical products, because it does not demonstrate real commitment to customers, and it does not educate customers. It increases vulnerability at the corporate level if companies only make green that which is profitable. But if a company commits to a corporate-wide strategy of green chemistry, the company will be respected.

One participant said the environmental performance and life cycle costs should not be put into an MSDS sheet, because an MSDS sheet is more regulatory and compliance based, that green chemistry deserves its own sheet.

Berkeley Cue said green chemistry is the definition he is most comfortable with. It is the utilization of a set of principles that reduces or eliminates the use or generation of hazardous substances in the design, manufacture, and application of chemical products. He added that many people think green chemistry is just about organic chemistry. Analytical chemistry, physical chemistry, inorganic chemistry, biochemistry, all of the disciplines that interface with chemical synthesis are covered by this definition, Cue said.

He reminded the participants of the 12 principles of green chemistry as articulated by Paul Anastas and John Warner, the most important being prevention. "It is better to prevent waste than to have to deal with it once you have produced it," Cue said. He listed atom economy, less hazardous chemical synthesis, safer chemicals, design for energy efficiency, renewable feedstocks, catalysis, and finally, design for degradation. From the pharmaceutical industry perspective, this is the biggest challenge. The challenge is for the molecules to be stable when they are synthesized, stored, and incorporated in the dosage form. They then should have at least a two-year shelf life where there is no appreciable degradation. They should be stable in the patient when they ingest them, because the active drug has to get to the site of action. Then, as the drug leaves the patient through the biological processes, it would be ideal to have them completely degrade into innocuous materials.

There is also a series of 12 green engineering principles that go along with the green chemistry principles. Material and energy inputs and outputs are as inherently non-hazardous as possible. Processes and systems designed to maximize energy, space, mass, and time efficiency, embedded atrophy and complexity, should be viewed as an investment when making design choices. We should target durability and not immortality. Design for all unnecessary capacity capability, one-size-fits-all solutions should be considered a design flaw.

Brad Allenby used CFCs (chlorofluorocarbons) as an example to show how the understanding of what is green has changed. CFCs are a classic example of green chemistry because they substituted for fairly toxic, dangerous materials. "If I apply any of the metrics, the heuristics that we tend to use in green chemistry—lower toxicity, lower impact on workers, safer for users, more stable—I would love CFCs," Allenby said. What made CFCs desirable on one scale—their stability—made them undesirable when they got up into the upper atmosphere and began to break up the ozone. He also pointed out that this happened on a very small scale. "If you were looking at volumetric chemical consumption in the United States, you would not have looked at CFCs," he said. They were a minor trace atmosphere and yet, because of the dynamics of the system, they turned out to be extremely critical. "So, a green chemical de-stabilized major earth systems with effects that we are probably not entirely familiar with at this point," he said.

CFCs show us that at the time, we did not have the ability to know how to think about what was or was not green, Allenby explained. This means there are gaps in the way that chemistry and its impact on global systems is thought about. But Allenby also said the response to CFCs was positive; alternatives were found, and used where CFCs had been employed, in the electronic sector, cleaning circuit boards, cleaning piece parts. This means the other lesson from CFCs is not to go into paralysis mode just because a green chemical may be potentially harmful some years down the line.

Another example is to reflect on green chemistry network components, Allenby said. None of these products exist by themselves. They all tend to be used in a particular context, a network structure, especially something like a telephone. "If you just have a telephone and there are no towers and nobody else has a telephone, then you have got a really kind of interesting paperweight and that is it," Allenby said. The technology of designing a telephone and designing the way different components and materials work in a telephone is very complex.

One of the mistakes that is made in policy, teaching, and thinking is that there seem to be things that are so bad a ban is immediately needed. There are some cases where that has worked well; lead in gasoline is a classic example.

Allenby recounted moving to corporate intranets at AT&T. This significantly reduced the material demand of the company in terms of paper. But corporate intranets also add to the value of the whole set of material-based products, like telephones with lead in them. "Is that good or bad? Is that green or is that not green? I don't know," Allenby argued.

Part of that is the refusal to understand that green chemistry does not operate at the scale of the bench or at the scale of the reaction. It operates at the scale of regional and global systems. "To me, that is an irreducible responsibility of green chemistry and it is one that so far, I think, has not been adequately addressed," Allenby pointed out.

Allenby said green—not environmental science, but green—is a fairly normative kind of concept. Green chemistry injects the normative into the heart of what has traditionally been a physical science. He reminded the audience of C.P. Snow and his theory of social science versus physical science, which are thrown together in green chemistry. "It is a very, very interesting sociological phenomenon, which is not what I think green chemistry intends to be, but I think it clearly is," Allenby said.

He went on to point out that given the scale of human activities, scientists are actually doing earth systems design and engineering. He gave pharmaceuticals as an example. A pharmaceutical is designed to have a specific impact in a specific human system but, at the scale at which any successful pharmaceutical is used, through any metabolic processes that result in products that are released into aqueous systems, it is also designing aqueous systems in developed countries.

Data from a number of different fields shows this link clearly, although it is not clear from the way pharmaceuticals are thought about, or regulated and taught. "Unless we understand that something that is designed at bench scale will, in fact, in many cases, impact systems at regional and global scale, we have not yet begun to grapple with what is already occurring in our world; not what is going to occur, what is already occurring," Allenby said

Allenby said it is important to learn to how to pay more attention to scale, to know that metabolic products are going to end up widely dispersed in the environment. "We should ask if we should be designing not just the pharmaceutical, but also the metabolic product," he stressed.

Earth systems engineering and management is where the serious business of green chemistry begins, and it is an area that hasn't really been focused on enough at all. "Where is our sense of responsibility? That doesn't mean simply retreating to ideological structures. Ethics and values need to be comprehensive. We need to learn how to dialogue with these systems, and we need to develop the institutional capability," he said.

Green chemistry is classic white space, it imports a lot of concepts from social science and in particular, historically contingent viewpoints into the practice of chemistry, which is very much a white space practice. Unfortunately, Allenby said, we are not really good at dealing with white spaces. A strongly disciplinary scientist or engineer, will tend to view white space work as being fluffy, and an admission by the person doing it that they couldn't handle the discipline. It is awfully hard to get interdisciplinary work funded. The staff at the NSF tends to appreciate the importance of interdisciplinary work, but the peer review committee thinks a multidisciplinary researcher is a complete flake, and the process breaks down.

DEMAND AND PRODUCT DESIGN

Lauren Heine gave the participants some background on GreenBlue, and cradle-to-cradle design. She talked about some of the drivers and obstacles for green chemistry, product formulation, and gave some examples of projects that are designed to facilitate adoption of green chemistry.

Lauren Heine talked about the furniture flame retardency partnership and the Design for Environment (DfE) Green Formulation Initiative for cleaning products. She also gave an example of a company using green chemistry as a strategy for product development. The furniture flame retardency partnership was an EPA project, part of the DfE program.

GreenBlue is about a year and a half old. It is a not-for-profit organization in Charlottesville, Virginia, that was founded by William McDonough, a well-known green architect, and the German chemist Michael Braungart. They wrote a book called *Cradle to Cradle*: *Remaking the Way We Make Things*. The book argues that industry and the public can use the following design principles: using current solar income, celebrating diversity of people, products, geographies, cultures, needs, and design, and that waste equals food. The waste equals food theme is very powerful, Heine explained, as biological materials can be perceived of as nutrients, flowing within biological metabolisms, and technical materials such as metals or polymers can be perceived of as technical nutrients, flowing in technical metabolisms.

The value of these materials gives rise to the thought of designing an entire system, and a biological metabolism may be the environment in the broader sense or it also may be a wastewater treatment plant. There has to be thought about designing the biological material, so that it can be metabolized. Sometimes the focus is on designing materials for existing metabolism, and sometimes on designing metabolisms for materials.

In the application of these ideas, the first step is to analyze the chemical composition of materials used, to select materials based on safety to humans and ecological systems, and then to design these materials to be nutrients, for high-value recovery or other beneficial uses. Energy recovery could be considered one of the recoverable values, Heine argued.

Heine talked about the cradle-to-cradle model. There is value in a big picture mental model, like cradle-to-cradle design, she said. While it initially may sound hokey to an engineer, it is powerful because it engages technical and non-technical people alike. Secondly, it provides a vision, but not a prescriptive approach. Thirdly, the focus on materials and metabolisms points to the importance of systems, and collaboration with others within the value change.

GreenBlue sees this as a short-term strategy to move companies and organizations toward sustainability. How well the strategies will work 10 or 20 years from now is not clear, as there may be more important strategies to take.

Heine then named some of the obstacles to integrating green chemistry into product formulation. First, change is always difficult, she said. There are huge manufacturing and market challenges. There is a big customer disconnect. Manufacturers will say, we have the brain power, we can make anything, but our customers are not asking for green materials. They might say, we make green chemistries, but our customers aren't buying them. There is a big disconnect there. A lot of human and ecological toxicology and life cycle impact data is missing that could support decision making. There is a lot of data out there, but it is not necessarily in a form that can support decisions.

Two examples are material safety data sheets (MSDS) and technical fact sheets. People look to these to help support decision making, but they are not always very useful. Heine showed an MSDS for a green product that did not show any ingredients. MSDS's are often wrong, they are generally incomplete, and there is no standard format for them. There is an American National Standards Institute (ANSI) format that is a very good format, that includes environmental attributes, but there are no requirements that everybody needs to use the same MSDS format, and they only have to report what is hazardous anyway.

Technical fact sheets can be very useful to formulators, because they give an idea as to whether or not it is useful to try this ingredient, based on performance properties. However, they are very inconsistent. Environmental attributes very often are not listed in technical fact sheets, and only the information the manufacturer sees as most relevant can be found. "It would be very helpful, I think, to have environmental attributes consistent, whether they are positive in that case or not, available to people to compare," Heine said.

Heine talked about the drivers of green chemistry, for example a recent phase out of penta- and octa-brominated diphenol ethers (PBDEs) and a pending national regulation requiring flame retardancy in furniture.

First she talked about flame retardants and the DfE-formulated flame retardant partnership. People desire to avoid making the same mistakes as they did with PBDEs. The Furniture Flame Retardancy Partnership was formed with the purpose of providing up-to-date toxicology and environmental information on flame retardant alternatives to the penta-brominated materials used in polyurethane foam and to identify environmentally preferable approaches to designing furniture that meet the pending fire safety regulations.

The impending tasks of the effort include identifying and evaluating the existing chemical substitution for penta-brominated materials, targeting research and data needs, investigating non-chemical additive approaches, such as barrier technologies, construction techniques, batting fill, alternative formulations of foams, and possibly posting targeted DfE innovation challenges to identify chemical and non-chemical solutions.

Heine then showed some of the information sheets. The sheets allow manufacturers to look at a particular flame retardant chemical and compare it on different end points. For example, one can examine whether the flame retardant is additive or reactive, which affects the exposure potential. The two-and-a-half page matrix is the distillation of about 450 pages of research on the chemical alternatives, done with the EPA and Syracuse Research Corporation.

The sheet allows consumers to choose which attributes are important to them. Acute aquatic toxicity could, for example, be less of a concern, while very low persistence and bioaccumulation potential could instead be the highest priority. "None of the existing options are perfect, but at least this model, I believe, is a really nice way of presenting data to help people make choices," Heine pointed out.

Heine then went on to talk about the Green Formulation Initiative for cleaning products. The drivers for green chemistry in product formulation are an executive order for government purchasing called Greening the Government Through Waste Prevention, Recycling, and Federal Acquisition. The U.S. Green Building Council LEED program has an existing building program that gives points for green cleaning products and for green cleaning programs.

Eco-labels are growing, Heine said. Green Seal has certified about 130 different cleaning products. Canada has the Environmental Choice Program and Europe has its programs.

Heine introduced the U.S. EPA Design for the Environment formulator program, which is a partnership where companies can partner with DfE. The companies submit their formulations to the EPA's technical expert staff for review. This team reviews all ingredients in the formulations and identifies ingredients of concern. The manufacturers are then responsible to finding alternative chemicals and reformulating. If successful, they can use the DfE logo on their product labels. This is a very powerful learning experience for the formulators who engage in this partnership. "They really love this program, and are very proud of the success of the partnership," Heine said.

GreenBlue has a related project, in part because there is so much demand for that service at EPA, and it is a very small program. GreenBlue is creating a resource to promote green chemistry in the design of industrial and institutional cleaning products and to enhance environmental and human health and safety. It is a multi-stakeholder process with about 170 or more formulators, raw material suppliers, industry associations, and NGOs working together to establish the relevant attributes and supporting data needed to identify ingredients that can be used to design cleaning products with potential environmental benefits.

GreenBlue is starting with surfactants. Steps include: identifying the attributes, building the database, soliciting ingredients and supporting data, and then posting this information to a public website to promote the greener chemistries. The initial attributes of concern for surfactants will be biodegradability (including consideration of breakdown products), aquatic toxicity, skin irritation, and additional product features such as percent bio-based. The attributes may be of toxicological, regulatory, policy and/or of eco-labeling significance. It will be a fact-based resource for formulators that allows them a one-stop opportunity to select ingredients to enhance the environmental profiles of their products and to communicate ingredient information.

The information will liberate manufacturers. Putting the data out there will allow formulators to consider environmental information when making their choices. Formulators do not want to be told how to use a particular ingredient and whether or not it is "green". They want to see the information so that they can make their own choices and determine the environmental benefits based on the application, Heine said.

Heine went on to talk about a small formulating company, Coastwide Laboratories, in Oregon that has used a green chemistry strategy in developing their products. They have established positive criteria for product efficacy and environmental health and safety by creating a product development standard that is publicly available on their web site. They thoroughly assess all candidate ingredients to understand their potential human and environmental health impacts. Then they formulate and re-formulate new and existing products to meet the standard. The company has received external verification of their products' environmental profiles through eco-labels and the DfE Formulator Partnership

Their full corporate commitment—not to just a few green products—but to all product development has paid off, Heine says. Their sales growth from 2003 to 2004 went up 430 percent. People are asking to license their technology. The company is educating all of their sales, marketing and technical staff as well as customers in their community about the value of green chemistry in their products.

Heine said programs like EPA's Formulator and Furniture Flame Retardancy partnerships are voluntary programs that are funded by minimal amounts. However, they provide a huge educational experience for industries, especially smaller companies.

Heine said she has a small company in mind when she talks about a strategy of green chemistry "I am not sure how you implement that at a very large company, but I think the principles will hold as well. You need a green chemistry strategy and a corporate goal—to say where you are trying to go," Heine said.

TECHNOLOGIES

Berkeley Cue talked about the importance of green technology to chemical enterprises, and the business argument that needs to be made to convince companies to be more active in green chemistry. He narrated some green chemistry success stories, and gave an overview of some technologies that enable green chemistry and engineering. He also talked about some of the barriers to adopting new technologies in green chemistry and engineering.

Cue introduced the concept of the triple bottom line, which was articulated by Elkington in the late 1990s, and is generally regarded as an important consideration in business success. It states that simply focusing on economic success without equally focusing on environmental stewardship and social responsibility is not the right business model for sustainability. "In fact, some people have said that the companies that largely focus on this are simply green washing the issue, and they are not paying attention to the important parameters that they should," he added.

There is a double economic penalty in sustainable production, Cue said. Only ten percent of the raw materials taken out of the earth actually wind up in goods and services. Ninety percent of them wind up as waste, and re-enter the environment as pollutants. Companies pay to use them and pay to dispose of them.

But even a 10 percent conversion factor would be great for the pharmaceutical industry, Cue said, which has a conversion factor of less than one percent. The industry has always argued that they produce more complex molecules, through more complex synthesis, with lower overall yields, so it is no surprise that it would be like that. But, Cue argued, it might not have to be.

One of the other driving factors is the presence of what Cue called "six billion consumption machines." If everyone had the same quality of life as the population of United States or Western Europe, three planet earths would be necessary in order to provide sufficient raw materials.

That combination of a ten percent conversion rate for raw materials, and the need for three earths for the emerging countries suggests the need for at least a three-fold improvement in the conversion of raw materials to goods and services. Since the demand grows as the global population grows, "there is a certain amount of urgency involved here to addressing these issues," Cue said.

Change may have to be the initiative of the companies themselves. For a long time companies have tried to live in a compliance mode; they reacted to regulations that were promulgated, which was feasible until about the 1960s, Cue said. But any company that believes it can exist by simply trying to comply with regulations, including regulations that have yet to be promulgated, is probably following the wrong business model, Cue said. This compliance costs U.S. industries over $200 billion, $200 billion that could be better used elsewhere, investing in R&D to discover new products or newer valuable products, Cue pointed out.

Responsible care is another important business driver for adopting green chemistry and engineering principles. That is a binding obligation of the chemical industry: self-responsibility in the area of health, safety, and the environment.

Another important driver is REACH (Registration, Evaluation and Authorisation of Chemicals),[5] and the European regulations that are being introduced. The European Union with its 450 million citizens outnumbers the U.S. economic market now, and those regulations will have an impact on the United States if the U.S. is not more proactive in terms of

[5]2001 European Commission *White Paper on the Strategy for a future Chemicals Policy* (COM(2001)88) available at: *europa.eu.int/comm/environment/chemicals/whitepaper.htm*

addressing some of the shortcomings. But companies may also gain through REACH. "One of the things our customers are going to learn, as they work through REACH, is that the gain from going from 70,000 chemicals on the chemical inventory, to 15,000 chemicals on the chemical inventory is going to be an enormous gain to them," John Carberry said. The regulatory process is going to drive chemical simplification toward chemicals that are known to be safe, which is a big switch from chemicals that are not known to be hazardous.

Another reason to promote green chemistry is homeland security as this would reduce hazardous waste that could be used by terrorists as a weapon. "A rallying cry would be terrorists hijacking a tanker truck with 8,000 gallons of hazardous waste, driving it to Times Square, and kicking open the valve," Cue said.

Waste reduction could be a big incentive for green chemistry in the pharmaceutical industry. The pharmaceutical industry pointed to the petrochemical industry for a long time, and said: "We don't make large quantities of material, relative to those guys." However, it does produce an awful lot of waste overall. Cue calculated that the pharmaceutical industry could be producing somewhere between half a billion and 2.5 billion kilos of waste for every kilo of active drug produced.

This amount can be reduced, Cue argued. By applying green chemistry principles companies could see a dramatic reduction in waste, by an order of 10-fold. Cue lauded Glaxo for doing a very nice job in life cycle analysis, which not many pharmaceutical companies do. Cue then called for one of the outcomes of the conference to be an increase in cross-talk between the pharmaceutical industry, the oil industry, the fine chemical industry, and the bulk chemical industry, in order to share best practices and to learn they each address these important issues.

Some of the success stories of green chemistry are legislative ones. Cue described a bill pending last year designed to integrate the federal government approaches to green chemistry by the EPA, the Department of Energy, National Institutes of Health, and NIST. It passed the House of Representatives, over 400 yea, to 14 nay. It was sponsored by Senators Snow and Rockefeller in the Senate but did not get called to vote before the last congress expired. It has to go through again.

Cue also called the Presidential Green Chemistry Awards a great tool for encouraging more green chemistry and engineering in the chemical enterprise industries. He recounted the experience of working for a company that won one. "It is one of the most motivational things that you can ever experience, and will really drive the entire company to look for other examples of success stories to submit for applications," he said. There are five award categories, including small business, academic investigator, alternate synthetic pathway, alternate reaction conditions, and design of safer chemicals. In the pharmaceutical industry, Lilly, Roche, Pfizer, and Bristol received awards. It is important that the pharmaceutical industry be very active in these areas because their mission is to bring innovative health care solutions to patients, but if that happens at the expense of a healthy environment, that is an incomplete mission, Cue said.

The award for Bristol—won in collaboration with Phyton—was given for an improvement in the manufacturing of paclitaxel, for plant cell fermentation from renewable nutrients such as sugars, amino acids, vitamins, and trace elements. The company ferments paclitaxel directly, without a need to stockpile needles. Overall, they have eliminated 10 solvents and six drying steps.

Some of the enablers of greener manufacturing process will be biotransformations, process analytical technology, robotics and automation, crystal engineering, separations technology, green solvents, microwave chemistry, equipment cleaning, and bio-based raw materials.

As an example, Cue talked about the work of Codexis, a biotransformation company in California. The company isolates genes from natural enzymes or substrates, which facilitate biotransformations. They then cut them up with DNA shuffling, generate a library of novel genes by recombining them in random methods, screen them for yield improvement, and find novel genes with improved properties. The president of Codexis claims that if the yield can be detected, they can develop a manufacturing process with a high yield.

The basic building block of cephalosporin antibiotics—7080CA—was made this way. It starts out with penicillin G, which is made from fermentation of feedstock and phenylacetic acid. Using the proprietary technology, they basically found a more streamlined conversion. In terms of yield efficiency, and *in vitro* activity, which is very low with the traditional process, there is about a 40-fold improvement in overall yield in the engineered process.

There is a need to look for potentially relevant technologies outside of the chemical industry, Cue said. For example, Foster-Miller is a company that manufactures a military robot to investigate potentially hazardous materials, and the same technology allows them to design lab automation for the pharmaceutical industry for a totally automated, analytical laboratory.

One of the challenges is the science of scale. One goal is to go right from the lab to the 4,000-gallon reactor. Another way is to run a whole bunch of small reactors, and that is what Velocys does with their micro channel reactor approach. It has some advantage including high yield and selectivity, and eliminating the need for catalyst recovery, because the catalyst is embedded. So, based on how much you need to produce determines how many modules you need and, at the individual reactor level, they are small and inexpensive.

Another important technology is product purification and particle size control through impinging jet crystallization. A synthesized molecule has to be recovered in a pure state, which is a process that is energy-, solvent- and waste-intensive. The pharmaceutical industry not only needs the crystalline form but also a precise particle size. In impinging jet crystallization, there are two streams of solvent. One stream carries the material to be crystallized, the other is an anti-solvent. The streams are slammed together, and the concentration and velocity determine the particle size.

Simulated moving bed, or multiple column chromatography is another area that is getting a lot of attention in pharma. The costs have come down for the equipment and the column material, a substantial reduction in solvent, and the FDA is much more comfortable with the technology now. Companies are using it to produce commercial quantities of material, and in the early stages of clinical supply synthesis. There are a lot of predictions that in the future, drug companies are going to need this technology more and more.

Microwave chemistry is another area of great interest. Right now it is an interest that is still in the laboratory stage, because there is a bias that it is not going to be engineerable and scalable.

Solvents are getting a lot of attention in green chemistry and engineering. Ionic liquids, for example, are seeing a tremendous growth in the number of publications. Near critical and super-critical solvents, for which Liotta and Eckert won a green chemistry award last year are very interesting. There is no reason, with proper engineering technology, that those temperature and pressure ranges are impossible to operate at, and some new chemistry that will lead to new products may be uncovered.

Equipment cleaning is a further important field, as a large amount of solvent or water waste is generated in cleaning chemical and manufacturing equipment. Right now, spray balls are kind of the gold standard, at least in the pharmaceutical industry. Some companies have looked at using ultrasonics, but the problem is that the detergent used is abrasive to the glass that lines many of the reactors.

The metrics of green chemistry are another big challenge, Cue said. He said an agreement on the metrics, the definition of the metrics, the measurables, and how to measure them would be important. The drug industry has a bad track record with incorporating technology, and this could actually be a negative. People could assume it hasn't been successful up until now and question the success of a new technology.

LIFE CYCLE ANALYSIS

Richard Helling talked about some of the drivers for sustainability metrics in general and life cycle analysis in particular, and some of the key challenges revolving around data quality and availability, the art of impact assessment and how it is done from a methodology point of view. "In order to change something, you have to be able to measure it, and you have to be able to do it quantitatively, and life cycle analysis gives us one way of doing that," Helling said.

Helling first explained which characteristics make a good metric. A good metric needs to be scalable, understandable, reproducible, and be able to describe all three dimensions of the sustainability environment. For economic metrics, there are a number of well-established descriptions for performance and accounting standards. A recent innovation is to look at what is called total cost accounting, which is looking to the future to quantify some of the noneconomic factors and convert them into dollar terms, so that a comparison based on a common dimension, dollars, is possible. "It is great in principle, a little hard to do in practice, because there is a lot of subjectivity and forward looking uncertainty with that," Helling said.

Life cycle analysis is still not well established, and there is not a globally agreed-upon set of metrics. In general, LCA starts by looking at the intensity of energy use or mass use or pollutant emissions, such as the kilograms of CO_2 per kilogram of product, or by looking at the economic side—the dollar value of production per megajoule of fossil fuel use—as an eco-efficiency. These values can be quantified in life cycle analysis.

Sociometrics is another relatively new area of research. While there is less consensus on what makes a good sociometric, it is clear that, when something is measured, people's behavior can be changed. A clear example is to look at industry's tracking of work place injuries, which have been reduced by the order of a magnitude over the years.

Many metrics have been developed for nations, or for looking at the status of the planet, rather than for individual companies or projects. But it is unclear if there is a need to find the best set of metrics for the chemical industry or to find separate and distinctive measurements on the social dimensions for each case.

Life cycle analysis is an analytical tool for the systematic evaluation of environmental aspects of a product or service system through all stages of its life cycle. Importantly, it is quantitative and looks at the full life cycle and does not just move waste or problems from one stage to another. It is a comparative tool, with standards from the international standards organization (ISO). The framework of classic life cycle assessment from the ISO standards defines four parts in the process. There is the goal, scope, definition, and inventory analysis.

Impact assessment asks the question of how the product and the emissions relate to mortality, and the interpretation asks what to do with the data. "The how is very well defined by these standards. The what, though, is really left to the particular study that you are trying to do," Helling said.

But in looking at LCA results, one has to consider the very specific question that the authors are trying to answer, because they may not be trying to answer the exact same question that you are interested in. The inventory calculations need a tremendous amount of data or time, or usually both. Then, in the impact assessment there are a lot of different choices to be made of how to relate emissions on a mass basis to impacts, either midpoint on global warming potential or on mortality, for example.

The first challenge for a new LCA practitioner is picking the right software tool. There are many tools available; universities, national labs, and companies have developed their version of the tools, all of which can vary in terms of their specific strengths, weaknesses, and costs. BEES and TRACI both exist on web sites or are publicly available. OMNITOX is being created in Europe and should be coming out soon. But there is a risk to software that is not self-developed, in that a certain amount of faith or understanding in how it is going to work is needed. While it is very easy to generate numbers, it is more difficult to understand what those numbers mean.

Helling presented an example of life cycle assessment, looking at a flexible foam polyol, such as might be used in seat cushions in cars. It concerned the possibility of using a soy-based material and comparing that to petrochemical alternatives.

A very key first step is to define the functional unit, the level of performance that will be compared, and the different options for meeting that level of performance. In this case, it was very important for the product to have certain mechanical properties. The soy-based route was not 100 percent soy based, and a certain amount of petrochemical derived ethylene oxide was required to get product properties identical to those currently used.

The study was done as a cradle-to-gate impact assessment, meaning that the end use, fate, and disposal of the product were the same, regardless of the route. This limited impact assessment, as some impacts were stopped at midpoint, such as global warming potentials. It also did not estimate any health or toxicity impacts.

The basis for making polyols in Europe was used as the reference case for the petrochemical route. This is based on a survey of 12 different sites using three different technologies in 1998 in four countries. Another route based on patents published by BASF, using hydrogen peroxide as an oxidant instead of chlorine, was also used.

A typical result from a life cycle analysis might show the megajoules of gross energy consumed per kilogram of product. The 1995 data, the BASF patent information, and the two different farming models for the soy polyol were available. In summary, the soy polyols gave a very exciting opportunity to reduce the total energy of the product to about 65 to 70 percent of what it is today. In looking at just the fossil feedstock component, they require only 40 to 45 percent of the energy intensity, which is better than a lot of potential biomaterials.

The BASF route, by not using chlorine, decreased mass intensity and, more important, freed this route from chlorine infrastructure. The use of chlorine can be very economic if the infrastructure is in place but, if not, it is rather expensive, and there are concerns about dealing with chlorinated by-products.

There was a big difference between the greenhouse gas emissions from the two different farming models for making soy-based polyols. This is due to the different assumptions of the generation of nitrous oxide from the use of fertilizers in the farm. The two different groups took two different approaches. They both looked at the same data but came to different conclusions, and this has a big impact on the overall view of the process.

Helling then talked about some of the challenges facing the chemical industry. There is an opportunity to gather and share information more effectively on the broad scope of the chemical industry. A lot of databases have been set up for specific applications, like in plastics for building materials, but not necessarily for the breadth of the chemical industry. Sharing information really started with the APME work and on the eco–profiles from Europe. It is continuing now with the American Plastics Council work in order to do the same thing as part of the U.S. life cycle database initiative being led by DOE and NREL, and Dow is fully contributing a lot of data for that effort. There will probably still be segments of the chemical industry that aren't covered by that because the focus is plastics, though. The need for access to data is also recognized by the UNEP SETAC life cycle initiative, which is another recently launched initiative.

In the area of impact assessment, a consistent procedure is needed. This means the most appropriate impact assessment methodology for chemical processes should be found. Helling credited BASF, who has done a superb job advocating for eco-efficiency analysis.

Some of the participants wanted to know why the tools come from a negative perspective. They were interested in balancing costs or greater negatives with greater benefits. They were looking for a way to add a benefits analysis along with cost assessment. Helling said it was a matter of definition. "Do you want zero to be good or infinite to be good?" he asked. Terry Collins said he was not aware of a single case where a pollutant put out in the environment has had a good effect, the inverse of toxicity or eco-toxicity. He added the damage that was done to American society by lead in paint and gasoline is incomprehensible, and it will never be quantified, because there will never be the experiment of having a civilization without lead.

Richard Scott asked if LCA took the scale of technologies into account when they are adopted on a widespread basis. Richard Helling answered that any time Dow looks at a new product, they look at its unit cost, and at total capital cost to get into that business, or the total market size, which will be unit cost times some hopefully very large number. The same approach is taken to look at the LCA results.

STRUCTURE-ACTIVITY TOOLS

Robert Kavlock talked about computational toxicology, which uses the best of modern chemistry, information technology, and biology to do a better job at assessing risk. He talked about how the EPA views this research strategy and presented some of applications the EPA is using.

The EPA views the world through this source to predict outcome paradigms, Kavlock said. An event takes place in the environment, a transformation followed by an exposure, which is a contact of a chemical with an organism. That is translated into an internal dose, which becomes a biological event, and eventually an adverse outcome, which the EPA regulates.

That has been the driving force in coming up with a computational toxicology program, Kavlock said. There is a lot of data for some kinds of chemicals. For example, the EPA asked the regulated industry for about $19 million in studies for pesticides, but there are other cases in which the EPA does not have legislative authority to ask for data.

Congress constantly gives the EPA new lists of chemicals to worry about, like endocrine disrupting chemicals, pesticidal inerts or high production volume chemicals, Kavlock said. The EPA has no way to sort through these and look at the risk-based criteria for setting testing priorities. So it really needs a different way of evaluating the way it approaches prioritization, screening, and testing.

Kavlock gave one example of the problems EPA faces. This has to do with so-called pesticidal inerts or nonactive ingredients. These substances are not necessarily chemically or biologically inert, but they are not the active ingredients. The EPA issues what are called tolerance exemptions for these. To do that, the agency conducts a risk assessment, for which there are no data requirements. "Basically, what we wind up doing is a margin exposure estimate, where we calculate what the likely human exposure is going to be," Kavlock said. This is done through literature research and toxicity estimates. The burden of proof is that there is a reasonable certainty of no harm. The problem with this is that there are 850 pesticidal inerts being used. There are no testing requirements, and the agency has been told to finish this work by August 2006.

This list goes on, Kavlock said. There are 350 non-food use antimicrobial agents in the same category, and 3,000 food use inerts. Because of that, the EPA four years ago began to think about how it could approach doing a better job of looking at these kinds of hazards.

Now, finally, this year the National Center for Computational Toxicology will open, Kavlock announced. It will have a small group of systems modelers, computational chemists and bioinformaticians. Concordant with this, there is a request for applications for a center for environmental bioinformatics, which will cost $1 million a year for the next five years, to help sort through the enormous amounts of data that this program will generate.

The EPA is planning to use computational chemistry tools and proteomic, genomic, or metabonomic technologies and apply them to risk assessment. This will aid the agency in screening and prioritizing chemicals through an understanding of the toxicity pathways with which these chemicals interact. In five or ten years the agency hopes to have faster and more accurate risk assessments.

There are two objectives in the framework, Kavlock pointed out. The first is to improve the linkages and their source to outcome paradigms. The FDA has been good at looking at individual steps of that paradigm, but not predicting what will happen at the next stage, Kavlock explained. There could be freight and transport models. There could be physiologically–based pharmacokinetic models. There could be biologically–based dose response models, or a version of system biology models, which basically show how a chemical interacts with the normal biology. The second objective is to provide predictive models for hazard identification, and this involves quantitative structure activity determinations. The final step is enhancing quantitative risk assessments. These technologies can cross levels of biological organizations. The goal is to find out how looking at the cell level can inform the organism or population level, Kavlock said. Other questions are how to translate from high doses to low doses and how to extrapolate across species.

The concern is not just with human health, but also with wildlife health. The EPA is using some molecular biology tools to sequence, express, and clone estrogen and androgen receptors from a variety of ecologically relevant species. Chemicals are then tested against them to see the similarity with estrogen or androgen receptor binding.

Kavlock talked about the national center for computational toxicology. It will have about 20 people in it when it is fully formulated this year and function as sort of a think tank to the agency. "The center will have a strong emphasis of developing partnerships, because in the era of the U.S. government, we have to stretch our resources as far as you can go, and there are a lot of other organizations out there that have very similar motivations," Kavlock said.

Likely focus areas are information technology and prioritization. "How do we get into that list of 850 pesticidal inerts and tell the agency, these 63 are the ones you should worry about, and you should worry about 21 of them for birth defects and 32 of them for cancer effects, and be able to put some kind of a priori knowledge in the system?" Kavlock explained. Quantitative risk assessment models are primarily focused around physiologically–based pharmacokinetic models, and how they can be more routinely used in risk assessment.

The center has already developed some partnerships. The Department of Energy has helped with some of the genomic work. For instance, there is no gene chip available for the fathead minnow. The Department of Energy has helped sequence part of the fathead minnow, so that the EPA can develop microarray chips and be able to do some of the same kinds of studies in wildlife species as you can do now with rodents.

Kavlock also talked about some of the other partnerships. The Department of Defense has several ongoing efforts such as new program in eco-toxicogenomics. The EPA is also working closely with the National Center for Toxicogenomics and the national toxicology program to do genomics and prioritization techniques.

One example is the work with hormone activity. In 1996, Congress passed the Food Quality Protection Act that stated the EPA needed to screen chemicals for estrogenic activity. The agency employed an expert panel that came back with a number of screen assays based upon whole animals for looking at estrogens and androgens as well as thyroid hormones. There were a number of assays recommended, and their total cost exceeded $250,000 to $300,000 per chemical, with the number of chemicals screened in the range from 1,000 to 1,500.

The EPA has tried from the start of the program to think about *in vitro* studies to short–circuit some of the testing, and *in silico* studies to actually avoid the use of tissues altogether. Kavlock said the assay might be recommended for replacement of an animal test.

The agency is also pursuing a number of activities with quantitative risk assessment. Basically, it is developing a three-dimensional plot of the TSCA (Toxic Substances Control Act) inventory. The challenge is to predict the binding of chemicals that are out here. One of the challenges is just to understand what that chemical space is, and then develop strategies for sampling chemicals out in further domains so that more robust and quantitative structure activity models can be developed.

Another of the agency's approaches approach is completely *in silico.* One of the EPA's researchers is collecting crystallized nuclear receptors for androgens, estrogens, and thyroid hormones. The scientist extracts the ligand computationally. Using computational models, he can put other chemicals in that receptor and see what the dynamics are and how they fit. About 40 chemicals have been studied across a number of different mutant receptors with this approach, and it is actually correlating and binding very well.

But there is more to do, as it is not good enough to look at the parent chemicals, Kavlock pointed out. Even for simple chemicals like bromobenzine, the metabolism can get fairly complicated. The metabolites could be causing the toxicity. One of the projects in the EPA's Athens laboratory is a metabolic simulator, and it predicts likely metabolites and gives the probability that they are going to be present, and whether they are terminal metabolites. Another display will show the metabolic profile of the probability of different ones being formed, and it can be made into a QSAR model. Then it will be possible to say: "Well, it is the metabolites that we think are going to be more active or less active". It is a more comprehensive approach of structure activity relationships, Kavlock explained.

Kavlock then talked about some of computer databases that are useful for computational toxicology. ECOTOX, for example, is not a product of the computational toxicology program but holds information sources on ecological effects. It has over 500,000 scientific records covering several thousand species and close to 10,000 chemicals. It is available on the web. "You can go there, you can query your chemical, and you can see all the known literature that is available on these chemicals," Kavlock said. It is a peer-reviewed database with very strict standards for data acceptance.

Another project is called DSSTox, distributed structures searchable toxicity database. It captures available public toxicity databases, cleans them up, annotates them for clinical structure, and then provides them in standard data format files.

Kavlock then talked about a toxicogenomics database that deals with a group of chemicals called the conazoles or fungicides with which the pesticide office has been concerned. Although the substances are all conazoles, they have very different toxicity profiles. Some are liver carcinogens in mice; others are testicular toxins in rats. To determine why these chemicals cause different profiles, the EPA is trying to use a combination of genomics, proteomics, and metabonomics to understand that.

Using acute genomic expression profiles, the agency hopes to sort through chemical toxicity and look for toxicity pathways more efficiently. Two companies actually have the same kind of approach with much bigger databases; one is Miconics. They now have looked at almost 600 chemicals, and have come up with these genomic fingerprints that they state are predictive of chronic health effects from acute exposure. Kavlock ended by saying toxicology and green chemistry both have a lot in common. "Have you made one monster from another, have you traded one devil for another devil?" he said.

CURRENT FOSSIL FUEL DEPENDENCE AND FUTURE ALTERNATIVE FEEDSTOCKS

Stanley Bull first talked about the history of feedstocks. Historically, feedstocks were dominated by wood. "We were in the renewable feedstock business once upon a time, but then we discovered things [such as] oil and natural gas," Bull said. Nuclear, hydro–, and some non–hydro renewables soon followed, Bull said.

Bull stated that oil is in many ways the biggest challenge. The first tier of countries that have oil are not necessarily friends of the United States. At the same time, the U.S. has a large appetite for oil.

Despite that, Bull said, there is good news. The world energy consumption and energy intensity is getting better. It has been improving at one percent a year, and in the United States, at double that rate. In other words, energy efficiency or energy conservation has grown at about two percent per year. Still, this is not adequate to keep up with our energy demand. The energy goes to several different end users. The end use sectors are industry, buildings, and transportation, which all use roughly a third of the total energy. A certain fraction, about 32 percent, is delivered by way of electricity. The feedstocks are petroleum, followed by coal, natural gas, and nuclear.

Further good news is that renewable energy is on the map, Bull said. It breaks down primarily to about 45 percent hydroelectric, and bit more than that in biomass. In previous years hydroelectric held the number one spot, but it is losing ground primarily because of continuing drought in the west.

The two fastest growing renewable energy sources are wind and solar, even though they are a small part of the total at the moment. The key drivers for renewable energy and energy efficiency are energy security, climate change, air emissions, and then electrical liability.

Public acceptance of renewable energy is large, but public understanding of it isn't. Solar is tangible. "I think they are starting to get the idea of wind, because wind is growing rapidly," Bull said.

Bull then talked about the role the five renewable sources—solar, wind, geothermal, hydroelectric, and various kinds of biomass—can play in efficiency. Efficiency should be done first, Bull pointed out, as energy not used is the best energy. Efficiency can and should be a factor in all three end use sectors, Bull stated. Wind is primarily an electricity producing technology, but it can also be viewed as a link to the end use sector through hydrogen. Solar and biomass can also go through the hydrogen route. Solar is likely to be more distributed, whereas wind can be essentially deployed and utilized in larger quantities virtually all of the renewables go through the electricity route to the end use sector. Biomass electricity is another approach, and it is also useful as a renewable fuel, which adds to its appeal.

Bull named some of the challenges facing feedstocks. One is the anthropogenic production of carbon dioxide that has accelerated in modern day, and the second is the release of carbon dioxide into the atmosphere in the future. "Depending on your perspective, I believe most scientists believe we need to be doing something about this," Bull said. The population challenge is another important factor.

Bull then went on to talk about biomass. The public doesn't understand what the term means, he said. In addition to that, an enormous amount of biomass is still put in landfills. "Cardboard, waste paper, grass clippings, broken branches, we put a ton of things in the landfill, that I am embarrassed," Bull said. Woodchips and forest thinnings are another important biomass resource. Agricultural crop residues are also an important biomass resource. Corn stover is the one program area that the Department of Energy is currently looking at, which also could be combined with the harvesting of corn. Then there are energy crops of various kinds, like switch grass, poplars, as well as alfalfa. "Ultimately, once you use the waste, then you would think about migrating to the use of energy crops," Bull said.

With the crops at hand, the next step is to think about the equivalent of petroleum refineries, Bull pointed out. All biomass is not equal, and there are various forms of biomass in terms of chemical constituents. Furthermore, every piece of biomass needs to be utilized to make biomass an economic business, and it is expensive to bring it to a processing plant. "We need to be doing the same thing [as] the petroleum folks, and that is get every value . . . of every product possible out of it," Bull stressed. The Department of Energy's program is now focused on this point.

Biomass is the only renewable source that produces carbon-based fuels and chemicals. Non-cellulosic biomass is traditionally starch, corn, wheat, or other starches. Sugar complexes that are easy to hydrolyze are currently used for ethanol. Oils, such as soy or cornoil, are also relatively easy to process and to deal with. This leads to its current use as biodiesel, which benefits from the advantage that a significant element of the current fuel supply is already diesel.

Transitioning to biomass fuels is another challenge. The transition will either effect a change in engine type or a change in the fuel supply.

Then there is non-cellulosic biomass with proteins that can be used for soybean meal and other chemicals and materials. Byproducts from corn meal, for example, are animal feed and other food products. The processing of glucose is as follows: hydrolyzation of glucose, before its fermentation to ethanol.

For cellulosics the constituents are both an opportunity and an intense challenge, Bull said. There are three main constituents, the first one being lignin, which makes up 15 to 25 percent of the biomass. Lignin contains aromatics, but since they are oxygenated, they may not be easily developed. Currently there are thoughts about just using it in a fuel, or gasifying or pyrolizing it. Ultimately, though, it should have a greater value as a chemical constituent. Hemi-cellulose is another component, making up 23 to 32 percent, and is made up primarily of 5 and 6 carbon sugar polymers. It is easier to hydrolyze. Six carbon sugars are easy to deal with but five carbon sugars are a greater challenge. The cellulose component is up to 50 percent. It is a polymer of glucose, and is generally hydrolyzed by using enzymes, which then makes it easy to ferment to ethanol. One participant pointed out that a number of technologies that are needed to process lignin or cellulose do not exist, and that there is a big need for R&D.

But fuels cannot be the only focus of these processes. The Department of Energy's programs primarily concentrate on ethanol, electricity, and possibly heat. For this to be an economically viable operation, products in the form of chemicals, materials, food, feed, and fiber have to be developed.

Bull named some examples for producing by-products. There is a partnership with Dupont that is working on integrated quantitative biorefining. This process uses not only the starch, but also the cellulose, the corn, and the corn stover. It produces chemicals, bioethanol, and power, and it feeds the production of Dupont's Sorona® polyester.

Another area is the forest, pulp and paper industry. Bull said this industry should think about producing not only pulp and paper, but also ethanol and other chemicals by stripping the hemi-cellulose away and using cellulose for the pulp manufacturing. The lignin and other residuals can be subjected to a thermochemical process, and a variety of chemicals can be produced from there.

Bull said industry in general does not associate the word biomass and its possibilities with their products. The challenge is to make their industry more viable and at the same time, really start up this business of a biorefinery. Genomics, proteomics, and bioinformatics are going to be key technologies in the biomass industry, Bull said. It may be new chemistry, but it is related to chemistry.

One of the areas that need to be worked on is producing chemicals to subsidize the ethanol production. The projected cost today to build a plant would be on the order of $2.50 a gallon, compared to corn ethanol at $1.20. Bull said a cost reduction is feasible in the future through improvements in technology and processing. Adding chemical products and materials would bring cost down at a more rapid rate.

While it is easy to think of biomass as the primary alternative feedstock, water could also fit that category. Hydrogen does not exist in nature nor can it be mined. However, it can be obtained from fossil energy. Hydrogen is embodied in biomass, and it is also in water, but energy is necessary to obtain it. This energy has to come from somewhere else, like nuclear, geothermal, solar, or wind. There are two key routes: One breaks down the hydrocarbons to elemental hydrogen and usually CO_2. A cleaner and neater way is to generate hydrogen from water, for example, by electrolysis.

There are several ways to produce hydrogen, Bull said. But if it is derived from natural gas, coal, gasification, or other forms, then all the problems that conventional fossil fuels have are not avoided. However, there is the option of using biomass and reforming it. "You can gasify it, pyrolize it, and get there," Bull stressed. Photo-optochemical water splitting with direct sunlight is another possibility. There is enough energy in sunlight to split water, but lakes bubbling hydrogen do not exist. This is because the water is transparent to the sun, and there is not enough absorption. There are two ways to bypass this problem. One method is to use a combined photovoltaic system and electrolyzer as a single device. By doing this, the system can be at least 30 percent more efficient than a two-step system in which a solar panel produces electricity to electrolyze water to hydrogen. The second method employs photosynthetic algae. The idea would be to have ponds of algae to efficiently absorb sunlight and manipulated to produce hydrogen.

Klaus Lackner raised the possibility that competition for agricultural land would arise between growing biomass and feeding the world's population, which may reach between 10 and 20 billion people. This is especially pressing in the light of the fact that many people in China and India move away from these diets toward ones which involve more meat.

Stanley Bull replied that the U.S. economy could handle that, as the food supply is adequate. He said that was why there is significant attention on cellulose parts, because they may in principle not compete head-to-head with fuel. Switch grass can be used on marginal lands; it can grow and sustain itself and maintain productivity for up to 10 years. Food would always be provided first, because that is going to be more economical, Bull said.

One participant asked if municipal waste contains many contaminants that may be difficult to deal with like PVC or fluorescent light bulbs. Trash that has been separated works best, Bull said. "So, I think that is really the best answer, is to do as much source separation as you can," Bull stressed. "That is why the public doesn't like it, because you put it through an incineration plant and you have got stuff that is really hard to control coming out," he added.

Valerie Thomas asked if it would be effective to have the kinds of subsidies that exist now for corn ethanol and for some of the other fuels.

Bull said without some significant advantages, like used equipment or free feedstock, a plant could not compete. He said the price drop in enzyme cost has helped to reduce the total cost. Technology is important, the industry will need incentives, things like the production tax credit, Bull pointed out. He gave wind as an example. Electricity can be produced from wind at five cents a kilowatt hour, which is competitive but the utilities want an additional margin to feel comfortable in putting their future in that technology. The 1.8 cents per kilowatt hour incentive fills that gap, Bulls pointed out. When that production tax credit is in place, the wind industry booms, but when it is in a hiatus, everybody stops. "Of course, part of the reason they stop is, they think the tax incentive is going to come back, so why go build something until it is going to come back. It is a chicken and egg thing a little bit," Bull said. Translating this to the biomass world would mean that more tax incentives will help stimulate the industry. "Our whole target is to get it to be cost competitive without tax incentives of any form, but we need it today," Bull said.

James Wishart mentioned that one of the other potential competitors to hydrogen as a basis for a fuel economy is methanol, which has been advocated by some people, including George Olah. He added that while the route to methanol from biomass is more difficult than with ethanol, methanol could be used in a closed cycle for forming fuel by photoelectrochemical or photochemical activation of CO_2. Methanol has the advantage of being a liquid form of chemical energy as opposed to hydrogen, which is a gaseous form, and difficult to store. Methanol can be obtained by gasification and doing methanol synthesis from that. There are also researchers working on CO_2 catalytic conversion to methanol, but thus far, no results have appeared. Unfortunately, methanol is not as friendly a fuel from a toxicity point of view as ethanol.

There is a problem with too many fuels that are not compatible or immiscible, because infrastructure for everything is not affordable. "The problem is, who is going to play God and decide which one of them we are going to focus on. Right now, the President is saying it is hydrogen," Bull said.

Richard Wool said that to meet 100 quads of energy in the United States in terms of solar energy, a piece of land 100 miles by 100 miles would have to be covered in today's solar collectors. Solar is at least twice as expensive as gas. However, as niche applications are used more and more, and manufacturing is geared up, the costs will continue to come down and "one day we will all be using solar," Bull predicted.

SUSTAINABLE FUELS AND CHEMICALS

Mark Holtzapple talked about the MixAlco process. The process fixes solar energy in the form of biomass and then runs through a biorefinery.

The refinery produces alcohol fuels, which are burned. This releases carbon dioxide, which is fixed into the biomass through photosynthesis. This cycle doesn't add new carbon dioxide to the atmosphere. As long as the sun shines, there will be a perpetual source of energy, Holtzapple said.

Holtzapple proposed ideal features of a biomass process. As a source, any feedstock, such as trees, grass, agricultural residues, energy crops, municipal solid waste, sewage sludge, and animal manure could be used. The alcohol potential from waste biomass is about 135 billion gallons per year in total. Gasoline consumption is 130 billion gallons a year, and diesel 40. This means that alcohol from biomass could have the potential to replace a significant amount of our liquid transportation fuels.

Ideally, high productivity feedstocks could be used. Right now, corn is the source of biomass and it only produces about 3.4 dry tons per acre per year. Compared to alternatives such as sweet sorghum and energy cane, it is not a productive crop.

Ideally, farming would be an economical activity. Right now, a farmer sells corn at $2.40 a bushel, which generates $340 per acre as gross income. If they were to grow sweet sorghum at $40 a ton, they would double their income. If they were to grow energy cane at $40 a ton, they would triple their income. Furthermore, the environmental impact, in terms of water, fertilizer, pesticides, herbicides, and soil erosion would be lower.

Holtzapple then talked about aquatic biomass, which is phenomenally productive. In addition, water hyacinths, for example, are a very beautiful crop. If they are grown without any CO_2 enrichment, the yield is up to 70 dry tons per acre per year, which dwarfs energy cane. Enriched with carbon dioxide the yield can be 100 dry tons per acre per year.

Next Holtzapple described the ideal refinery. Ideally, it would not be sterile, because it is very hard to maintain sterility on a large industrial scale. It would be preferable not to use genetically modified organisms because of public concern, which would be costly due to disposal methods that prevent their release into the environment. The process should be adaptable to varying feedstocks. Ideally, it would not need enzymes or vitamins, because they incur costs, and there would be high product yields. The process should not be based on the economics of co-products, such as proteins. Currently, corn–derived ethanol has a protein byproduct that is responsible for about a third of the income.

Lastly, the fuel itself has to be competitive in terms of the octane rating, the volatility, the ability to ship it through pipelines, its energy content, the heat of vaporization, and whether it will damage the ground water if accidentally released. MTBE is problematic, but ethanol is considered to be a good alternative. It has a very high octane rating, and it is considered an innocuous chemical, a highly desirable characteristic if it is accidentally released into the ground water. However, it has some major drawbacks. For example, it raises the vapor pressure of gasoline. Also, it cannot be shipped through pipelines since it can pick up water and causes problems when used in downstream applications. It has a fairly low relative energy content (about 84,000 BTUs per gallon), and there can be cold start problems with pure ethanol. "What I would suggest is that mixed alcohols are superior on all of these various features," Holtzapple said.

The MixAlco process produces a product that has all these ideal features, Holtzapple argued. He first described the process in its original version. First, the biomass is treated with lime. This treated biomass is then fermented with a mixed culture typically derived from soil. "[L]iterally, you just throw dirt on the biomass and let it rot," Holtzapple said. What comes off the rotting biomass is a carboxylate salt, and some calcium carbonate is added to neutralize the acids. Acetic acid, propionic acid, and butyric acid are then added during the rotting process. The carbonate reacts with the acids to make calcium acetate, propionate, and butyrate. The water is removed from the salts, which are then heated to produce ketones such as acetone and, if hydrogen is added, alcohol, such as isopropanol. "We are turning cattle manure into salts of vinegar, nail polish remover, and rubbing alcohol," Holtzapple said.

Holtzapple said he believed the hydrogen economy could viable through the MixAlco process, because this process hydrogenates biofuel. Biofuel is a hydrogen carrier, and it converts the energy of the hydrogen into a liquid transportation fuel that is completely consistent with the current infrastructure. As much as 35 percent of the energy content of that alcohol can come from the hydrogen. This means it is a very safe, reasonable way of getting to the hydrogen economy, Holtzapple said.

To assess how well the technology works Holtzapple uses an *in situ* digestion method. Scientists take about two grams of biomass and put it in a container resembling a tea bag. The tea bags are put into a porous sac, and the porous sacs are placed into the rumen of a cow by way of a surgical hole called a fistula. The bags are incubated, washed, dried, and weighed. Digestion yields are measured based on the mass of biomass remaining. For example, if the experiment starts with two grams and one gram is left over, it was 50 percent digested.

More recently, Holtzapple has come up an advanced lime treatment process. For this, he built a big pile of biomass with lime in it and then aerated it to get the combined effect of oxygen and lime. The addition of air is a necessary step, for without the air, a third of the lignin will not be fermented. The next step is the fermentation. Organic acids naturally occur everywhere, including within the rumen of cattle, sheep, deer, and elements, sewage digesters, swamps, and termite guts. Nature favors the production of organic acids, because the process is thermodynamically driven. As a result of the fermentation, acetic acid as well as propionic and butyric acid are produced. Methane can also be produced, but Holtzapple adds an inhibitor that blocks methane production. As a result, the energy that would have been lost to methane is accumulated into the higher acids.

The product distribution is a function of the temperature. At mesophilic conditions—at the temperature of a cow—the distribution is about 41 percent acetic acid. If the temperature is raised to 55, the process highly favors acetic acid production. The process utilizes a proprietary marine organism that is resistant to the high salt concentrations. The microbe is used in the inoculum, leading to high product concentrations.

The grand vision is to build the pile with biomass, lime, and calcium carbonate. During the first month or so, air is ventilated up through it to remove the lignin and make the biomass digestible. A tarp cover is then thrown on top, the microbe-infused dirt is added, and the pile allowed to rot and produce organic acids. The next step is the de-watering step. Vapor compression is the preferred de-watering method, since placing a vacuum on a salt solution will cause it to boil, producing distilled water and concentrated salts.

The thermal conversion step is next. The calcium acetate becomes acetone, and the higher acids become higher molecular weight ketones. A 99 percent conversion at about 440 degrees Celsius takes about 25 minutes. Finally, the hydrogenation step takes place, in which the ketones become the corresponding alcohols. This step uses a Raney nickel catalyst in liquid phase. The process is geared toward ethanol at the moment, as that is where the tax credits are. The calcium acetate solution is run over several steps to produce ethanol.

Holtzapple then introduced the economics of the process. The ketones sell for about 60 or 70 cents a gallon, providing a substantial profit margin at the moment, as the current price of acetone is $3.50 a gallon. Alcohols are around 80 cents a gallon. The acetic acid, for example, is in the six cents a pound range, and it sells for about 25 cents a pound. The alcohols—in this case mainly ethanol—are in the 60 to 70 cents a gallon range. These prices are calculated for a corn price of $40 a bushel.

A possible scenario is taking the sugar cane, extracting the sugar, and then producing alcohol from the fiber. The sugar could be used to make a range of products, such as biodegradable polymers, rubber, or even fibers such as Dupont Sorona®.

Holtzapple then named the factors for replacing gasoline. With current engine efficiency, 248 biorefineries would be needed, and a land area of 300 by 300 miles would be required for sugarcane. At double the efficiency, the required area is reduced to 200 by 200 miles. At triple the efficiency, it shrinks to 174 by 174 miles. In comparison, the land requirement for sweet sorghum would be 340 by 340 miles. Holtzapple is currently testing an engine that could be 49 to 55 percent efficient. This translates into a gas efficiency of 75 to 100 miles per gallon in a full sized car.

One participant wanted to know the time scale for realization of the project. Holtzapple estimated that a small demonstration plant should be running by the end of 2005; a full scale commercial plant might take two or three years.

Another participant asked if sustainable agricultural practices were part of the project. Sugar cane has been growing in Cuba on the same land for hundreds of years, and the land still maintains its productivity. "So, if you do it right, the soil doesn't wear out," Holtzapple said.

Frank Flora asked how the process is controlled. Calcium carbonate is self-buffering, it maintains a pH range of 5.8 to 6.2.The temperature is controlled by circulating liquid through the pile, which can then go through a heat exchanger. "[A]ll the control that we need is just temperature, pH, and keep that inhibitor in there so that we don't degenerate to methane," Holtzapple said.

ROUTES AND COMMODITY CHEMICALS FROM RENEWABLE RESOURCES

Douglas Cameron spoke about Cargill's work in the area of green chemistry and sustainability. He also talked about two carbohydrate-based examples of the chemistry bio-refinery, lactic acid, and 3-hydroxypropionic acid (3-HP).

Cameron predicted that biomass feedstock prices will continue to drop in real terms, due to improvements in agronomic practice and in biomass conversion technologies. Process technology has to continue to evolve in order for this to happen, and government funding is needed to help spur this along. Novel catalysts are going to be important, he said. Product development and selection of the right products are important, as are platform chemical concepts and partnerships between companies like Cargill, who understand agriculture and chemical companies.

Cameron then introduced some examples. He started with the production of polylactic acid (PLA). The concept is to make lactic acid by fermentation of sugars, which is extremely attractive. It is then chemically converted to lactide. Starting mainly with the L,L form, the product is primarily L,L lactide with a small amount of the D,L lactide and an even smaller amount of the D,D lactase, which can be removed by vacuum distillation. The polylactic acid is recovered through ring opening polymerization.

Cargill now has a large production plant, where it makes various types of fibers, clothing, and other applications that are being developed, such as carpets and tile squares. PLA has the property of dead fold, so it can be used in wrapping, typical biodegradable type applications, and bottles. Recently, a company in Colorado started selling bottled water made out of PLA bottles.

Cargill is now the biggest producer of lactic acid, and its process utilizes a wide range of renewable sugars, including glucose. Lactic acid produced by an anaerobic fermentation, which means it is not energy intensive since oxygenation is one of the most energy intensive parts of fermentation. The theoretical yield of lactic acid from glucose is 100 percent, which compares favorably with the theoretical yield from other glucose-derived products, such as ethanol (51%). There are two functional groups in lactic acid, which means that it can act as a platform molecule for other chemistry.

One potential product from lactic acid is hydroxypropionic acid, which may primarily be 2- or 3-hydroxypropionic acid. This acid is not widely available through the chemical industry, not even from Sigma Chemical or Aldrich Chemical. Since it is not readily available, its possibilities have not been extensively explored. Cargill also determined that no microorganisms had previously been used to make it.

This case exemplified the concept of green chemistry design that potentially looked attractive, Cameron said. However, in practice, there were many unanswered questions. Cargill evaluated hydroxypropionic acid in terms of its properties and its safety. Like lactic acid, it could act as a platform chemical; for example, it could be oxidized to malonic acid, a pharmaceutical intermediate currently manufactured through a chemically messy route. It could also lend itself to polymerization and hydrogenation to 1-3 propane diol, which would provide an alternative route to make a chemical ingredient for the Dow product Sorona®. Hydroxypropionic acid could also be dehydrated to acrylic acid, which is a seven billion pound product with a rapidly growing demand; it is the basis of superabsorbent polymers used in diapers and other products.

What this could potentially do is give Cargill a renewable route to a compound like acrylic acid and a whole host of other materials. Since it had not previously been investigated, Cargill researched some of its applications. One of the things the company found is that the calcium salts of 3-hydroxypropionate are very highly soluble relative to many other organic acids. This provided an opening for unique opportunities for this acid in cleaning applications such as removing "scale" (substance buildup) from various materials. In addition, the corrosiveness of hydroxypropionic acid is much lower than that of a number of other acids, making 3-HP or its salts a potentially good antifreeze agent.

While Cargill now saw opportunities with hydroxypropionic acid, there was yet no microbial method to make the chemical. Cargill wanted to determine if they could design and build metabolic pathways to do this. Criteria for the process included a 100 percent theoretical yield, the availability of necessary genes and enzymes, and several other design factors. To begin, Cargill mapped every possible metabolic pathway from glucose to 3-HP and found the most intriguing one to be the beta alanine pathway. This route only requires a microorganism to ferment glucose to pyruvate and an additional four steps to make beta-alanine directly from pyruvate. These additional steps could potentially be engineered into the microorganism.

How does the pathway compare to the criteria? Energetically, it is very favorable. The theoretical yield of this pathway translates into one gram of 3-HP per gram of glucose under anaerobic conditions, with identical thermodynamics to those of lactic acid production. The one major challenge in the pathway is that it requires a catalytic step that doesn't exist in nature. However, enzymes exist in nature to convert alpha-lysine to beta-lysine.

Ideally, the pathway could be transferred into an organism like *E. coli* and the various byproducts could be eliminated. "So, you would have an organism that makes 100 percent 3-HP from glucose, and that is what we are proceeding to do," Cameron said.

Vegetable oils are another important research area for Cargill. One of the current business divisions is involved with industrial oils and lubricants, and they study how to produce hydraulic fluids, transformer fluids, and various other codeines and things made from vegetable oils. For example, vegetable oil is used to make biodiesel in Europe, and a byproduct of biodiesel is glycerol. "So, there are opportunities to figure out what to do with that," said Cameron. He also mentioned that Cargill has a very active research program in polyurethane polyols, and there are some compelling reasons to make polyols from vegetable oils. For example, polyols are used for the production of polyurethanes for automotive seats.

Cameron said Cargill uses fatty acids and performs various chemical reactions with them, such as metastasis chemistry (the interchanging of double bonds). This is done in partnership with a company called Materia. Dienes for rubbers, or alpha olefins for polyethylenes, can be made from unsaturated fatty acid starting materials.

When asked about toxicity studies on 3-HP acid, Cameron said the data shows lower toxicity than lactic acid both in fathead minnow aquatic toxicity tests as well as in various animal feeding studies. However, the concern is that it is quite easy to dehydrate 3-HP acid to acrylic. He added that the chemical is a component of what is called the 3-hydroxypropionate cycle, which is present in many bacteria species, leading researchers to think that it could be rapidly metabolized in nature.

SUSTAINABILITY, STOICHIOMETRY, AND PROCESS SYSTEMS ENGINEERING

The chemical industry has been driven by material substitution for decades, Jeff Siirola said. Products are mostly made from methane, ethane, propane, and aromatics. Eighty percent of all manufacturing energy, and 80 percent of all manufacturing wastes, are associated with the processing industries. Today, even though the chemical processing industries are considered to be energy intensive, energy cost has not actually been a dominant economic factor, not even in distillation processes. Siirola said that in his company products that cost more than 5,000 BTUs per pound are not made. With coal priced at 80 cents per million BTUs, energy does not comprise more than five percent of the sales price, which means that it rarely costs more than two, perhaps three cents per pound of product.

The cost of energy has gone up by an order of magnitude, but the relative ratio of energy to capital is unchanged and has remained so for the last century. But sometimes, certain sources of energy change in price relative to others, Siirola said. For example, the price of natural gas today is really more expensive relative to coal.

There will be an increase in the global demand for energy, Siirola predicted. The increase in the world's population to between nine and ten billion people will increase the GDP (gross domestic product) by a magnitude of six to seven times. At the same time, most commodities, most materials of construction, and the chemical industry will increase by five or six fold. The energy demand is expected to increase by a factor of about three and a half, which translates into a growth rate about half that of GDP growth. This growth rate has remained fairly constant for the last several decades due to technological innovations.

According to Siirola, the imperative of not harming the environment and not increasing the impact on it would be the basis of his discussion. He then asked what it means to not limit the choices available to future generations. He discussed how a choice should be made between two different sources of a raw material or energy with two different costs for the chemical industry. "Should I only use the more expensive one and leave the cheaper one to future generations, [or should] I extract from both sources in the same percentage that I find them so that I leave the future generation the same problem that [I've] got?" Siirola asked. He argued that the cheaper one will be exploited, resulting in a price rise and leaving the future generation to fend for itself. "No customer will pay extra to exploit something more expensive so that future generations are left with a cheaper alternative," he said.

Siirola then spoke about raw material selection for the chemical industry. Selection characteristics or criteria include factors such as availability, concentration, extraction cost, competition for the material, other alternatives, and how close the raw material is in chemical or physical structure and in oxidation state to the product.

The oxidation state of material is a particularly important factor, especially for carbon. Carbon has eight oxidation states, which range from –4 (methane) to +4 (carbon dioxide). Free energy changes between [e]ach of those states are almost exactly equal, amounting to about 25 kcals per milliliter per oxidation state. Most of the polymers in the world lie somewhere between the –2 and –0.5 state, and most oxygen organics exist between –1.5 and zero oxidation state. Methane is –4, ethane is –3, many hydrocarbon type materials are –2, and many oxygenates are a little bit higher, with acetic acid at zero. Carbonate salts are found at the bottom of this chain. Carbon in the +4 state is acidic and can be neutralized, and its salt has a free energy state some 40 kilocalories per milliliter lower than that of the free acid.

Siirola then counted up the available carbon on earth. There are about 75 gigatons of carbon in natural gas, 120 gigatons of carbon in oil, 900-plus gigatons in recoverable coal and about 250 gigatons each in oil shale and tar sands. There are about 2,500 gigatons that are recoverable at prices higher than today's prices. This means tighter oil or tighter gas supplies, as coal seems currently too thin to mine. Carbon is also found in methane hydrates with an estimated tonnage range from a few thousand to a number so large that they could not have been generated biogenically. The total biomass on the top of the earth is 500 gigatons, and the amount of carbon located in the soil one meter below the surface, plus peat, is four times as high. The total amount of biomass produced each year on the earth is 60 gigatons, and an equal amount is destroyed. More than half of that amount is located in the tropical rain forest and the tropical savannah. The total amount of chemicals produced in the world is three tenths of one gigaton of carbon.

Upon looking at oxidized carbon atoms, the total amount of CO_2 in the atmosphere at today's concentration supplies 750 gigatons of carbon. There is twice as much coal as there is biomass, and there is more coal than there even is CO_2 in the atmosphere. There are approximately 40,000 gigatons of carbon that exist as dissolved carbonates in the ocean and an additional 100 million gigatons of carbon found in limestone, chalk, and dolomites.

In sum, this means that the world is not running out of carbon atoms, Siirola said. Many of them are in a reduced state or in their oxidized state. If the raw material for carbon is in a lower oxidation state than the product, it has to be oxidized. This may occur through direct and indirect partial oxidation. The oxygen source is almost always atmospheric oxygen, and the reactions overall are oxylformic. Selectivity is sometimes an issue, purification is oftentimes an issue. Sometimes a proportionation reaction will form the desired oxidation state. The carbonaceous material is oxidized and at the same time co-produces hydrogen. Often, almost all the hydrogen produced is used, often for environmental purposes, for example to remove sulfur from raw materials. In carbonylation chemistry a molecule is oxidized to carbon monoxide, which then reacts to the desired oxidation state, and this is the only oxidation that is very easy to reverse.

If the raw material is at a higher oxidation state, it has to be reduced. The reduced state ultimately produces hydrogen. Hydrogen production and the reduction reaction frequently occur in tandem and are net endothermic. This means energy has be added to reduce carbon. Starting with an intermediate oxidation state, a disproportionation process can be a good choice. It drives part of the carbon into a lower state. Fermentations, for example, work that way. Glucose will make ethanol at the -2 state while oxidizing an equal number of carbon atoms to the +4 state to produce energy.

In the total synthetic reduction, the energy comes from the sun and CO_2 which co-produces oxygen. To make a milliliter of hydrogen, either water has to be split or a carbon atom has to be oxidized by two states. In steam reforming to methane or in biomass gasification, a material at raw oxidation state reacts with water to make hydrogen and CO_2. Splitting water into hydrogen and oxygen can be done by electrolysis, and there are experiments to achieve this directly by photosynthesis.

Taking this into account, there is a question of what is the most sustainable raw material for the chemical industry, Siirola said. “Should it be the one that is the most abundant, which means that we would make everything out of limestone? Should it be the one for which a natural process already exists to do some of the energy change that would be required to exploit it, which would be atmospheric carbon dioxide?” he asked. Oil might require the least addition energy to process it into the most final products. Methane or condensate are likely to be least contaminated with unwanted elements like sulfur and nitrogen. Glucose or lignin might be structurally closest to some desired products.

If the world population stabilizes at a number below 10 billion with subsequent GDP growth and energy needs, there will be new energy demands of 2,500 quads. This demand distribution breaks down to one third transportation, one third electricity, and one third domestic heating and industrial requirements, which will mean close to 5,000 gigawatts of new power. This is not a great demand for power, and it would mean one gigawatt power plant every three days for the next 50 years, or about 1,000 square miles of new solar cells at 10 percent efficiency and annual sunlight conditions similar to a cross between those of Tennessee and Nevada. It means carbon emissions climbing from today’s seven gigatons a year to maybe 26 or 30 gigatons a year. That assumes the same fossil and nonfossil mix and the same mix of fossil fuels. "Actually, if we run out of methane, the amount of carbon [produced] will be even greater than this for the same amount of energy," Siirola pointed out.

There are 6,000 gigatons of fossil fuels available, counting the biomass, peat in the ground, unrecoverable reserves, but not including the hydrates. At some price more and more—but not necessarily all—will be exploited, growing to three times the current demand of seven gigatons per year. "Will we run out? Yes, at this rate we will, but not tomorrow, [and that] is the point," Siirola said.

Siirola counted the number of options for sequestering CO_2, such as burial or absorption into geological formations, into coal beds, the deep ocean, saline aquifers, or into tight formations, all of which he deemed not entirely satisfactory. There are even fewer options for the energy involved in transportation. In transportation, mass counts, so technology to absorb CO_2 on board light weight vehicles does not exist. Even the lightest absorbent known, lithium oxide, is still too heavy to be useful.

Siirola then talked about non-fossil options. Biomass costs too much in terms of cropland. The total world's net production of biomass is close to 60 gigatons. The total world's crops currently are six gigatons, and that is likely to grow to nine gigatons as the world's population approaches nine billion. Most of the cropland will be needed to feed the people. The current energy crops currently comprise a hundredth of a gigaton. The projected energy need will be 26 gigatons per year by the time the population levels out, and the projected chemical needs, at the same time, might rise to 1.5 gigatons per year. However, there are 60 gigatons of net biomass which could be utilized, but it means having to harness half of the annual biomass produced on the planet for energy needs. "So, could you do it? Yes. Are you likely to do it? I kind of doubt it. I just don't see an infrastructure to collect 50 percent of the biomass," Siirola said.

If CO_2 cannot be captured, fossil fuel cannot be a viable option, Siirola pointed out. Solar power could be a worthy alternative. Compared to biomass, solar power has a much higher energy density. Siirola calculated that the power density that could be obtained by turning biomass into pyrolized coke would be four tenths of a watt per square meter, assuming no energetic cost of growing the biomass. A solar cell on average provides between 20 and 40 watts per square meter, 20 in a place like Tennessee where it is cloudy, 40 in a place like Nevada.

But the difference in capital costs between the two choices becomes an issue. The capital costs for planting hundreds of square miles of biomass could be minimal compared to the capital costs of photo well tanks, which are nearly an order of magnitude higher than the capital costs for making a coal fired power plant of the same production.

Solar energy must be collected and stored. It could be stored in atmospheric pressure gradients as is done for wind. It can be stored in elevation gradients as molecular hydrogen or as carbon in the zero oxidation stage. It may also be stored as latent or sensible heat in thermal storage. "All these things are possible," Siirola said.

Hydrogen has many advantages, Siirola pointed out. First of all, it produces fewer pollutants and no CO_2 at the point of use. But molecular hydrogen is not available, is difficult to store, has a very low energy density, and is an energy carrier rather than an energy source. "If hydrogen comes from reduced carbon, then the same amount of CO_2 is going to be produced whether or not we just burn the carbon or make the hydrogen and burn the hydrogen," Siirola argued.

Solar and nuclear are the only long-term energy solutions, Siirola concluded. "By a factor of 105 there are far more carbon atoms in the high oxidation states than the low oxidation states," he calculated. The environmental impact of having the rest of them oxidized may be smaller than is currently thought. There is plenty of available carbon in the low oxidation states, and it exists close to the activation state of most of the desired chemical products. In addition, the high availability and the existence of photosynthesis do not necessarily argue for starting from CO_2 as the principal raw material as it requires too much energy to be added to the system to obtain the products. "We can, however, get to any carbon oxidation state from any other, but going down an oxidation state costs you energy," Siirola said.

One participant objected to nuclear being called a viable option. Siirola said he did not spend time talking about nuclear because the risk is a very large number multiplied by a very small number. But he said he suspected that in the end the product is going to be such that it is going to remain among the alternative choices. Siirola said the problems of storage were serious, but not insurmountable, in terms of being able to handle the long-term sequestration of solids. One of the participants added that nuclear looked very much like a green energy.

Klaus Lackner said there might be more carbon reserves than accounted for. He stated that there may well be that there are 20,000 gigatons available. However, that still would not change Siirola's conclusion. If anything, he argued that this point supports his opinion. Finally, Siirola offered that the amount of oxygen in the atmosphere is a key to estimating how much CO_2 was reduced.

ENZYMES

Glenn Nedwin talked about how enzymes can help to achieve a sustainable future. "In the last century, we have had the industrial revolution, and what we believe is that we want to get to the industrial evolution," he said.

Enzymes are ubiquitous. They are used in detergent, starch, textile, fuel ethanol, pulp and paper, baking, brewing, wine, juice, food specialties, and animal feed. Nedwin listed enzymatic properties that contribute to sustainable development. First, they are biological catalysts with very specific properties that drive chemical reactions in living cells. They work at mild conditions in small quantities and are fully biodegradable. They are made by fermentation from renewable resources, and the excess biomass waste is used as a soil conditioner and fertilizer.

Enzymes can improve product quality and save water, energy, chemicals, and waste while speeding up production processes and enabling new products. Most enzymes come from microorganisms in the soil, with nearly half the enzymes in the world originating from bacteria and the remainder found in fungi.

Enzymes can be tailored to different uses, such as in laundry detergent where the conditions of the water in different places can vary. To find a substitute enzyme, scientists search within organic environments that mimic desired reaction conditions. For example, for cold temperature conditions, an organism that thrives in a cold environment is ideal. If it can't be found in nature, it is evolved in the lab.

Native enzymes can be altered to change their activity in different areas, making them more alkaline, thermally stable, or pH-sensitive. After an enzyme is discovered, it has to be made at very high levels by large-scale fermentation of microorganisms, which are initially streaked on a petri disk and inoculated into gradually larger volumes of nutrient-rich broth. From these fermentations emerge the purified enzymes: proteases, amylases, cellulases, carbohydrases, lipases, esterases, and oxidoreductases. The challenge lies not only producing them at high levels but also in finding uses for them.

How are enzymes involved in sustainable development? The detergent industry is an important example, as a mixture of proteases, amylases, lipases, cellulases, and manonases is used in detergents. The use of these enzymes has allowed the washing temperature to be lowered from 60 ºC to 40 ºC. In Denmark alone, this has resulted in a savings of 28,000 tons of coal per year.

Enzymes also help save on the use of other chemicals and render detergents more effective. By using enzymes, fewer phosphates and other chemicals are needed while simultaneously making laundry cleaner. The enzymes are fully biodegradable and gentler to fabrics. If the average washing temperature in Europe is decreased from 40 to 30 degrees, about a third of the household electricity consumption can be saved.

Another application is textiles. The average pair of jeans consists of cellulose fabric woven into denim. Previously, it was dyed but required additional chemical and mechanical treatments to remove the remaining starch in it and obtain the desired "look." Historically, oxidizing agents or sodium hydroxide pressure-cooking were needed to get rid of the starch. Now, amylases are added. Cellulases in laundry machines replace the pumice stone that was originally used to make stone washed jeans. The bleaching process now operates with lactase instead of chlorine and other bleaching agents.

To demonstrate that the environmental burden of making the enzyme is outweighed by its sustainable applications, Novazyme performed a cradle-to-grave life cycle analysis. For the analysis, the company compares two systems: a combination enzymatic/chemical system and an enzyme-only system.

Scalazyme, a pectin ligase enzyme that breaks up pectin in cotton, was presented as an example for the life cycle analyses. It was incorporated into the entire process from cotton processing to knitting. First, a scouring step is required to bleach the cotton and prepare it for coloring, a process which normally requires sodium hydroxide, acetic acid, surfactants, energy, and voluminous amounts of water. Novazyme examined this step and found that the scalazyme enzyme could provide a tremendous reduction in the amount of resources that are used in the original process. With the enzymes, the energy demand is reduced by 25 percent, resource consumption is decreased by more than 25 percent, and water use is cut by 65 percent. If the process by which all cotton in Europe is scoured could be converted to this scalazyme process, it could prevent the pollution of enough water to supply 400,000 people. In 2001, Novazyme won a Presidential Green Chemistry Award for the process.

Another example for waste reduction is phytase, an enzyme that breaks up phytic acid in plant material. It can be used to replace the addition of inorganic phosphate to animal feed. Animals fed from phytase-treated feed need less inorganic phosphate in their diet, which results in less phosphate released to the environment. A significant reduction in nutrient salt pollution is also seen. If 23 million pigs in Denmark were given phytase-treated feed, the estimated reduction of aquatic phosphate pollution would be enough to supply an additional amount of potable water for 300,000 people.

Another example is amylase in baking, which is used for extended shelf life of bread. Bread treated with amylase has a modified structure of starch such that it doesn't recrystallize, effectively preventing the bread from going stale. This reduces waste in terms of transportation and wheat production for the supply of bread. "If this was used in all the white bread in the United States, you would probably save the CO_2 effects of 50,000 people," Nedwin said.

A future use of enzymes could be in the production of bioethanol, which is made from corn starch, and the challenge is to make it this way as economically as possible. Bioethanol is sustainable and is an almost CO_2-neutral energy source. It can replace MTBE as an opting booster in gas. Ten states have successfully banned MTBE, which creates a 1.4 billion gallon per year market right now. Fuel ethanol as a fluid energy source for the transportation sector is the only alternative to gas, except for biodiesel and gas. Today there are blends of 10 percent ethanol, and 20 percent ethanol biofuel is used in Minnesota.

In the year 2000 alone, it is estimated that the ethanol industry added 22,000 new jobs and more than $15.3 billion to the gross output of the American economy. Replacement of all MTBE used in gasoline comprises about six percent of total gasoline substitutions, which amounts to a need for 10 billion gallons of ethanol a year. The current corn ethanol production is about three billion gallons a year, an amount that can only provide ethanol gasoline substitution for 30 percent of all gas in the United States. Furthermore, the total MTBE replacement would consume about 30 percent of the farm land growing corn.

These facts prompted the Department of Energy to fund a very significant research project with Novazyme and Genencor to evaluate alternatives, operating on a budget of about $18 million over four years. Corn is currently broken down by amylases to corn starch and glucose. The alternative to corn-derived cellulose material is the use of corn stover, which consists mainly of cellulose and hemicellulose. NREL worked out an acid pretreatment process for corn stover, which delivers 56 percent cellulose. The cellulose is further broken down by using a mixture of cellulases. Unfortunately, the corn stover/cellulase process is 50 to 100 times more expensive than the corn/amylase route.

There are several different ways of making enzymes less expensive, Nedwin said. These include reducing enzyme production costs by reducing the cost of feedstocks and enzyme recovery processes, by employing onsite production of enzymes where the corn is grown, by increasing the fermentation yield, or by increasing enzyme activity on a program basis.

All factors point to novel enzymes that can be genetically engineered to be tailor-made to specific industrial processes. Enzyme candidates can be integrated into an expression host, characterized biochemically, and tested on the conversion of pretreated corn stover to ethanol. The enzyme cost to make a gallon of ethanol from corn starch is between five and ten cents. The enzyme cost from biomass was $5.40 at the onset of this project, and it is now down to 27 cents,[6] which is a 20-fold reduction. The ultimate goal in order to compete with cornstarch is about 10 cents. For this work,

[6]This figure was current at the time of presentation in February 2005. However, at press time, Novozymes announced that the enzyme cost had been lowered to $0.10-0.18 per gallon ethanol, a 30-fold reduction.

Novazyme received two awards in 2004, the Scientific American 50 award and, together with NREL and Genencor, an R&D-100 award.

Nedwin said pretreated corn stover is about the furthest advancement in terms of technology today. The future needs other pretreatments and mixes of enzymes with different types of substrates. "If we look at making the biorefinery happen in a big way out of biomass, we need government support. If we look here historically, the government has had tremendous help in pushing industry, in the railroads, in the Detroit automotive industry, and even the biotech, by changing patent laws," he pointed out.

Nedwin summarized the role of enzymes in sustainability. Today, only five percent of fine chemical, polymer, bulk chemical, and specialty chemical industries are impacted by enzyme processes or wholesale microorganisms. McKinsey & Company estimated that by 2010 this number can be up to 10 to 20 percent, which translates into sustainable development to produce less pollution using enzymatic routes. He added that knowledge of enzymology in the chemistry industry needs to be broader, as does the awareness of applications and demand. But in the end, enzymes must be price competitive.

Participants asked about enzymes in nonaqueous environments, as enzymatic hydrolysis is found only in aqueous environments. Glenn Nedwin said there are some breakthroughs being made in that area, such as lipases which work in organic solvents and immobilization of lipases and other enzymes.

MEMBRANE PROCESSES

William Koros talked about membranes and separation processes and their energy saving potential. He showed that this technology has great potential with the help of some examples; nevertheless, it is nonetheless still underdeveloped.

Separation technology is a possible application to save energy. In the United States, around 33 percent of the total energy use is in the industrial arena, and 40 percent of that fraction is used for separation. This translates into about 15 percent of the total energy use. If this number could be lowered, it would have an enormous impact. This is a huge opportunity, because global capacity will grow over that period of time. If the capacity that is installed today is based on current, largely thermally-driven technology, then membranes will not sustain it as the world stabilizes at a population of 10 billion. "[W]e are buying what we are going to live with in terms of thermal separations if we don't do something," Koros said.

Membranes have great potential as energy savers, Koros said. Looking across the separation spectrum, membranes are the low energy intensity enablers that can allow energy conservation in the chemical industry. In an ideal sense, this technology is not thermally driven, but instead mechanically driven. "So, one avoids a lot of the second law restrictions that are currently plaguing separation processes," Koros said.

But the technology is insufficiently developed. Although membranes have the greatest potential to facilitate low energy processes, they are by far the most immature in terms of technical development. The reason for their lack of application is due to a failure to implement improvements for installation of those membranes.

Koros pointed out that membranes could be used in large-scale processes. Many times people are under the mistaken impression that membranes do not scale, Koros said. Other very selective processes like chromatography and affinity methods do not scale very well, but membranes and adsorption do. In fact, membranes and adsorption are a very powerful "one-two punch," because adsorption can deal with very dilute solutions, while membranes can deal with more concentrated solutions. In many cases, hybrid systems incorporating these two technologies are very attractive.

There are two fundamentally different kinds of membranes. One operates primarily on the basis of hydrodynamic sieving, which is not actually a filtration process but rather a more subtle process. The size of the rejected entity ranges from 20 Angstroms up to chunks of dust, and it is very easy to shear away and strip away a suspending medium. Usually it is an aqueous organic suspending medium passing through the membrane, and in which some undesirable component is rejected.

Something very different happens when the scale of what is being stripped is on the same order of magnitude as the medium from which it is being stripped. Separation of an aqueous suspending medium with salts or organic components is very energy intensive to separate. In a process called ultrafiltration (or microfiltration), a physical pore is built into a membrane in order to separate particles that are less than 20 Angstroms in diameter. A transmembrane pressure drives the suspending fluid via current flow through the membrane, while the rejected biomolecule is separated because it can't fit through the pores.

This technology is a very powerful energy saver. As calculated by Koros, capturing a cubic meter of water using this technology costs about 6.7 kilowatt hours per cubic meter (assuming 33 percent energy efficiency) compared to about 73 kilowatt hours per cubic meter using an optimized, fairly efficient triple effect type evaporator method. The real cost, in terms of mechanical energy, is about 2.2 kilowatt hours per cubic meter.

The problems of this process boil down to the need to obtain better control of pore size and uniformity. If the process involves larger solids or more complicated feeds, such as renewable feedstocks, it becomes very important to control the physical chemistry at the membrane surface. If one takes a step into the next part of that spectrum and considers stripping away micromolecules from micromolecules, or ions from water, it becomes an extremely expensive and energy intensive proposition. Water must want to be in the membrane more favorably than does the ion or the organic molecule being rejected. In addition, once it is in the membrane, there has to be more favorable molecular diffusion process to cause that separation.

While this technology exists as a functional one, it is only known to work well for aqueous systems in a highly evolved state, Koros pointed out. Seawater reverse osmosis is the only well developed example. This is very compatible with wind generation, because it could be off-shore and wind could drive the pump to bypass some of the second law restrictions regarding thermal generation of energy. The energy cost is about 10 times more efficient than that for the thermal option.

This could have implications on a worldwide basis. Around the globe, there are about a billion people who do not have adequate drinking water. About nine billion gallons of water are desalinated every day around the globe, half of which performed thermally in plants that were constructed before membrane technology existed. Due to investment in research, most of the new de-salination plants are now membrane-based. The savings could be about 1.4 quads a year, Koros calculated, which is essentially a payback on the roughly $1 billion of research that was invested in the membrane option over the last 40 years.

There is a whole array of other kinds of membrane applications such as olefin paraffin separations which remove sulfur and benzene from gasoline or isomer separations that distinguish between normal and more bulky isomers. These kinds of separations can be performed but not very well with the current generation of membranes. To have an impact on the energy use, they would have to be as efficient as a reverse osmosis unit.

Koros looked at another example of separation: propane and propylene, a significant market of about 25 billion pounds a year with a growth potential on par with the GDP. Currently, it is a very expensive and energy intensive process conducted through cryogenic distillation. A new unit costs about $50 million, but membranes could cut both energy costs and the capital costs, Koros said. The problem is whether such a membrane actually exists. Propane and propylene are very similar; propylene has a compact and a bulky end, but propane only has a bulky end. The difference in size is about half an Angstrom. "If you simply take a polymer and turn it into a carbon molecular sieve at 500 or 550, all of a sudden, you get an enormous selectivity because it becomes possible to do size and shape discrimination that is simply not possible by a polymer alone," Koros explained. Tenths of Angstroms can be easily distinguished.

However, cost is still a problem. This process is about a thousand times more expensive per square meter of membrane than the polymer process. "I think the only thing that can be done is analogous to walking on both legs. You don't count on all your left leg or your right leg. Organics or polymers are very easy to process," Koros explained.

Both technologies need to be developed. Inorganic- and carbon-based membranes are extremely selective because of their rigid size and shape discriminating ability. There must be investment into the development of the next generation of membranes that retains this exquisite size and shape separating capability. In some cases, organic polymers do fine, such as in reverse osmosis. However, as there is a need for increasing selectivity, the next generation technology is being pushed almost to a pure inorganic glued together by a polymer.

It can be achieved, as early work in the last couple of years has demonstrated. It is possible to put a million of these fibers into a module that is about a foot in diameter and about a meter long with the surface area of a football field. If the hybrid material can be put on the outside of the fiber while maintaining the inside as a flexible material, "it thinks it is a polymer in terms of mechanical properties but, in terms of its separating properties, it thinks it is a molecular sieve, or at least a hybrid material," Koros said. The idea is to integrate this material into a practical process in which mixtures of molecular sieve entities and polymers are made up as a "dope." It is spun into a hollow fiber about 200 microns in diameter, placed through fluid exchange, and dried. Instead of a thousand-fold higher cost, the estimate is about $5 a square foot or $50 a square meter.

"This technology is about where I would say aqueous reverse osmosis was in the late 1960's. It was clear that it worked, but it didn't work very well, and there still has to be a significant investment made. We are making a decision. We are either going to invest in something that has this ability to cause an order of magnitude reduction or we won't," Koros said.

Participants asked if membranes offer an opportunity to separate a molecule the size of water from a 300-, 400-, or 500-gram per mole pharmaceutical, for example as in a waste water treatment facility. This process would be somewhere between a true solution diffusion process and one that has aspects of a filtration process, Koros said. There are membranes in this dimension, and they are not difficult separations in aqueous systems.

Separations for hydrocarbons have the problem that hydrocarbon molecules are dissolved on the surface of the inorganic membrane, one of the participants noted. A major interest is in organic membranes because they withstand very high temperature conditions. There are some thoughts that, by cutting the surface of the membrane material, the adsorption factor could be eliminated. Koros replied that membranes are variations of that idea, which are easier to process. Usually, depending on what the hydrocarbon is, it is possible to have the material tight enough that it won't allow large molecules in. The membrane already does part of the separation, and it acts as a sort of a raincoat for the membrane that is doing the fine separation. "Now, in terms of being able to use a pure inorganic or carbon, I won't say that that will never happen. I am afraid that what has to be done is, we need to get onto the field with some technology that actually works, so that people don't invest in these high energy intensive things," Koros said.

GREEN CHEMISTRY FOR CARBON MANAGEMENT

Klaus Lackner talked about the challenge of using fossil fuels, a new fuel economy, and how to intelligently and safely dispose of CO_2 produced by the world's population.

The situation of fossil fuels is precarious. If 10 billion people—the potential future global population—start consuming energy at the same rate as the United States, Lackner said that CO_2 emissions will lead to climate change on an unprecedented scale. He stated that there is a high likelihood that there will be shortages in oil and gas and pointed out that the global population has been faced with the situation of 30 remaining years of reserves for the past 100 years. "The other unfortunate point is [that] all of that oil is concentrated in the Middle East," Lackner added.

He said two problems—climate change and the end to global oil reserves—will become acute at the same time, which will occur some time in the middle of the century. He emphasized that fossil energy is absolutely vital to the economy. "It is about 85 percent of the total, and I have a very hard time seeing that, in the short term, it is going to be replaced," Lackner said.

But the scale of energy consumption is so large that it might be difficult to find alternatives. The three big alternatives are solar energy, nuclear energy, and fossil fuels. Solar energy is not likely to provide a complete substitution anytime soon; only one ten thousandth of the solar energy on earth is being used. Nuclear energy is the other big player. People argue that the uranium reserves might be too limited. However, if the technology were better, it would not be a problem, Lackner said. With current research, there is a decade or two left for the world energy consumption to use fossil fuels. Lackner projected that there will be fossil fuel for the next 100 to 200 years at a price similar to today's prices. To underscore that point, Lackner recounted South Africa's situation under embargo, a time when the country still managed to produce gasoline for about $45 a barrel.

From a raw resource point of view, Lackner argued there is no guarantee that fossil fuels will run out in this century. Unfortunately, the environmental havoc will be horrendous if the CO_2 problem is not resolved. This means that the fossil fuel cycle has to be engineered; products must be benign and safe, either for use, or for ultimate disposal. It also means that fuel has to be produced from *all* fossil resources, and advances in gas to liquid and solid to liquid transformations must be made to bring prices down.

Disposing of the carbon dioxide is a major challenge, Lackner said. Lackner stated his point of view that any chemical returned to the environment should be in its ground state. This requires a thermodynamic transformation from CO_2 to an even lower state, the carbonate form.

The amount of CO_2 in the atmosphere is increasing. In 1800, it held about 550 gigatons of carbon. It is now in the 750 gigaton range. Current consumption of fossil fuels is about 600 gigatons per year, which is equal to the entire standing biomass. But it is not clear if fossil fuel use will increase by three or four times as much in the coming century. Nevertheless, the CO_2 output could potentially amount to orders of magnitude that are huge compared to soil and biomass content. It is already large compared to the storage capabilities of the ocean. In other words, there may be 39,000 gigatons of carbon dioxide dissolved into the ocean, but it cannot be removed or added without drastically changing the pH of the ocean. A pH change of 0.3 would be equivalent to roughly 1,200 to 1,400 gigatons of dissolved CO_2.

Some hypothetical disposal grounds for CO_2 are the ocean, biomass, and the soil. If 30 percent of the ocean's volume were to be acidified, it would cover some fraction of CO_2 disposal, and if biomass could be increased by 50 percent, the disposal of carbon in soil could be increased by another 30 percent. None of these options are ecologically acceptable, feasible, or practical with current technology, Lackner said, and that still wouldn't come close to covering the emissions if business ran its course as usual.

Even in a no growth scenario, CO_2 will be a huge problem. The last 200 years has produced 300 gigatons of CO_2, and there will be another 300 gigatons released before 2050. "So, this, in a nutshell, is the problem. The fossil carbon pie, in some sense, is rather limited," Lackner said.

To cope with these problems, Lackner said all three major energy options had to be left open since current solar capacities could not be counted on as a full replacement strategy. Nuclear energy, on the other hand, is far too complex and too expensive to replace fossil carbon. "We simply cannot abandon in the foreseeable future the one option which currently works, but I don't want to belittle the problems," Lackner said.

This still requires massive changes. An entirely new energy industry has to be built, and CO_2 emissions between now and 2050 must be held constant. It also means the establishment of an energy economy at the current, or double the current, size that will not emit CO_2 while simultaneously allowing the current CO_2-emitting energy economy to exist.

Lackner cautioned against depending on rising efficiency. "If you throw every efficiency and every trick in the book into this game, you might be able to hold things constant until 2050. The problem is, at that point, when the options run out and CO_2 levels start rising again naturally, the effect is effectively zero by the end of the century," Lackner said.

This is why there is a need for new technologies to keep CO_2 levels constant. CO_2 has to be collected and disposed of at the big concentrated sources in a permanent and safe manner. At the same time, CO_2 has to be captured from the air in order to deal with the waste produced by the transportation sector.

Lackner then discussed the options for disposing of carbon dioxide. One of the proposed routes is storing it in the ocean. Since the oceans will simply acidify, Lackner said that idea has been discredited. Furthermore, the turnover requires an 800-year time scale, which means the greenhouse gas problem is merely postponed to be dealt with by future generations.

The second option is to put CO_2 under the ground. This is done today, as the United States buries some 20 to 30 million tons of CO_2 for the sake of enhanced oil recovery. CO_2 can also be pumped on to coal bed methane or into saline aquifers. Most people suggest 300 gigatons of carbon can be stored in these ways. "But by the scale we are looking at, this is not enough," Lackner pointed out. Furthermore, there needs to be a minimum of 10,000 years in securely storing the carbon.

The third possibility could be going to the thermodynamic ground state. Carbonates are in a lower state than carbon dioxide. Carbonic acid dissolves serpentine rocks, and the serpentine reacts, forming silica and magnesium carbonate. It is an exothermic reaction, producing about 63 kilojoules per milliliter and giving free energy points in the right direction, even with ambient CO_2.

But there are still some drawbacks, Lackner said. While the reaction is spontaneous and will stabilize itself, it takes about 100,000 years to occur. As a result, there is a need for an industrial process to bring the reaction time to under an hour. Claiming the rock and dealing with metallics are both affordable. Reclaiming the mine is also affordable, and all this can be done for less than \$10 a ton for CO_2, but the reaction is simply not fast enough. Using energy would be self-defeating, but at this point, with a 40 or 50 percent energy panel, it can be done for \$100 per ton of CO_2. That is a factor of three or four higher than the desired cost of about \$30 per ton of CO_2, "at which point you add maybe two cents to the kilowatt hour and about 25 cents to the gallon a gas," Lackner said.

There is a need for the right catalyst and the right preprocessing step. Lackner suggested using a weak acid to first dissolve this material, making the magnesium salt, and then switching it to the carbonate to recover the acid. The weaker the acid, the easier it is to recover, but it also corresponds to a smaller reaction rate. Determining how to gain another factor of three to five, perhaps even ten, in this process would make all the difference between success and disaster, Lackner said. From a policy point of view, it is absolutely critical because it signals an open door. "The only one of the methods which… opens the door to the next 100 to 200 years is this dramatic step of forming carbonates," Lackner stressed. There is plenty of peridotite rock, which contains olivine, serpentine, and magnesium silicates. Oman alone has more serpentine than would be needed to deal with all the carbon reserves in the world, but it is highly distributed all over the world, Lackner said.

The obvious place to store CO_2 is in power plants, Lackner said, which could also be hydrogen plants. Since hydrogen is likely to come from fossil fuels for a long time. Lackner estimated a price range in gigajoules of energy for various fuels to back this prediction. At a gigajoule, coal on average usually costs less than a dollar. Oil is $6 per gigajoule at $30 per barrel, and electricity, at five cents, is $14 a gigajoule. If hydrogen is to be made from electricity, the cost will be at least $20 a gigajoule for hydrogen. From natural gas or coal at today's prices, it is $6. The obvious prediction is that hydrogen will be made from the cheapest source—coal. Hydrogen can also be derived from tar, coal, shale, or biomass, but it is very unlikely in the foreseeable future to come from wind, photo well tanks, or nuclear energy. "Unless you put on your burner one cent a third kilowatt hour, which I think is an achievable goal for photo well tanks in the long term, you cannot make hydrogen from it," Lackner said.

Bypassing the CO_2 problem by using windmills may not be possible. The energy that feeds the wind is about 20 times the energy the world consumes today. It is not clear how much wind energy can be harvested without having an impact on the wind field and thus perhaps on climate. Furthermore, a windmill would require at least 80 square meters of rotor-swept area in order to supply enough energy for a single person in the United States. In comparison, the CO_2 output per person would flow through an opening the size of a television screen. Therefore, a device to capture the CO_2 produced per person would be a factor of several hundred times smaller than one to collect wind energy for that same person. With the ability to capture CO_2 from the air comes the option of either making hydrogen from fossil fuels and collecting the CO_2 at the hydrogen plant or running your cars on gasoline and capturing an amount of CO_2 from the air that compensates for the emission. In addition, if renewable energy becomes affordable, it is possible to create synthetic carbon-based fuels from CO_2 and H_2O by using the energy to reduce carbon and hydrogen.

Even hydrogen might not be feasible. If the cost drops to $30 per ton of CO_2, hydrogen will still not be competitive because the distribution system for the hydrogen will be very expensive. If hydrogen is piped from a central power plant which collects its own CO_2 to destinations across the country, it will cost a lot of money.

However, the dream of the hydrogen economy is to close the loop and have a renewable energy source to split water into oxygen and hydrogen, giving hydrogen to the consumer who then recreates water. If CO_2 can be captured from the air, the same loop is slightly more complicated. The CO_2 and hydrogen can be used to run an old-fashioned fissure trough to make gasoline. This means the ability to capture CO_2 may actually open doors for carbon in any of its hydrocarbon forms to become an alternative energy carrier. The world may then no longer need fossil fuels if this alternative energy carrier to hydrogen can be used in a vehicle.

The future might hold a spectrum of pure carbon to pure hydrogen and, in that spectrum, there is a fuel of choice that can be oxidized. "At the point where you use it, you make CO_2 and water, and you give it back," Lackner said. In a situation where it is very easy to obtain hydrogen for an application—for example, a city bus in a bus fleet—hydrogen might be preferable. This opens up a whole new chemistry of sorting out what fuels are appropriate for the right circumstances and how many different ones can be supported.

New power plants, recovering CO_2, and the chemical transformation of CO_2 into a stable deposit, will all open doors. But there will have to be an energy revolution in the next 60 years. "If we did what we did the last 50 years, which was essentially doing the same thing slightly better, and incrementally more and more and more of it, we cannot repeat this for another 50 years," Lackner said.

E

Summary of Workshop Breakout Sessions

SUSTAINABILITY SCIENCE AND LITERACY

1. What is the intellectual and conceptual content required to form a solid educational foundation on which green chemistry—and other (related) sustainable research and technology—might rest?

General/philosophical/ethical

- Adopting an obligation to leave our descendants a habitable planet
- Making decisions on the right time scale in order to influence change.
- Knowledge and basic awareness of the environment we live in—
- Presenting an appreciation for nature to a generation that accesses information through electronic media
- Understanding ethics and how they create barriers
- Awareness is needed before literacy.
- Teaching complexity at multiple levels.
- Taking advantage of the introductory level of complexity found in children's curiosity to begin teaching about sustainability.
- More effectively building on what adults already know
- Present sustainability message from corporate leaders to customers, shareholders, employees.
- Knowing who the relevant "public" is that needs to be reached and provide them with simple evaluation tools for making decisions.
- Teaching cycles (economic, life, etc.) assessments at many levels
- Understanding of interacting systems and the ability to look at

things from a systems perspective— at all educational levels and for policy makers

- Understanding what function product ultimately serves and how will it be delivered

Chemistry

- Effectively conveying the basic fundamentals of chemistry and chemical engineering to the general public.
- R&D facilities awareness of green chemistry at the corporate level
- Understanding that chemistry is not going away, but is disseminating into all other disciplines.
- Providing more chemistry for engineers—a better understanding of chemistry and product design is needed.
- Incorporating a sense of design and systems perspectives into the chemistry curriculum. .
- Introducing the life cycle component into chemistry and chemical engineering thinking.

Business and Economics

- Presenting economics as an essential element of literacy—which drives industrial production.
- Understanding of perceived benefits and perceived risks
- Understanding how industry operates.
- Identifying Markets.
- Customer understanding of green chemistry and sustainability in order for there to be a "pull-through" effect—analogous to the construction effect. (People want "green" houses because they understand the benefits—both social and environmental—that come with living in them. This drives the construction of "green" houses.)

2. **What do the informed engineer, chemist, and other related subfield specialists (not to mention business, law, and medicine practitioners) need to know that current educational institutions fail to communicate?**

- Holistic Approach
- Systems Integration
- Life Cycle Assessment
- Sustainability Ethics
- Multidisciplinary Education/Course Content
- Relation to the Industry
- How to Cope with the Industry Demand

- Toxicity & Eco-Toxicity Concepts
- Problem-Based Approach

3. How might this foundation be continuously expanded as we move forward in order to stay current with rapid technology advances and new science applications for design, process, and products?

- Understanding of biological organisms as chemical producers
- Understanding the waste balance between human and environmental generators

4. What are, and what explains, the key areas of resistance to introduction of sustainability research and technology into materials and product design as well as educational curricula?

Culture

- "culture eats strategy for breakfast every day of the week"
- Lack of support from accreditation agencies
- Inertia in an aging industry–"why change?"
- Perception that green chemistry is not "real" chemistry
- Stovepipes
- Lack of understanding of the importance of sustainability
- Multidisciplinary and cross-functional nature
- Question is currently not natural
- Need individual incentives to adopt sustainable practices; incentives will be different for individuals in different roles
- Lack of acceptance from students, who are worried they are not going to learn what they need to get into medical school or other programs
- Inherent problem with long-term thinking (intergenerational issues) and with definitions that tend to raise value issues that are difficult to handle
- The ethical question is a bigger question–more so than the science and technological capabilities.
  - One cannot divorce ethics and S&T; we must consider tradeoffs in making decisions. How do we begin to arrive at making these choices?

Money

- Funding constraints at federal, state, etc. level
- Unwillingness to pay for green chemistry
- The need to design for economic competitiveness and profit must be considered when developing sustainability practices and form-

ing regulatory rules. Otherwise, the willingness to be clean will be absent.

- Perceived lack of financial incentives
- Slowness in the turnaround time for economic payoff for green chemistry

Metrics

- Inadequacy of societal impact evaluation
- Lack of metrics

Structure/Nomenclature

- There is no clear definition of green chemistry to articulate to people outside of chemistry. We need a clear definition of green chemistry to allow us to talk to different audiences.
- Perhaps we should refer more often to "sustainable products and processes." "Green chemistry" may be too narrow a term
- There is also disagreement about whether green chemistry should be a separate discipline or if it should be a framework for addressing chemistry
- Complexity itself

Other

- Do environmental implications challenge creativity?
- What we perceive as green now may not be so in the future—how do we avoid the case of CFCs?

5. Where should efforts be targeted if sustainable research and technology are to be incorporated into the chemical industry? Should it be towards consumers, student chemists/chemical engineers, and other scientists in training, business executives, MBA students, etc?

General

- We need to communicate the complexity of sustainability and the web of life. Perhaps engage the artistic community? In other words, we should try to reach an audience who is scientifically less-knowledgeable.
- The scale of the effort differs for different audiences (e.g., chemist vs. process engineer).

Business/economics/corporate leaders

- The thinking around sustainable consumption needs to be coupled in a systems way.

  - We need to demonstrate that the ability to make profits does not disappear with green chemistry.
  - This message needs to reach consumers, business executives, and middle management.
- CEOs can set the tone. Real leadership provides resources to back up its words, and this would provide incentives if the market for such thinking exists (e.g., hybrid cars).
- We need to convince leaders of the business/leaders of production of the economic and environmental benefits of sustainability.
- Purchasing agents in chemistry should be targeted for education.

Future practitioners/Research Community:

- We should take advantage of the tremendous opportunity to train at the undergraduate and graduate level. Currently, industry is doing all the training.
  - There would be more incentive if sustainable skills are in demand at the Ph.D. and undergraduate levels.
  - We should also think about educating K-12 students
- Types of thinking skills that should be taught:
  - Critical decision-making tools
  - Technical skills
  - Systems-wide consideration in thinking skills
- Universities can also play a role in sustainability education at the high school and middle school level. Unfortunately, this topic is not on everyone's front burner.
- Business Schools

Current and future consumers

- There is a tremendous lack of understanding among consumers about sustainable products and processes.
  - E.g., market for organic foods, genetically modified crops
  - Who is responsible for educating the consumer? How is it done, and how should it be funded?

Government

- The government needs to get involved in raising public awareness and enthusiasm for sustainability (e.g., the space program/Sputnik).
- We need to educate legislators and tailor the message to different audiences. The issue of complexity needs to be introduced within this message.

Professional societies and Nonprofit/Nongovernment Organizations

- The topic of green chemistry is missing from ACS's 2015 visioning exercise.
- Relations between nonprofit organizations and industry should be established or improve (e.g., GreenBlue Institute).

6. What, if any, policy can be implemented to encourage better degrees of sustainable chemistry and chemical engineering practices?

"Carrots"
Culture/leadership

- Create a culture that reinforces the message of sustainability (e.g., procurement, buildings, preferred purchasing, etc.). People respond to aspirations, goals, and positive rather than negative messages.
- Can we learn from nano- and biotech (HGI?) initiatives?
- Offer awards and monetary incentives for improving or practicing sustainability (e.g., targeted gifts for universities).
- Reward partnerships between government, industry, NGOs, and universities. Facilitate interdisciplinary research and interactions.
- Determine how to improve profitability in sustainable practices.
- Develop a sound intellectual property position.
- Determine how to reduce liability.
- Reduce the regulatory burden (industry).
- Compare U.S. efforts on sustainability with other international efforts.

Education

- Develop an NSF-IGERT-like program for sustainability research and practices.
- Form sustainability centers (e.g., GUI partnerships, centers for product design, Shell center for sustainability at Rice University).
- These centers need to be centers of excellence, working on key problems.
- Include NGOs
- Increase recruiting capacity.
- General information: The EPA is performing a benchmarking of sustainability in all engineering departments.

Green chemistry can be used to innovate and make new products and compounds that other methods can not. This will create markets and drive green practices.

- Meet downstream consumer's demand.
- Provide green chemistry federal funding.
- Incorporate green chemistry into regulation—to create an opportunity for innovation.
    - Create capacity and willingness to change through an effective regulatory environment.
    - Improve the management of chemicals in commerce.
- Complexity is inherent in whole systems. To determine where decision points lie in chemical processes and reactions, one first needs to understand this complexity.
- Elevate green chemistry to the level of green engineering. This brings us to systems-level understanding that is more easily measured through metrics. It also allows us to begin acquiring the ability to make comparisons of whether one thing is more sustainable than another.
- Understand toxicity. For example:
    - Look at the need for chemicals within different products (e.g. flame retardants within furniture).
    - Examine the use of adhesives (formaldehyde vs. bio-based).
    - ACC and EPA have an agreement to screen HPV chemicals.
    - We should examine the EPA-IRIS system. We need to have information management, comparison metrics, and other consistent ways to convey information.
- We need to address the lack of information on chemicals. How do we obtain it? The lack of data is one of the drivers for REACH.
    - Europe is phasing out chemicals, but without much thought for the ramifications. For example, what are the broader impacts, what will the replacements be, and what are the impacts of those replacements?
    - Problems lie in regulation by people with only cursory knowledge of the issues. For example, the MTBE decision was made by legislators (and the population at large) for reasons that were not scientifically based.
- Why are some educational departments developing curriculum and others aren't?
- How do we move green chemistry and sustainability into commerce? Green chemistry may be a tool to move society and trade towards sustainability.

"Sticks"

- Mandated green chemistry courses in universities—degree requirements vs. integration of subject throughout the curriculum.
- Purchasing policies:
  - Mandated government and university purchasing
  - Leadership purchasing programs
- Green Tax Reform
  - One potential idea: introduce tax credits to encourage sustainability
- Greater penalties for mistakes

ENABLING TECHNOLOGIES THAT DRIVE THE APPLICATION OF GREEN CHEMISTRY AND ENGINEERING

Introductory Discussion/Commentary: What are the enabling technologies that drive the application of green chemistry and engineering?

- There is a need for good metrics in green chemistry; we do not have the ability to address, or to assess, whether changes are made for the better.
  - How does one measure progress?
    - We first need to know what measurements are important.
    - We should also try to have metrics from the chemical level to the systems level
    - Whenever you have metrics, you must have a system in mind or one that is already defined.
  - What's the next frontier for life cycle?
  - Tools are needed to determine prices of chemicals and related products. The chemical industry is not so concerned with toxicity or environmental impact because they have developed technologies to control these risks.
  - There must be a way to use current knowledge to help make better decisions for today and the future. Today's decisions should not be based on the past.
  - There is a need to gather, list, and prioritize hazards, but current abilities to accomplish this are very inadequate. The ideal steps of metrics:
    1. Gather, list, and prioritize.
    2. Replace.
    3. Update continuously.

Suggested table for identifying metrics:

For whom?	For what purpose	At what physical scale	At what timescale
Government	human safety, natural systems stability, to guide regulation	Physical: Technology, institutional, regional (e.g., watershed), global	Today vs. Tomorrow- person to-global
Business (Supply chain, Company, Product)	compliance, etc . . . ultimately to create innovative solutions to be successful economically		
Education	Awareness, intelligence, integrity —well-trained		
General Audience—Public			

- The desire to reduce information down to a single number is not useful; it creates value that may provide useful information. We should be able to deal with large amounts of information (e.g., nutrition labels, etc.) where we can weigh trade-offs.
- Heine's table visualization (from her presentation) is useful. Perhaps perform a similar exercise in consideration of what makes a successful proposal at NSF, e.g., pattern recognition.
- Categories and taxonomy of impacts are needed:
    - Include examples of bench-level activity that seems small scale but could have significant large-scale impact (e.g., photovoltaics).
    - Is it valid to evaluate the intrinsic toxicity of a material's molecular content?
    - Context is also important; a benign chemical can be used inappropriately.
    - Example: Progress would be made if the photovoltaic industry incorporated green chemistry principles (use benign chemicals, etc.)
- Global Impacts: Europeans and Japan are very far ahead of us on thinking about green chemistry metrics and life cycle analysis

(LCA), but how they utilize the information is not necessarily beneficial (going to single score).
  - Global standards set by other countries will impact trade.
  - The U.S. also has to create our own culture. Currently, California leads sustainability thinking and policy, and the rest of the country follows.
  - The potential that current chemicals may be deauthorized under REACH is an extremely effective driver for industry. There has to be a real incentive to scale from the benchtop chemical processes considered to be business risks.
  - In addition, any research investment by the U.S. government over the next 5-15 years must be conducted with a comprehensive understanding of what has happened and what is happing in Europe (REACH).
- Education and Public Perception
  - There is no degree program in LCA; colleagues are going to South Africa and elsewhere to get degree.
  - There is a lack of communication between subfields; the design aspect is usually assigned to engineers, while the molecular aspect is assigned to chemists.
  - Look at models for collaborative research:
    - ✔ Collaborative Research in Chemistry (NSF) brought many disciplines together to solve complex problems. Are there a sufficient number of scientists to do this?
- Motivation for Better Policy and Research Funding:
  - Thinking green globally helps us to recognize where our shortcomings are and leads to needed research —to the enabling technologies.
  - There is a growing consumer concern about chemicals in the environment, especially as it relates to health.
  - The market fails to deal with the externalities (e.g., impact of ethanol). Products should be priced according to impact on society.

1. What tools are required to identify shortcomings in chemistry or chemical engineering in terms of reducing environmental/health risks?

These tools should allow us to:

i) prioritize areas or activities requiring better sustainability (strategical products, independent resources, . . .)

ii) identify these area/activities from different perspectives, including economical development (local, national)
  - environmental security (fixing problems; improving situations)

- long-term quality of life (cultural, societal) for surroundings

Research Tools:
- Molecular design tools
  - What is the structural relationship to function?
  - Address the disconnect between macro and micro scale.
- Transformation toolbox
- Separations
- Assessment (LCA, scenario tools, etc.)
  - Lack of standardization in the compilation of data mean that different research results can't be compared.
  - Performance metrics and decision trees for making the right decisions
  - Consideration of the environment in which the design is to exist
- Prediction tools (toxicity, bioactivity)
  - Chemists need to access chemical toxicology information earlier during the product design process.
  - The EPA ecotox database may be sufficient but is relatively unknown to chemists and chemical engineers.

Research Grand Challenges:
- Switches in stability/ the ability to turn on instability
- Physical advantage of heterogeneous/selectivity of homogenous catalysis
- Elimination of batteries
- Elimination of toxic chemicals in everyday products (lamps, computers, etc.)
- Incorporation of toxicity training into research
- Safer energy – photovoltaic technologies that are safe
- Diversify the feedstocks (e.g., CO_2)

Policy
- We need mechanisms or tools to provide incentives for industry to incorporate sustainability into chemical processes and products. Should industry or society by targeted initially?
  - We should educate consumers so that they make better sustainability decisions.
    - ✔ Sell sustainability to the public.
    - ✔ Sell positive messages to kids about sustainability.
- Agreement upon important values and standards for public policy research are needed.
- Scientific proof vs. peace of mind.

2. What kind of guidelines should be incorporated into the LCA to which every process and product should be subjected before it is commercialized?

Suggested impacts include:

- Resource accessibility, disposal, and renewal
- Energy production and renewal
- Product manufacturing, including production conditions
- Product end-of-life analysis (impact of disposal) and after-life management (waste treatment and recycling)

- There should be a clear delineation of assessment boundaries:
  - Is tire wear of the truck that brings coal to the electricity plant counted?
  - Guidelines are different for products/materials (e.g., end-use consumer products vs. chemicals).
  - Does the boundary include the use phase?
  - There is a need to understand the definition of the product. For example, do we assess a whole tractor, or do we count the reuse of the indestructible engine?
- Different languages or measurements are required for each leg of the stool. We need to put these externalities on a common basis, such as dollars, so that they can be traded off one for the other.
  - E.g., value of a quality-of-life year—This can be valued very differently from country to country.
  - How is allocation amongst multiple products in one facility measured?
  - How is allocation of ancillary benefits measured?
- What is the set of environmental impacts that should be considered in the LCA? This requires information on interactions between environmental factors (law of unintended consequences). We will need to bridge the disciplinary divide between engineers and environmental scientists to develop these.
- Who sets the criteria for final decisions? Values, ethics, etc.
- Tools need to be global in their scope and considered beyond an American-centric type of thinking.
- A qualitative approach may be more desirable. (Ask the right questions)

Criticisms of LCA:

- Utilization of LCA in the chemical industry is critical but not feasible at this time.

- LCA analyses are proprietary; one can only make an assumption of results.
- LCA is not being widely used.
- Results from LCA were found not to be credible or useful to most companies.
- Data from LCA expires; there is poor data quality (supply chain data).
- Products not regulated by compliance are not measured by LCA.
- LCA is a good comparative tool, but it can be misused as a design tool.
- There is no such thing as a "final" LCA—inputs can change (i.e, energy costs).

3. What are the priority problems that routinely come up during the life cycle analyses of chemical products? What alternatives could be suggested for meeting these problems?

Priority Problems:

- Strategic approach of LCA in terms of:
  - Validation of the methodology
  - Priorities
  - Management of unknown parameters
  - Criteria for LCA values
  - Risk assessment—agreement on acceptable risk, evaluation, communication.
- Validation of the LCA process and control of the data implementation
- Failure to capture systems level impacts
- Data as the limiting factor—Uncertainty is dictated by the amount and quality of data.
- Visualization/viewing of the high dimensionality of the data in a manner that is understandable
- Quantitative vs. qualitative data for LCA
- Where does green chemistry fit into LCA?

Suggestions to Improve LCA:

- Perhaps we should broaden the scope of LCA (for example, to capture social and cultural values).
- In the pharmaceutical industry, values are governed by human toxicity (one species), backed up by rat and mouse toxicity data.
- Research dollars should be focused upon data collection for LCA. Data collection needs to be a coordinated effort. The data is avail-

able, but it needs to be inventoried. We need a central, refereed source of data

- We need heuristic tools to guide the boundaries of data for LCA.
  - We need a standard format for delineating what is entered and what is obtained from LCA.
  - Agreement is needed on a weighting system for various components of the analysis.

4. To assess the health and environmental impacts, how can the following problems and issues be resolved?

Development and validation of new assay methods, including computerized approaches, to enable human and ecosystem toxicity evaluation

- Encourage cross-talk between industries.
- We should develop the ability to predict life cycle profiles, including toxicity values, based on a priori models.
- Again, this is limited by the quantity and quality of data available.
- *For future consideration*: what about secondary interactions (e.g., synergy)?

Identification of priority compounds, including assessment of quantities, long-term effects vs. environmental half-life, etc.

- EPA has recognized the need to begin this task.
- How are compounds determined to be toxic? What is the process by which these compounds are identified?
  - Who are the leading toxicologists? Are they in academia or industry?
  - The different fields need to interact—more crosstalk with the chemical community, joint training programs are needed.
- Development of high-throughput analytical methods to measure toxicity and other chronic and multi-generational effects.
  - Screens, especially the reference materials used as standards
- Develop alternative methods of measuring toxicity and other impacts.
- Develop modeling that analyzes systems level impacts. There is a need for large-scale system modeling.

Risk assessment methodologies, including incorporation of missing data

- Better/more toxicological data.

Solutions to the mixtures problem (deviation from the additivity rule)

Measurement of environmental impacts (methodology, parameters, food chain contamination, …)

Adequacy and availability of technical solutions to environmental impacts, including actual R&D developments)

- We need to balance negative effects with positive impacts.
- We should trace materials in effluents of wastewater treatment plants
- Under what circumstances should a state-of-the-art LCA be required? Currently no standard exists to evaluate these circumstances.
- What are best practices?

Final Discussion/Commentary:

- MSDS sheets not useful for chemists. Do we need a separate environmental sheet? It may depend on data content
- Source Database contains carcinogenic information, etc. of all compounds.
- Green chemistry database consisting of what happens from production to dispersion into the environment.
- Suggestion: workshop on Grand Challenges in Green Chemistry
- Before conducting this workshop, address grand challenges in chemistry to connect molecular structures with material products.
- Methodology from Bhavik Bakshi (professor at Ohio State University).

NEW CHEMISTRIES AND PROCESSES THAT LEAD TO COMMERCIALLY VIABLE ALTERNATIVE FEEDSTOCKS TO FOSSIL FUELS

1. What plant derived feedstocks and building blocks provide the most viable alternative to fossil fuels?

Plant-derived feedstocks and building block suggestions

- Energy cane may be utilized. New plants should be constructed near the sources of these feedstocks.
- Hydrothermal depolymerization allows the use of carbon wastes which, when mixed with hydrogen, can be converted into useful fuels.
- Other brainstorming ideas:
  - Algae as a viable feedstock
  - Soybeans, corn, and sugar cane (from DOE workshop)
  - Corn stover (pre-treated)—best for fast commercialization
  - Lignin—can be broken down into useful aromatics, may give

rise to a new industry as well as providing substitution for current chemicals (e.g., vanillin)
    - Peanuts
    - Potatoes
    - Beet pulp
    - Manure (e.g., animal waste in general—pig waste, chicken waste) and other rendered animal by-products—may need to use caution, particularly with BSE concerns
    - Chicken feathers (6 billion lbs/yr)
    - Jatropha (a type of tropical tree)—may be grown in Florida, other tropical climates.
    - Waste stream from agriculture—see hydrothermal depolymerization suggestion above
    - Tobacco
    - Urban Solid waste (pre-sorted)
    - Flax (as a waste by-product)
    - Oil seeds
- Perform a technology assessment to determine the downstream consequences of developing the aforementioned options.

Ethanol Issues
- Scientifically, should ethanol be our focus? Is it currently driven by politics?

Biomass Issues
- Burning agricultural residue for energy needs may be a better near-term goal (e.g., palm oil, sugar gases, husks from palm oil).
- How should we address the seasonality issue of biomass production against the year-round need for products?
- Flexible infrastructure and processes may allow use for multiple types of biomass.
- Can biomass production be linked to restorative technologies, such as water hyacinths and "energy cane?"
- The high moisture content of biomass is problematic; we need drying technologies to help deal with this issue.
- Biomass economics are still strongly linked to fossil fuel economics

General Comments
- Is there enough information available to identify plant-derived feedstocks? Should further research be performed to make these decisions?
    - Gather research experts in this area to collect information.
    - There is sufficient information to identify substitute feed-

stocks for fossil fuels. To identify feedstocks and/or processes for specific platforms, more research may be needed. (Biochemistry, microbial information are potential research areas.)

- The U.S. vs. global economic outlook makes a difference.
  - U.S. tariffs exclude Brazilian cane-based ethanol.
  - Cellulose is not cost competitive on its own merits.
- We need to investigate economic options, such as new incentives and risk reductions for industrial investment.
- Most technologies are niche or regional technologies. This may have to be the approach; perhaps there is no one-size-fits-all strategy. This may involve significant changes in business models with a more distributed infrastructure.
- Perhaps we should focus on compatibility between fuels with the current infrastructure. However, the current infrastructure is also a burden.
- Diesels have particulate problems; this may not be the best focus for long-term efforts.
- The best products from alternative feedstocks will depend on the particular feedstocks utilized.
- Systems analysis are required to determine the best inputs, routes, and products—emphasis should be placed on research challenges that must be met to enable such analysis.
  - Extracting materials from very dilute solutions (e.g., boiling off water) becomes an energy issue. We need total LCA or LCI.
  - Has LCA been performed on alternative feedstocks to compare them to the current (petroleum-based) processes?
  - PLA has been compared to nylon, PET, etc. using LCA. LCA is useful in identifying weak points in the processes (e.g., farming practices).
  - What should be the demarcation points for LCA analysis?

2. What new chemistries and processes will enable the use of plant-derived feedstocks and building blocks as viable alternatives to fossil fuels?

- Engineered microorganisms to allow new bioconversions, e.g., how can the top 10 chemicals be produced biologically?
  - Investigate whether a systematic approach exists towards using microorganisms for recovery of higher-value chemicals from bio-based feedstocks
  - Biocatalysis and enzymology

- Metabolic engineering and energetics: more research in metabolic pathway design and construction is needed.
  - This will require both biology/biotechnology and chemistry research. It will involve a better collaboration between these disciplines.
- Energy-efficient water removal and other separation technologies
  - Recovery of organic chemicals from aqueous/fermentation solutions
  - May be process-dependent
- Green chemistry alternatives to production of large volume materials such as solvents, salts, acids, and bases. This may involve:
  - Green transformations from defined platform chemicals
  - Green transformations using alternative technologies
- Source separation—paper vs plastics, etc.
- Identification of technical nutrients, ie., things that are not biodegradable but can be recycled numerous times
- Development of methods to obtain sugars from carbohydrates (hydrolysis of cellulose)—a large limiting step
- General lignin chemistry/convergence
  - Recovery of aromatics from plant lignin
  - Establishment of research centers to address this problem
  - Reference: John Frost (fermentation research)
- Development of pre-treatment chemistry or of processes that eliminates the need for pre-treatment
- Advances in fuel cell technology (e.g., methane instead of hydrogen, which may create a use for urban waste)

General Discussion and Comments

- What does viable mean? From what point of view?
  - Use of this technology may cause greenhouse warming (true for any carbon based fuel).
  - CO_2 by-product must still be handled
  - We must develop a carbon-neutral fuel (e.g., hydrogen)
- We must perform cost-benefit analyses to examine economic trade-offs. Studies should be robust and standardized.
  - Strategic study should not be constrained by short-term economics, benefits, and risks.
  - Cost-benefit analysis
- Compare the quantity of water use in bioprocesses relative to that used in fossil-based processes
- Perhaps NSF and other government agencies should establish programs to fund this type of research.

- Example: DOE program to promote development of building blocks from carbohydrates, lignin, and vegetable oil

3. Are there green chemistry options?

Improve energy efficiency: devise efficient designs for

- Industrial processes
- Building construction
- Transportation materials
- Insulation materials
- Development of new catalyst systems in bio-refining

Lower toxicity

- Understand the environmental fate and effects of producing/using new chemistry from a toxicity perspective.
- Perform life cycle analysis (LCA) to determine if an approach is intrinsically "green" and how to optimize it.
- Include the final downstream products produced from the platform chemicals.

Improve recycling design and implementation

- Perform extractions and separations where solvents are recycled or supercritical fluids are used.
- Incorporate biomass from agricultural resources as a feedstock, which can safely be returned to the environment.
- Use energy cane, which also stabilizes soil erosion.
- Formulate a Top 10 DOE wish list

Economic analyses

- Determine what the sensitivity of the current systems are to petroleum costs:
    - Are there infrastructure costs that will rise as the petroleum costs rises?
    - Is the system in question resistant to the inflationary consequences of rising petroleum costs?
- Evaluate the effect of a subsidy on gasoline; determine the impact of biomass-derived fuels and whether support can be directed away from petroleum.
- Reevaluate large processes (i.e., paper industry) in light of green chemistry principles.

4. Which areas of application require the most attention, or will provide the greatest opportunities (e.g., specialty intermediate and complex molecule synthesis)?

Focus should be placed upon:

- More efficient/less energy-intensive conversion of lignin to aromatic molecules via better catalysts/enzymes
  - Lignin applications: burned as fuel for pulp mills
- Process intensification; for example:
  - Continuous fermentation
  - Simultaneous saccrification and fermentation
  - Separation processes (e.g., removal of alcohol as it is produced to avoid reaction inhibition)
- Biotechnology; examples include:
  - Extremophiles (e.g., cold tolerance)
  - Genetic engineering of plants
  - Genetically modified goats that produce pharmaceutical drugs
- Biofuels (bio-ethanol, bio-diesel, etc.)
- Biofilms
- Conversion of biomass directly to heat and electricity as well as higher-value applications:
  - If efficiently performed, this could significantly reduce petrochemical productions.
  - However, although this is very efficient, it is also the lowest value output from the biomass.
- Replacement of the most hazardous materials and processes with greener alternatives.

Breakthrough technologies

- Production of large volumes of clean, pure, and simple molecules from biomass
- Improvement of CO_2 sequestration and possible utilization of it as a value added commodity: does a form exist where CO_2 can be sequestered in a safer or greener manner than dumping/burying it?
- Low-energy separations in aqueous solutions (this research is vastly underfunded).

Discussion/Commentary

- We should target the “low-hanging fruit,” which is dependent on the target goal (energy reduction, recyclables, utilization of biomass to replace fossil resources).

- Also, what are net sustainability impacts? For example, where do the petrochemicals go if they are not being used to manufacture chemical products or gasoline? Will there be a net gain?
- Feedstocks originating from biomass are different from existing feedstocks. They will enable new products and chemistries and produce molecular diversity.
  - Basic chemistry research will be required. (Potential question: what can one do with these novel molecules?)
  - Products and their use will be based on available plant materials.
  - New plant-based materials may be engineered or bred.
  - What should be done with residual biomass?
  - We also need to consider how to replenish the soil for sustainable production of biomass.
  - Perhaps consider applying biomass feedstocks to chemicals production.
- Inventory chemicals present in biomass to determine available opportunities (e.g., taxol)
- Is there enough dialogue between academia and industry?
  - Academics should be allowed to work on fundamental research for the sake of knowledge. Applied research will result from discoveries.
  - Industry should be brought in early in academic research.
  - Relationships within the chemical industry must be strengthened.
- Investment in sustainable research and development:
  - Are there R&D issues that suggest a new institutional base (e.g., Sematech model)? Should institutional opportunities for collective research be established?
  - At what point is the imperative there to push investment? A social decision must be made to invest in promising "green" or sustainable sciences and technologies.
  - Given the capital investment in the plant infrastructure and the expense, we cannot expect to have new approaches coming out of the industry.
  - The industry has bought into globalization—fewer and fewer customers are willing to pay for R&D—more of a luxury—focused on solving current problems. The ability to do long term research has been reduced.
- Encourage multidisciplinary research:
  - Intermarriage of biology and chemistry
    - ✔ Several chemical engineering departments have integrated biology into their curricula.

- ✔ Emphasize opportunities for biologists and chemists to work together.
- ✔ Are there other areas of chemistry that should be encouraged for alternative feedstock research?
  - o Students do not recognize how to integrate biological processes into chemistry processes—this is an educational problem that should be addressed.
  - o Use case studies and real-life examples; AIChE encourages tying life cycle and bio-design issues into senior design project courses
- Should molecular platforms be investigated for sustainable production of chemicals?
  - o The notion of building blocks is tricky; should we use this type of plan to build up bio-based feedstock processes?
  - o We can identify the cheapest feedstocks using the idea of building blocks. The idea of using platforms and building off of them is also useful for identifying additional products and energy sources.
- Perhaps the search for sustainability should be focused on existing processes.
  - o Can more energy, products, etc. be produced out of current bio-based and alternative feedstock processes?
  - o Can additional products be derived from feedstocks that are already used?

5. What is the best way to address the regulatory approval challenges in implementing new chemistries and processes?

Research Agenda:

- Research should be focused by making a list of priorities based on chemical hazards to target.
- Develop a framework for identifying platform chemicals.
  - o Biomass to platform chemicals and fuels
  - o Start with high value materials
  - o Match availability of resources with potential applications
  - o DOE Platform Chemicals Report (*www.nrel.gov/docs/fyotosti/35523/pdf*) provides a good starting point
- Integrate these platforms chemicals into a sustainable process. In particular:
  - o Address the energy required for separations processes and operations.
  - o Determine how to extract additional high-value products from reaction mixtures

- Capture complexity from plant feedstocks.
- Perform selective oxidation/reduction reactions to accomplish goals.
- Guidelines for processes:
  - ✔ Performance
  - ✔ Genetically modified organism (GMO) concerns, e.g., "release" into agriculture, cross-breeding
  - ✔ Risk management and understanding
- Suggestion/example: Start with the simplest molecules from biomass and build the value chain of products from there.

- Examine post-process treatment of waste (ash, spent microbes): potential reuse value, disposal, and/or treatment as hazardous material
- Examine patent implications, which may restrict sharing of information.
- Address fundamental scientific challenges in a way that is economical, reliable, efficient, and cross-cutting. Challenges includes:
  - Analytical processes
  - Process chemistry and engineering, especially intensification
  - Biomimicry to harness complexity
  - Unusual chemistries across taxa: perform an examination or set up a database
  - Atom energy
  - Systematic benign design
  - CO_2 utilization, potentially as a fuel source
- Perform a risk analysis examining past, present, and future needs. Look for discontinuous changes as a opposed to incremental.

Perceptions of Sustainability

- Institutional barriers exist due to the perception of liability (e.g., garbage as a good source of biomass)
  - Perform social science research on facilitating acceptance of new technologies and new infrastructures (large compost piles).
- There is a negative opinion about sustainability; it connotes restrictive practices (a "list of don'ts"; sustainability = limits to growth).
  - This attitude is pervasive in both Congress, educational departments, and industrial companies.
  - This audience, especially legislative staffers, need to be enlightened to the fact that sustainability does mean growth.
  - Also, sell the business case for sustainability. For example, define a message: "Sustainability = yes (and then some)"

  - ✔ Profits
  - ✔ Job creation
- Does the business management establishment understand the arguments for sustainability? There is a communication gap between scientists and financial experts over sustainability.
  - Is the internal rate of return set by sustainability proponents understood?
  - What is the risk of business as usual?
  - The cost of energy is forcing companies to focus on the front end sustainability. Companies are also influenced by government programs and subsidies.

Regulatory Modifications

- Current regulations are focused on a centralized production system; examine how this must change for a distributed production system.
  - Plant site, permit, process, and zoning issues
  - State and local issues.
- The existing regulatory apparatus demonstrates a disconnect between the current approaches to regulating manufactured chemicals and the new technology being developed.
- GMP rules from FDA create barriers to new processes in the pharmaceutical industry..
  - It currently pits process specifications vs. product specifications.
  - Improved analytical techniques may make this approach obsolete.

The role of government in promoting sustainability

- Major government initiatives that are sustained over a long period of time are required. Sustained funding effort is needed.
- Congress should pass a green chemistry bill
- The government should address the need for infrastructure modifications when implementing biodiesel and biofuel usage.
- Perhaps focus on incentives rather than regulations; for example:
  - Small business incentives (e.g., ethanol model) to enable small regional chemical plants.
  - Local incentives to reduce energy usage.
  - Production tax credits, incentives, renewable portfolio standard
- Establishment of a gas tax to fund renewable fuel alternatives:
  - Potential drawback: Current gas taxes pay for highway upkeep. What would happens if these funds were redirected towards development of alternative fuels?

    - Use a small fraction, e.g., $0.02 tax on gasoline to invest in researching renewable fuels
- Establish standards, codes, and benchmarks.
    - Dramatically higher fuel efficiency standards
    - CO_2 emissions standards
- Expedite the permit process for developing sustainable processes or materials.

REDUCING THE ENERGY INTENSITY OF THE CHEMICAL PROCESS INDUSTRY

1. What is the business case for "reducing the energy intensity of the Chemical Process Industry (CPI)"?

- The reduction of capital costs will drive innovation in sustainable practices in the CPI:
- Unfortunately, the trade-off of reducing the energy intensity is higher capital costs. Higher capital costs may be justified if stockholders believe there is a benefit involved.
- Another issue: the developing world is not concerned with sustainability issues.

2. What approaches are needed to reducing the energy intensity of the chemical process industry?

- The efficiency and density of energy storage devices must be improved.
- Energy efficient separations (e.g., membranes) must be employed. Examples of important separation processes:
    - Removal of water from microbial solutions
    - Separation of active compounds from dilute solutions
- Cogeneration of energy with other processes could be devised (e.g., supercritical water oxidation).
- Highly selective chemistries coupled with improved separations are needed.
- Development of aqueous two-phase separation processes are also important.

3. Dr. Nedwin suggests the use of enzymes as one of the biotechnological answers to reducing the energy intensity of the CPI. What other biological or biomass-based opportunities deserve serious consideration?

- Production of simple aliphatics and aromatics from biomass is

less energy intensive but requires suitable separation technologies. Examples include:
  - Chemical conversion of biomass to polymers, including direct chemical conversion of biomass polymer into functional products
  - Conversion of vegetable oils to chemicals, polymers, and functional products
- Conversion of lignin to aromatics is another possibility. This is a tough problem, especially if progression beyond phenol compounds is desired.
- Whole organism biochemical conversion may be useful. However, this again raises selectivity and separation issues.
- The application of RNA aptamers for selective binding and separations might address energy-intensive separation problems. Advantages:
  - They may be optimized through selective evolution.
  - They are more easy to scale than protein-based methods.
- Other enzyme-related technologies and topics should be considered, such as:
  - Bioconversion in organic solvent-based systems
  - Generation of human metabolites from the API using enzyme systems
  - Separation applications based on selectivity of enzymes—e.g., lipases to separate enantiomers
  - Creation of a repository of information on natural enzyme sources as scientists scour the earth for natural products
  - Solids and other types of support for enzyme substrates

Other general and miscellaneous topics:
- Process industry synergy should also be considered. This involves reaching out outside of CPI, ie. collocation (using energy from pulp and paper, glass, steel, pharma,…)
- Is biotechnology a replacement technology, or does it signal an entrance into a new field or market area in which traditional chemistry fails?
- How should disposal and waste treatment of personal care products and pharmaceuticals be handled?
  - One solution may lie in programmed drug release. This would eliminate the need to separate drugs out of regular waste and reduce energy intensity of this type of separation.

4. Building on Dr. Koros's discussion of the use of membranes "as low energy-intensive enablers for energy conservation in the chemical industry," where do you see the breakthrough or game-changing opportunities for low energy-intensive separation processes for the CPI?

Membrane Applications/Technology:
- Major reductions in the cost of in-module membranes with extremely improved separation factors (by at least three orders of magnitude)
- Improvements in membrane technology for O_2 processes (to avoid poisoning, etc.)
- Development of mixed systems integrating membrane separation with adsorption
- Non-fouling or self-cleaning membranes (e.g., marry enzymes with membranes)
- Studying transdermal drug delivery of pharmaceuticals to better understand transport across membranes
- Use of biomimicry; for example, understanding:
- how cell membranes function in active transport to control flow across membranes
- how to mimic the production of bone material
- how different types of cellular membranes function, e.g. gills or lungs
- Membranes or enzymes for equipment cleaning (solvent recovery)

Alternative Technologies/Separation Materials:
- Development of ultra-selective adsorbents that can be regenerated with high efficiency and low energy input
- Application of reactive distillation fundamentals to biological systems
- Development and optimization of distillation alternatives in order to eliminate the use of heat in separation processes; for example:
    - Self-separating phases and/or products
    - Affinity chromatography
    - Simulated moving bed (SMB) and Multi-Column Chromatography (MCC)
- Application of evaporation–induced self-assembly for molecular separations (Sandia National Laboratories)
- Development of mineral-organic hollow fiber
- Development of solvent-free processes and solid-state synthesis

5. Dr. Lackner discussed several "novel chemistry, products, and processes for the management of CO_2 emissions." What other novel chemistry, products, and processes can provide effective management of CO_2 emissions? What are the R&D challenges in achieving commercialization of these processes?

Novel chemistry, products, and processes:

- Development of novel catalyst chemistries, e.g., Fischer Tropsch with CO_2
- Innovative electrolysis applications
- Direct photochemical hydrogen production
- Absorption of CO_2 from the atmosphere and general adsorption technology; for example:
    - Is there a CO_2 absorbent that will reversibly remove CO_2 from the atmosphere?
- Development and use of annually renewable resources for efficient and effective carbon management
- Algae for CO_2 fixation
- Sequestration in buildings, e.g., in cement (eco-cement)

R&D challenges for commercialization:

- Revisit older gas-to-liquid technology to circumvent proprietary issues; perhaps organize an industry roundtable to examine pre-competitive issues (SEMATECH model)
- Study and improve the kinetics of CO_2 sequestration with minerals
- Find ways to catalyze the formation of carbonates (e.g., calcium carbonate) for CO_2 sequestration
- Examine technical issues in the use of silicates for carbon sequestration (e.g., mining of silicate)
- Handle volume differences that result from sequestration (larger final volume vs. smaller initial volume) and its effect upon materials transportation and storage
- Study the energetics of absorption and desorption
- Study the economics of regeneration and recovery
- Identify alternative CO_2 removal chemistries at reasonable rates.
- Encourage wide scale fixative utilization of CO_2 (e.g., Climate Change Program)
- View CO_2 as asset rather than waste; for example:
    - Utilize CO_2 as energy carrier (carbon cycle)

General comments:

- The nation's capital should be spent today to address CO_2 management rather than spent over the next 50 years as the problem grows. We need to communicate a sense of urgency about the problem.

- We may be able to solve the chemical industry's energy problems but not those of the entire world. Also, if the focus is placed solely on the U.S. chemical industry, is it merely a matter of improving energy efficiency?
- The self-interest of chemical industry should drive their involvement in the decision-making process for future energy generation (e.g., new power plants, cogeneration, etc.). A chemical industry transformation must occur to respond the energy and CO_2 challenge
- We must consider Earth systems engineering (e.g., simultaneous management of multiple nutrient cycles). We should also encourage local solutions for this global problem.
- Implement noncarbon emitting processes and technologies:
    - Solar technology (storage and transmission technology for solar capture) to enable distributed energy production
- A possible grand challenge: Do renewable sources have suitable properties for use in commodity chemicals? Perhaps renewable sources with desired properties must be developed. This will involve a large capital cost in terms of money and energy.
- Encourage the production of chemicals onsite.
- Are commodities moving overseas because the customer base is overseas?

6. Final Thoughts

- Dissemination: Make sure that the final report gets into the hands of CEOs, or the most appropriate executives, in the chemical industry.
- Involve policy experts, economists, and politicians in these matters. They may be able to help by installing incentives to bring about major changes.
- From a Congressional staffer: So far, a case has not been made for sustainability to congressional representatives. The House Science Committee understands the problem, but a broader appeal is needed.
- The final report should contain an exciting and appealing executive overview. For instance, a good business case may be made using case studies or examples.

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Workshop Speaker Biographies

Braden R. Allenby is currently Professor of Civil and Environmental Engineering, and of Law, at Arizona State University, having moved from his previous position as the Environment, Health and Safety Vice President for AT&T in 2004. From 1995 to 1997, he was Director for Energy and Environmental Systems at Lawrence Livermore National Laboratory, and from 1991 to 1992 he was the J. Herbert Holloman Fellow at the National Academy of Engineering in Washington, D.C. He is currently President-elect of the International Society for Industrial Ecology. Allenby has authored a number of articles and book chapters on industrial ecology and Design for Environment; and is coauthor or author of several engineering textbooks, including *Industrial Ecology: Policy Framework and Implementation*, published by Prentice-Hall in 1998. Allenby received his B.A. from Yale University in 1972, his J. D. from the University of Virginia Law School in 1978, his Masters in Economics from the University of Virginia in 1979, his Masters in Environmental Sciences from Rutgers University in the Spring of 1989, and his Ph.D. in Environmental Sciences from Rutgers in 1992.

Stanley R. Bull is currently the Associate Director for Science and Technology for the National Renewable Energy Laboratory and Vice President of the Midwest Research Institute, has more than 35 years of experience in energy and related applications including renewable energy, energy efficiency, transportation systems, bioenergy, medical systems, and nondestructive testing. He leads NREL's RD&D which emphasizes renewable energy and energy efficiency technologies in support of DOE programs.

Bull has also held university faculty and private sector responsibilities, and has authored approximately 85 publications in diverse fields and technical journals, and presented about 103 papers at international, national, and other meetings. Professional recognition and honors include a Senior Fulbright-Hays Professorship in Grenoble, France, the Faculty-Alumni Award from the University of Missouri-Columbia, and the Secretary of Energy Outstanding Program Manager Award. Bull has a Ph.D. from Stanford University and has degrees in Chemical Engineering and Mechanical Engineering.

Douglas C. Cameron leads molecular biology and metabolic engineering R&D in the Cargill Biotechnology Development Center (BioTDC). From 1986–1998, Cameron was a professor in the Department of Chemical Engineering and an affiliate in the Molecular Biology Program at the University of Wisconsin—Madison. From 1979–1981 Cameron held the position of Biochemical Engineer at Advanced Harvesting Systems, a plant biotechnology company funded by International Harvester. Cameron is a Fellow of the American Institute of Medical and Biological Engineering (AIMBE) and of the Society for Industrial Microbiology (SIM). He is on the editorial board of *Metabolic Engineering*. Cameron served on the Minnesota Governor's Bioscience Council and is on the board of directors of MNBIO. He is a member of the MIT Biological Engineering visiting committee and is on the managing board of the Society for Biological Engineering (SBE). Cameron has a B.S.E. in biomedical engineering in 1979 from Duke University, Durham, North Carolina and a Ph.D. in biochemical engineering in 1986 from MIT, Cambridge, Massachusetts.

Berkeley W. Cue, also known as Buzz, consults with several technology companies who serve the pharmaceutical industry to create innovative solutions for pharmaceutical science and manufacturing challenges. Most recently, at Pfizer Cue was responsible for the departments (Analytical R&D, Bio Process R&D, Chemical R&D, Pharmaceutical R&D, Regulatory CMC & Quality Assurance and Pharmaceutical Sciences Business Operations) that comprise Pharmaceutical Sciences at their Groton R&D site. He created and led Pfizer's Green Chemistry initiative and has spoken extensively on this topic since 2000. Cue retired from Pfizer in April 2004 after almost 29 years, but he continues his mission of advancing green chemistry in the pharmaceutical industry. In 2004, he gave more than a dozen presentations on green chemistry in the pharmaceutical industry. Cue received a B.A. with honors from the University of Massachusetts-Boston (1969), his Ph.D. (Organic Chemistry) from the University of Alabama (1974), and completed Postdoctoral Research at the Ohio State University (1974), National Cancer Institute Research Fellow, University of Minnesota (1975).

Lauren G. Heine, is Director of Applied Science, at GreenBlue. As such, she guides the development of technical tools and approaches that help organizations integrate Green Chemistry and Engineering into their product and process design and development activities—eliminating toxics and the concept of waste, and moving toward economic, environmental, and community sustainability. She was previously Director of Green Chemistry and Engineering at the Portland, OR-based, Zero Waste Alliance (ZWA) and a Fellow with the American Association for the Advancement of Science in the Green Chemistry Program of the Industrial Chemicals Branch of the U.S. EPA in Washington, D.C. Lauren earned her doctorate in Civil and Environmental Engineering from Duke University.

Richard Helling has been focused intensely on economic and environmental life cycle analysis of products made from renewable resources for over 2 years, since his return from a 4-year manufacturing technology role for Dow AgroSciences in France. The majority of his 18 year career at Dow has been in process research, primarily in support of agricultural chemical manufacturing processes in California. He has worked on a wide range of classical chemical engineering technologies and management roles. His largest impacts at Dow have been in waste-reduction technology development and application, manufacturing process yield improvements and management of external manufacturing in Europe and Asia. He has a BS in Engineering (and History) from Harvey Mudd College, a M.S. in Chemical Engineering Practice from MIT, and a ScD in Chemical Engineering from MIT. He taught at MIT prior to joining Dow. He has had continued interest and research in waste elimination technology, chemical process modeling and simulation, and supercritical fluid technology since working in these fields at MIT.

Mark T. Holtzapple is currently Professor of Chemical Engineering at Texas A&M University, College Station, TX. From 1981 to 1985, Mark served in the U.S. Army and rose to the rank of captain. While in the Army, he performed research on water desalination and microclimate cooling, a method for cooling soldiers encapsulated in chemical protective clothing. Since joining the faculty Texas A&M in 1986, Mark has been well recognized for his excellent teaching and has won numerous teaching awards. Mark has authored nearly 100 technical articles and reports, plus a widely used engineering textbook. Further, he has over 22 issued patents, numerous pending patents, and over 80 disclosures. His research interests include fuels and chemical from biomass, food and feed processing, water desalination, air conditioning, high-efficiency engines, jet engines, and vertical-lift aircraft. In 1978, he received his B.S. in chemical engineering from Cornell University. In 1981, he received his Ph.D. in chemical engineering from the University of Pennsylvania.

Robert Kavlock is currently Acting Director of the National Center for Computational Toxicology. His research interests are oriented toward the development of improved hazard and risk assessment approaches for non cancer effects. Kavlock has held a variety of responsibilities for the EPA's research program on endocrine disruptors and more recently on computational toxicology. On the national level, he was a member of the Endocrine Disruptor Working Group of the Committee on the Environment and Natural Resources with the OSTP. On the international level, he has co-organized EDC workshops with the European Union and the Japanese Ministry of the Environment, and he was a co-editor of the Global Assessment of the State-of-the-Science of Endocrine Disruptors that was published by the World Health Organization in 2001. Kavlock is active in the Society of Toxicology, where he is a past president of the Reproductive and Developmental Toxicology Specialty Section and the North Carolina Regional Chapter and he was President of the Teratology Society (2000–2001). He received his Ph.D. in Biology from the University of Miami in 1977 and has been with the U.S. Environmental Protection Agency since that time.

Mary M. Kirchhoff is Assistant Director for Special Projects in the Education Division of the American Chemical Society, and previously served as Assistant Director of the ACS Green Chemistry Institute. She received her Ph.D. in organic chemistry from the University of New Hampshire and joined the Chemistry Department at Trinity College in Washington, D.C. upon completion of her degree. Mary spent nine years at Trinity College, where she served as Chair of the Division of Natural Sciences and Mathematics and Chair of the Chemistry Department. She became involved with green chemistry when she received an AAAS Environmental Fellowship to work with the U.S. EPA's green chemistry program. She has edited two ACS publications on green chemistry education, serving as co-editor with Mary Ann Ryan on *Greener Approaches to Undergraduate Chemistry Experiments,* and co-editor with Kathryn Parent on *Going Green: Integrating Green Chemistry into the Curriculum.*

William J. Koros is the Roberto C. Goizueta Chair in Chemical and Biomolecular Engineering at the Georgia Institute of Technology. He received his B.S., M.S. and Ph.D. in Chemical Engineering at the University of Texas and spent four years with the E. I. DuPont company. In 1977, he joined the faculty of the Chemical Engineering Department at the North Carolina State University. Koros joined the faculty of the Department of

Chemical Engineering at UT Austin in 1984, and served as Chairman of this Department from 1993 to 1997. He has served as the Editor-in-Chief of the *Journal of Membrane Science* since 1991, and he served as the Secretary of the North American Membrane Society from 1991–2004. Koros joined the School of Chemical Engineering at Georgia Institute of Technology in 2001. He has published over 250 articles and holds ten U.S. Patents in the areas of sorption and transport of small molecules in membranes and barrier materials. Koros was elected to the National Academy of Engineering in 2000, and he was named a Fellow of the American Association for the Advancement of Science in 2003.

Klaus S. Lackner joined the Earth Institute at Columbia University in 2001 as the Ewing-Worzel Professor of Geophysics in the Department of Earth and Environmental Engineering. He received his Ph.D. in 1978 in theoretical physics from the University of Heidelberg, Germany. After postdoctoral positions at the California Institute of Technology and the Stanford Linear Accelerator Center, he joined the Theoretical Division at Los Alamos National Laboratory in 1983. While mostly working in research, he also held positions in the Laboratory's senior management, among them as Acting Associate Laboratory Director for Strategic and Supporting Research representing one third of the Laboratory. Lackner is a founder of the Zero Emission Coal Alliance, an industry-led effort to develop coal power with zero emissions to the atmosphere. At present, he is developing innovative approaches to energy issues of the future focusing on environmentally acceptable technologies for the use of fossil fuels.

Glenn E. Nedwin is President of Novozymes, Inc., Davis, CA, a wholly owned R&D subsidiary of Novozymes A/S, where he is responsible for all scientific, financial, and administrative functions. He is a cofounder of Novozymes, Inc. (inception 1992) and has been with the Novo family over 13 years. Nedwin received his B.S. degree from S.U.N.Y./Buffalo and a Ph.D. in Biochemistry from U.C. Riverside. He did a post-doctoral fellowship in Molecular Biology at Genentech, Inc. He also holds a M.S. Degree in the Management of Technology from M.I.T. He is a co-editor of *Industrial Biotechnology*, a new journal with launch in 2005. Dr. Nedwin is also a member of several scientific and business associations and is on the Board of Trustees of the University of California Davis Foundation, an Advisory Board member to several U.C. Davis Departments, the Explorit! Science Center and on the Board of Directors of Air MD, Inc., an indoor air quality start-up company. Glenn is also lead guitarist with the Amplified DNA band, as well as Novozymes' CopenDavis band. He resides in Davis, CA with his wife and identical triplet daughters.

Jeffrey J. Siirola is a Technology Fellow in the Eastman Research Division of Eastman Chemical Company in Kingsport Tennessee where he has been for 33 years. He received a B.S. in chemical engineering from the University of Utah in 1967 and a Ph.D. in chemical engineering from the University of Wisconsin-Madison in 1970. His areas of interest include chemical process synthesis, computer-aided conceptual process engineering, engineering design theory and methodology, chemical process development and technology assessment, resource conservation and recovery, sustainable development and growth, artificial intelligence, non-numeric computer programming, and chemical engineering education. Siirola is an international program evaluator and past engineering accreditation commissioner for the Accreditation Board for Engineering and Technology. He has served on numerous National Science Foundation and National Research Council panels, and on the advisory boards of several journals and chemical engineering departments. Siirola is a member of the National Academy of Engineering and is the 2005 President of the American Institute of Chemical Engineers.

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