



## **Food, Energy, and Water**

Transformative Research Opportunities in the  
Mathematical and Physical Sciences

Mathematical and Physical Sciences Advisory Committee

**July 2014**



National Science Foundation



# **Food, Energy, and Water**

## **Transformative Research Opportunities in the Mathematical and Physical Sciences**

The function of Federal advisory committees is advisory only. Any opinions, findings, conclusions, or recommendations expressed in this material are those of the Advisory Committee, and do not necessarily reflect the views of the National Science Foundation.

# Contents

|  |    |
|--|----|
| Executive Summary .....  | i  |
| List of Figures .....  | ii |
| Introduction.....  | 1  |
| 1. Ensuring a Sustainable Water Supply for Agriculture .....                       | 4  |
| Introduction.....  | 4  |
| Expanding Supply through Wastewater Recycling.....                                 | 5  |
| (1) New approaches to wastewater recycling.....                                    | 5  |
| (2) Rapid, reliable measurement technologies to ensure water quality.....          | 6  |
| Increasing Water Supply through Desalination .....                                 | 6  |
| Improving Water Use Efficiency .....   | 8  |
| Energy from Agricultural Waste and Wastewater .....                                | 9  |
| Conclusions.....   | 9  |
| 2. Nutrient Life Cycle: Closing the Loop .....                                     | 11 |
| Introduction.....  | 11 |
| More Efficient Application and Uptake of P and N in Crops .....                    | 11 |
| Recovery and Reuse of P and N from High-Strength Organic Streams .....             | 12 |
| Capture and recovery of P and N from Agricultural Runoff .....                     | 13 |
| Conclusions.....   | 14 |
| 3. Crop Protection .....   | 16 |
| Introduction.....  | 16 |
| Biopesticides .....  | 16 |
| Gene-based Crop Protection .....   | 18 |
| Smart Application Systems.....   | 18 |
| Conclusions.....   | 19 |
| 4. Innovation in Processes and Materials to Prevent Waste of Food and Energy ..... | 20 |
| Introduction.....  | 20 |
| Magnitude of the Food Waste Issue.....   | 20 |
| Reducing Food Waste with Enhanced Packaging.....                                   | 21 |
| Recovering the Energy Content of Discarded Food .....                              | 22 |
| Conclusions.....   | 22 |
| 5. Sensors for Food Security and Food Safety .....                                 | 24 |
| Introduction.....  | 24 |

|  |    |
|--|----|
| State-of-the-Art Food Security.....  | 24 |
| Food Safety .....  | 25 |
| Conclusions.....   | 25 |
| 6. Maximizing Biomass Conversion to Fuels, Chemicals, Food, and Materials without Harming Food<br>Production ..... | 27 |
| Introduction.....  | 27 |
| Catalytic Conversion of Biomass to Fuels and Chemicals .....   | 27 |
| Heterogeneous Catalysis in the Liquid Phase .....  | 28 |
| Conclusions.....   | 28 |
| Summary .....  | 30 |
| APPENDIX A. Charge to MPSAC Subcommittee.....  | 34 |
| APPENDIX B. Members of the MPSAC Subcommittee for Studying the Role of NSF/MPS in Food<br>Systems (SFS).....       | 36 |
| APPENDIX C. List of Teleconference Speakers.....   | 37 |

## Executive Summary

The security of the global food supply is under ever-increasing stress due to rises in both human population and standards of living world-wide. By the end of this century, the world's population is expected to exceed 10 billion, about 30% higher than today. Further, as standards of living increase globally, the demand for meat is increasing, which places more demand on agricultural resources than production of vegetables or grains. Growing energy use, which is connected to water availability and climate change, places additional stress on agriculture. It is clear that scientific and technological breakthroughs are needed to produce food more efficiently from “farm to fork” to meet the challenge of ensuring a secure, affordable food supply. A Mathematical and Physical Sciences Advisory Committee (MPSAC) Subcommittee on Food Security was formed and specifically charged to evaluate current technology gaps that can be addressed by the National Science Foundation/Mathematical and Physical Sciences Directorate (NSF/MPS). To identify these gaps, the Subcommittee evaluated all aspects of food production, treating food production as a system. In addition, special consideration was given to the inextricable roles of water and energy in food production, noting that any developed technologies must be efficient with respect to both energy and water use. The Subcommittee gathered information from the literature and from leading experts in these areas.

The Subcommittee identified six areas in which MPS researchers could provide key foundational knowledge on which technology breakthroughs could be based: (1) Ensuring a Sustainable Water Supply for Agriculture; (2) “Closing the Loop” for Nutrient Life Cycles; (3) Crop Protection; (4) Innovations to Prevent Waste of Food and Energy; (5) Sensors for Food Security and Safety; and (6) Maximizing Biomass Conversion to Fuels, Chemicals, Food, and Materials. In all of these areas, the technical gaps that currently exist in maximizing, recycling, and reusing resources associated with global food production were identified.

A number of common research themes from these six areas were identified, including separations, catalyst materials and catalytic processes, chemistry at interfaces, new materials and chemical processes, new analytical techniques and sensors, computational approaches, and renewable energy. Fundamental research in these cross-cutting research themes will provide the foundation to yield future technologies for water desalination, use, and recycling; fertilizer production and management; novel methods for efficient pest control (such as selective biopesticides); food waste minimization and reuse; and even clean renewable energy generation and conservation. In addition, training next generation scientists in these areas to support sustainable food production was identified as another critical role for NSF/MPS.

The technical challenges in optimizing the sustainable production of food to ensure a secure, affordable food supply are daunting. The Subcommittee concluded that incremental advances in today's technologies simply will not be sufficient for meeting these formidable challenges. Rather, fundamental research is needed to provide the foundation for achieving technological breakthroughs required to provide safe, secure, and affordable food supplies globally.

## List of Figures

|   |    |
|---|----|
| <b>Figure 1.</b> The digital global map of irrigation areas, October 2013 .....   | 2  |
| <b>Figure 2.</b> This National Aeronautics and Space Administration (NASA) satellite photo shows crop circles in Finney County, Kansas .....  | 4  |
| <b>Figure 3.</b> Conceptual drawing of an SWRO desalination plant showing the various stages— seawater intake, pretreatment, reverse osmosis, post-treatment, and brine discharge— and their interactions with the environment..... | 7  |
| <b>Figure 4.</b> A bipolar electrode drives electrolysis reactions to create an electric field gradient that directs salt into one branch of a microfluidic network.....  | 8  |
| <b>Figure 5.</b> Ultraviolet- stable and self-healing plastics could provide for robust micro-irrigation systems...8  |    |
| <b>Figure 6.</b> Struvite ( $MgNH_4PO_4 \cdot 6H_2O$ ) is a source of P and N and can cause blockages in sewer pipes..13  |    |
| <b>Figure 7.</b> Eutrophication from field run-off and agricultural wastes causes excessive plant growth and decreases in water oxygen levels in surface waters.....  | 14 |
| <b>Figure 8.</b> Emerald ash borer (left) and a manufactured decoy (right).....   | 18 |
| <b>Figure 9.</b> RNAi offers a new means of pest-control.....   | 19 |
| <b>Figure 10.</b> Food energy and waste in America.....   | 21 |
| <b>Figure 11.</b> Annual contributions to US landfills.....   | 22 |
| <b>Figure 12.</b> Real time monitoring of nutrients, water and soil quality.....  | 25 |
| <b>Figure 13.</b> Fractionation of lignocellulosic biomass and reaction pathways to produce GVL from hemicellulose and cellulose.....   | 28 |

## Introduction

Access to a secure, affordable supply of food is a basic human need. As the world's population increases from the current approximately 7 billion people to a projected level of well over 10 billion before the end of this century, new technologies for food production are needed to meet increased demand. In addition, as standards of living increase in countries with emerging economies, the types of foods produced will change. For example, by 2020 meat consumption in China is expected to double from 2005 levels; the increase in turn places more stress on food production, because appreciably more resources are required to produce meat than grains or vegetables. Thus it is critical to identify technical gaps in current agricultural processes that could be addressed by fundamental advances in the physical sciences. These advances in new chemical processes and materials would underpin future technologies to produce food efficiently to meet future global demand.

In considering increased demand for global production of food, it is impossible to project strategies for meeting these demands without considering two other key factors: energy and water. Society is increasingly forced to choose, for example, between using land and fertilizer for food production or for bio-based or renewable energy production, and between using fresh water for energy production (e.g., hydraulic fracturing or growing corn for biofuels) or for irrigating food crops. Thus food, water, and energy are inextricably linked and must be considered together as a system.

The availability of fresh water is a major driver in food production. In many areas of the world, rainfall is insufficient and water must be supplied to crops by irrigation. Currently, 70%

of global fresh water consumption is used for agriculture, and total water consumption for agriculture is expected to increase by about 20% by mid-century. The increased demands for fresh water for crops and livestock production, together with other uses (e.g., energy production), will add significantly to the current stress on non-renewable groundwater sources. Food production also contributes to the contamination of fresh water supplies. Runoff from fields and feedlots introduces large quantities of fertilizers and animal wastes into surface waters, depleting oxygen and impacting aquatic life. As a result, there are prominent "dead zones" in coastal and inland bodies of water that have led to severe economic losses in the commercial fishing and tourism industries. Approaches are needed to reduce agricultural runoff and to capture and recycle nutrients before they reach water sources. Salt water and brackish water from inland sources represent a potentially significant source of fresh water for food production; however, the current desalination technologies are very energy intensive and expensive. New approaches for efficiently treating these water sources for agricultural use could greatly alleviate the stress on fresh water supplies.

Food production requires significant amounts of energy from "farm to fork." Nearly 10% of US annual energy consumption is used to produce food. This significant amount of energy consumption includes preparing, maintaining, and producing crops and raising livestock on farms (e.g., production of fertilizers and pesticides, use of fuels; pumping irrigation water), and additional processes occurring after the product leaves the farm, including transportation, food processing and handling, and storage. In California alone, agricultural irrigation uses 10 billion kilowatt hours of electricity annually. Improvements in sensors could reduce energy costs by precisely



delivering irrigation water when needed and could reduce runoff as well. The increased production of liquid fuels from agriculture represents another dimension of the energy–food relationship. Many crops currently grown to produce fuels require large amounts of additional fertilizer, pesticides, and water, which in turn require additional energy. For example, it is estimated that a gallon of ethanol derived from corn requires 1,400 gallons of water to produce. Finally, significant amounts of energy are lost when food is wasted. Thus improvements in food production technologies could also improve the production of biofuels. Food losses from the farm, transportation, processing, and home and commercial use, account for nearly 2% of US annual energy consumption; however, the waste food could be converted into energy, chemicals, and materials by the use of new catalytic processes. For example, one beef cow produces over 14 tons of manure each year, representing a significant

source of organic matter that could be used in energy production. In addition, nutrients found in livestock manure, including nitrogen and phosphorus, could be recycled as fertilizers if selective separation methods could be developed.

In all of these areas, it is clear that advances in the physical sciences—including new chemical processes and materials for separations, catalysis, sensors, and pest control—could have a significant impact on the development of next-generation technologies for meeting future food demands. A subcommittee of the National Science Foundation’s Mathematical and Physical Sciences Advisory Committee (MPSAC) (see Appendix A) was charged with identifying fundamental science areas that could underpin these advances. The Subcommittee Members (Appendix B) met by teleconference and video conference to gather information relevant to the charge. These meetings included presentations from experts in fields relevant to

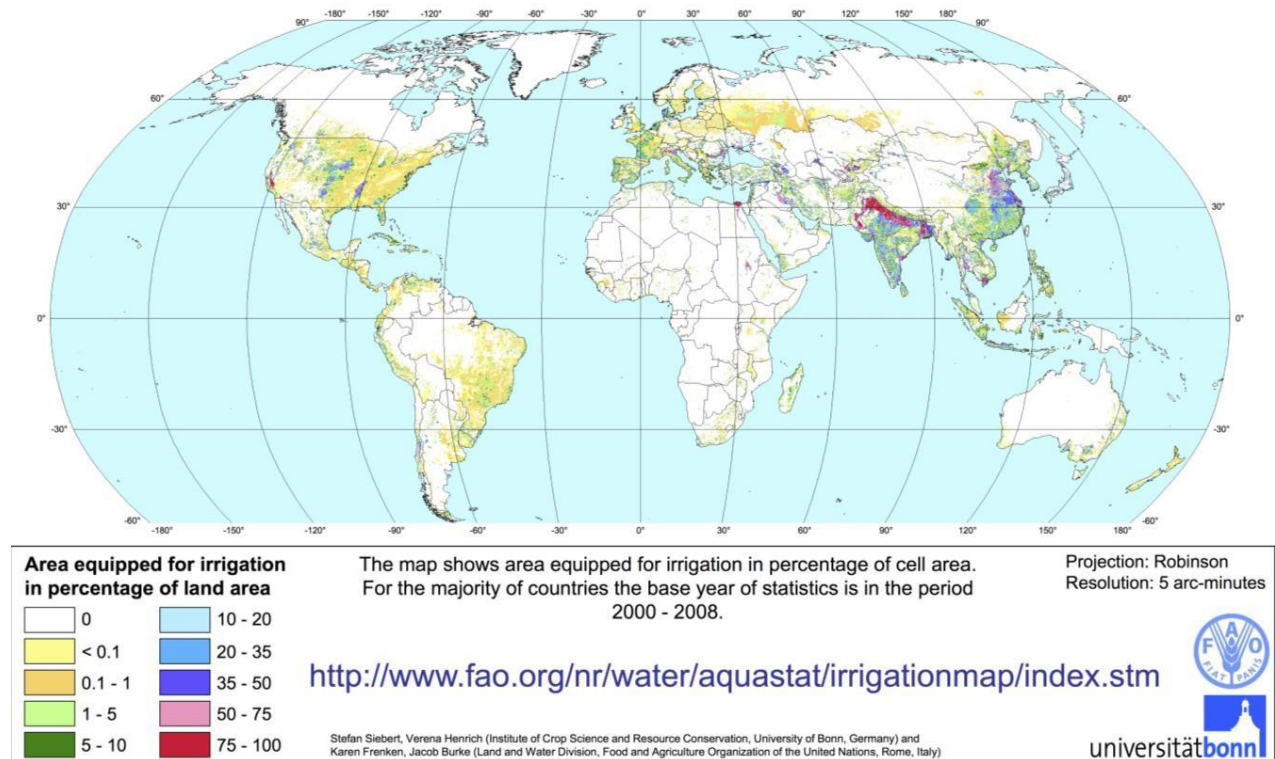


Figure 1.

the charge (see the Appendix C), who were specifically tasked with identifying technical gaps that could be addressed by advances in the physical sciences. The committee identified seven key areas in which the physical sciences could provide breakthroughs needed to address the pressing demand to enhance sustainable food production. These include (1) Ensuring a Sustainable Water Supply for Agriculture, (2) “Closing the Loop” for Nutrient Life Cycles, (3) Crop Protection, (4) Innovations to Prevent Waste of Food and Energy, (5) Sensors for Food Security and Safety, and (6) Maximizing Biomass Conversion to Fuels, Chemicals, Food and Materials.

The report is organized according to these six areas, and recommendations for each area are provided in the report summary. Although this report does not directly address other avenues to sustainable energy production and storage that compete with agriculture (such as solar energy), we note that scientific breakthroughs for energy technologies will also be crucial to food-system success, because the sustainable production of food and water is so intimately connected to energy.

# 1. Ensuring a Sustainable Water Supply for Agriculture

## Introduction

Water is a key resource for agricultural production, as irrigation is used to produce 40% of farm output worldwide (see Figure 1) [1]. The amount of food crops dependent on irrigation is higher in arid regions. For instance, irrigation is used for 60% of food production in Asia.

Currently, 70% of global freshwater consumption is for agriculture [2],

corresponding to a volume of over 2,500 km<sup>3</sup>. Water withdrawals for irrigation are projected to increase by 50% in developing countries by 2025, much of which will come from non-renewable groundwater use [3]. The United Nations estimates that to meet global food demand, total agricultural water consumption will need to increase by 19% by 2050 [4]. At current rates of water usage, up to 7 billion people in 60 countries will experience water scarcity by 2050, which will place additional stress on agriculture. Irrigation is also energy intensive. Regional-scale canal projects cost tens of billions of dollars and often require pumping stations to move water between watersheds. The energy cost of pumping water depends on fuel or electricity prices. Irrigation with groundwater can lead to energy costs in the range of USD \$10– 100/acre per year. In California alone, agricultural irrigation uses 10 billion kilowatt hours of electricity annually [5]. Freshwater withdrawals in the United States are rising, increasing the stress on regions that have limited supplies of freshwater (Figure 2).

Another important factor, not addressed directly by this report, is the effects of climate change. Models and recent climate data indicate that global warming will likely lead to changes in

precipitation distribution, soil moisture, and temperature. Such changes have already been observed over the last century: for example, there was a 50% increase in the frequency of days with precipitation exceeding 4 inches in the United States, which is statistically significant [6]. The impact of climate change is complex, but it has major relevance to agriculture because yields from staple crops, such as corn, are highly dependent on moisture and temperature during growth and flowering. The latest analysis using ten global hydrological models projects that direct climate impacts on corn, soybean, wheat, and rice will result in annual losses of 400–1,400 petacalories (8–24% of the present-day total) [7]. The effect of climate change on water stress and agriculture is a critical issue that factors into the relationship of food, water and energy.



Irrigation freshwater withdrawals for the United States in 2005

| Withdrawals<br>Million gallons per day<br>(1,000 acre-feet per year) |                    |                      | Irrigated land (1,000 acres) |                  |         |
|--|--------------------|----------------------|------------------------------|------------------|---------|
| Groundwater  | Surface water      | Total                | Sprinkler                    | Micro-Irrigation | Surface |
| 53,500<br>(60,000)   | 74,900<br>(84,000) | 128,000<br>(144,000) | 30,500                       | 4,050            | 26,600  |

**Figure 2.** This National Aeronautics and Space Administration (NASA) satellite photo shows crop circles in Finney County, Kansas. The irrigated plots are 800 and 1,600 m in diameter (0.5 and 1 mile). This area uses irrigation water from the Ogallala aquifer that underlies an area from Wyoming to Texas. Photo used courtesy of NASA; table used courtesy of US Geological Survey.

The physical sciences can provide the fundamental basis for new technologies required to optimize irrigation practices and expand water supplies through recycling and desalination. The technologies required to meet future agricultural needs include advanced desalination systems with lower energy demands. These will require advances such as improved membrane materials; new wastewater treatment approaches for enhanced water reuse; inexpensive sensors to measure soil moisture levels and crop conditions in real time; and robust, low-cost, self-healing polymers that can be used for micro-irrigation. The following six sections of the report identify areas in which mathematics and the physical sciences can provide the foundation for revolutionary technology solutions within the food/water/energy nexus.

### **Expanding Supply through Wastewater Recycling**

In North America alone, 19 trillion gallons (85 km<sup>3</sup>) of wastewater are generated each year [8]. Although 75% of this wastewater is treated, only 3.8% is currently reused for agricultural or other beneficial purposes. The total amount of wastewater relative to agricultural water withdrawals in North America is 42%, indicating that wastewater could help decrease stress on fresh water supplies. This is especially true for farms in urban and peri-urban areas: more than 800 million farmers are engaged in urban agriculture worldwide [9]. For example, in most West African cities, 60–100% of the vegetables consumed are grown in urban or peri-urban farms [10].

Wastewater comes from a wide variety of sources [11]. Some of the largest wastewater volumes result from energy applications and industrial processes, such as refining, oil/gas production, and paper manufacturing, in addition to municipal sewage treatment and stormwater

runoff. Thus it is critical to understand what types of wastewater are most treatable and useful for augmenting water supplies for agriculture. Furthermore, capturing and recycling water in agriculture can lower the dependence on already strained water resources. Recovering and recycling wastewater presents a number of daunting technical challenges, including removing pesticide contaminants, salts, and pathogens—all by highly efficient and energy effective means. Meeting these challenges will also require new approaches to measure water quality with respect to many pollutants in real time. For example, use of industrial wastewater and stormwater runoff offers opportunities to expand the water supplies available to agriculture; however, these sources introduce a broader variety of biological, organic, and inorganic pollutants. Understanding the presence and fate of micropollutants to ensure food safety is a major technical need. There are two major challenges that physical scientists must address to render wastewater usable for food production.

#### **(1) New approaches to wastewater recycling.**

The provision of safe water for food production begins with the development of efficient processes that can be incorporated into effective water treatment systems. Methods such as membrane filters, membrane bioreactors, and artificial wetlands are emerging technologies that show particular promise. However, improved membranes and alternative separation approaches are required to improve the selectivity and efficiency of these approaches, as well as reduce energy requirements and costs. In most cases, multiple stages of separation may be required to produce water safe for food use. For example, in artificial wetlands, many types of contaminants can be eliminated; however, the removal of phosphates is currently an unresolved issue. Further, selective chelators can be designed to remove trace metals at high

efficiencies. These molecules can be used to modify the surfaces of either adsorbents or membranes to enhance separation selectivity. Understanding the fate of biotic and abiotic contaminants in water as it is processed is critically important. Achieving this understanding will require the development of new analytical capabilities, including real-time monitoring of these contaminants. The physical and chemical interactions of micropollutants with soils and innovative soil amendments that could irreversibly capture pollutants are also critical for understanding how contaminants from recycled wastewater can be removed or sequestered.

Finally, to ensure food safety from field to table, the impact of recycled water on harvest and post-harvest processes, including cleaning, preparation, and storage, must be fully understood.

## **(2) Rapid, reliable measurement technologies to ensure water quality.**

Although some components in wastewater need to be removed, wastewater can host a variety of solutes and nutrients that can add value to agricultural purposes if their use is closely monitored. As an example, the wastewater widely used in the Tula Valley of Mexico possesses an inherent nutrient load that has led to significant increases in crop yields. The Atotonilco Wastewater Treatment Plant, currently under construction there, will be the world's largest wastewater treatment facility with the capacity to treat 800 million gallons per day, almost 60% of the wastewater produced by the metropolitan area of Mexico City. Treated water will then be used to irrigate about 200,000 acres of agricultural land. However, excessive or imbalanced nutrients can lead to undesirable plant growth, delayed crop maturity, and reduced crop quality. Integrating wastewater into agriculture requires the development of sensors and other analytical methods to provide

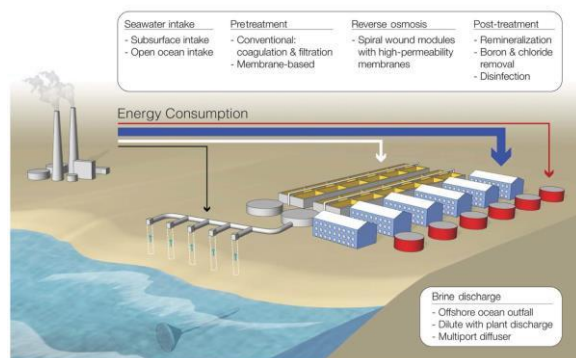
critical water quality data to farmers, public agencies, and consumers. In addition, a combination of analytical methods could be employed in epidemiological studies to assess water quality parameters that can be correlated to potential negative health impacts. Such studies will require new analytical tools and computational models based on the analysis of large data sets.

## **Increasing Water Supply through Desalination**

Outside of water reuse, desalination of seawater and brackish water is the only method to provide new water resources for agriculture [12]. Seawater desalination offers a potentially unlimited supply of water for agricultural areas located near coastlines. Desalination of brackish waters also can serve as a source of water for farms located in interior regions. Large desalination systems have been developed in countries where freshwater is scarce, including Spain, Australia, and several countries in the Middle East. For example, the United Arab Emirates produces 90% of its freshwater by desalination. There are two critical aspects to consider regarding desalination of seawater for agriculture. The first is recognizing that the theoretical minimum energy of desalination of seawater from thermodynamic considerations is  $1.06 \text{ kWh/ m}^3$ , a high energy cost [13]. State-of-the-art desalination plants use reverse osmosis in combination with significant pre- and post-treatment steps to maintain performance (Figure 3). High-flux reverse osmosis (RO) membranes have already achieved power consumption values of less than  $2 \text{ kWh/ m}^3$ . However, RO treatment of seawater to produce freshwater will always come at a high energy cost.

Second, current state-of-the-art, high-flux RO membranes allow chloride and boron to pass through with the permeate, prohibiting the use of

the produced water for agriculture without additional treatment. Chloride and boron removal currently requires expensive, high-energy secondary treatment methods. Pretreatment systems are also used in many RO plants and add to the total cost of water produced via desalination.



**Figure 3.** Conceptual drawing of an SWRO desalination plant showing the various stages— seawater intake, pretreatment, reverse osmosis, post-treatment, and brine discharge—and their interactions with the environment. The thickness of the arrows represents the relative amount of energy consumed at the various stages. [After M. Elimelech and W.A. Phillip et al., *Science* 333, 6043 (2011)]

Fundamental advances based in the physical sciences are needed to produce the technology improvements required for desalination processes and thus increase water supplies available for agriculture. For example, it has recently been shown that the movement of colloids toward the membrane surface is driven electrokinetically by the salt concentration gradient near the surface. The colloids can be driven in the opposite direction, inhibiting membrane fouling, by simply decorating the membrane surface with calcium carbonate particles [14]. This discovery grew out of an earlier fundamental study of the electrokinetic propulsion of micromotors and micropumps that were driven by salt dissolution [15].

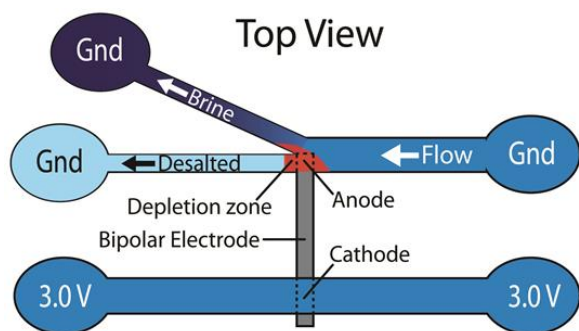
Achieving optimized materials and processes for desalination will also require the development of next-generation membranes and new separation

processes. First, eliminating pretreatment stages through the development of anti-fouling membranes would significantly reduce total energy consumption. Anti-fouling membranes may be developed by tailoring the surface chemistry of membrane materials without reducing membrane flux. Second, developing membranes that can selectively reject chloride and boron would eliminate expensive secondary treatment after RO. New concepts are needed for a new generation of membranes with improved selectivity and high flux that do not use a traditional solute diffusion mechanism for desalination. Third, other types of separation processes for water desalination must be developed. For example, in forward osmosis processes, thermolytic draw solutions (typically containing low-molecular-weight salts) are used to enhance transport of water from the contaminated source through a membrane into the draw solution. The salt is removed in a separate step to produce purified water. Innovative approaches to alternative membrane separations for agriculture could include using fertilizer-containing draw solutions, which would eliminate the additional separation step to remove the salts. Finally, new separation approaches need to be designed to decrease the energy-intensive steps used in current water desalination processes and to reduce equipment costs. Greater energy efficiency may also be realized by developing improved renewable energy production and the use of waste heat sources that can be indirectly beneficial to desalination for agriculture.

A novel desalination approach, illustrated in Figure 4, illustrative of the potential impact of fundamental research in physical sciences, involves taking advantage of electrochemical gradients on very small length scales that desalinate water with high energy efficiency, albeit in nanoliter volumes [16]. Although scaling up such a process is clearly a challenge,

a company (Okeanos Technologies) has already formed to explore the development and commercialization of “water chip” desalination.

Other innovative approaches to desalination and to the reverse, which is extracting energy from salinity gradients, involve cycling electrochemical capacitors and batteries [17–19]. This is an especially interesting interdisciplinary development because the basic concept was developed by a physicist [17] and is now being elaborated for power generation by engineers [19] building on battery and supercapacitor materials developed by materials scientists [18,20].



**Figure 4.** A bipolar electrode drives electrolysis reactions to create an electric field gradient that directs salt into one branch of a microfluidic network. [After K. N. Knust, D. Hlushkou, R. K. Anand, U. Tallarek, and R. M. Crooks, *Angew Chem. Int. Ed.* 52, (2013).]

### Improving Water Use Efficiency

Crop irrigation requirements vary depending on weather and soil moisture conditions. A survey by the University of California–Berkeley and the Pacific Institute found that irrigation scheduling based on environmental data can reduce average water use by 13% [21]. Many farms are irrigated by the flood or furrow method (i.e., water is flowed over the ground among the crop), in which it is estimated that only half of the water applied benefits the crop, as half is lost through evaporation, run-off, and other losses.

Conversion from traditional furrow irrigation to drip methods, combined with low-till

procedures, has been shown to reduce irrigation needs by about 50% while improving yields [22]. Eliminating water subsidies and providing incentives for the installation of water saving measures would lead to adoption of the technology. However, there are still other significant opportunities for improving the efficient use of water in agriculture by the development of new technologies that cost less and/or save energy.

Better understanding of water-soil interactions is needed to realize improvements in the capacity of various types of soil to retain moisture for longer periods of time. Further, improved materials and processes for manufacturing drip irrigation or micro-irrigation systems are needed to produce strong, self-healing materials to reduce costs and increase adoption rates by farmers (Figure 5). Such systems are much more water-efficient than broadcast irrigation systems. Of high importance for irrigation scheduling is the development of robust, low-cost sensors, perhaps based on spectroscopic or electrochemical methodologies that can provide real-time, spatially-resolved soil moisture data for farmers. Remote sensing data obtained from advanced satellite imagery, available on the internet, is poised to play an even more important role in irrigation scheduling. However, combining this information with a battery of local sensors providing information



**Figure 5.** Ultraviolet-stable and self-healing plastics could provide for robust micro-irrigation systems. [Source: Thinkstock]

about soil moisture and plant health could provide enhanced insight regarding soil conditions and ultimately reduce water usage.

### Energy from Agricultural Waste and Wastewater

Electrochemical materials and processes can be used both to produce power from agricultural waste and to purify wastewater. For example, microbial fuel cells can generate power at the same time that they generate purified water, but because they operate at low power density, their capital cost per watt is high [23]. Solar photocatalysis has been studied as a method of removing contaminants from water and generating hydrogen fuel, which produces water when used in a fuel cell. However, the process is currently inefficient, and stable, low-cost ultraviolet-absorbing photocatalysts are needed to make this process viable. The most efficient visible-light photocatalysts contain toxic elements, such as cadmium, and are themselves subject to photocorrosion. Approaches like these that address multiple needs associated with the relationship of food, water, and energy are particularly exciting; and advanced materials and chemical processes can provide the needed breakthroughs in catalysis, separations, and other technologies.

### Conclusions

Data from many sources point to water scarcity as being a major challenge in the future. Predictions of increased water requirements for the level of agricultural production that will be needed in the future indicate that food supplies will be in jeopardy. Fundamental research that underpins technology advances will be essential to develop a sustainable water supply from diverse sources. Overall, fundamental research in the following areas has been identified as the

high priorities for developing technologies required for water production, recycling, and use in agriculture.

- Development of a new generation of highly efficient, selective, low-energy separation processes, which requires:
  - fundamental understanding of separation processes, including computational methods for simulating transport and optimizing separations; and
  - improved membranes, including anti-fouling and self-repairing materials.
- Fundamental understanding of materials chemistry and chemistry at interfaces for separations.
  - New metal ion ligand chemistries and other approaches for metal separations.
  - Other separation strategies, including novel adsorbents, bio-inspired materials, and molecular recognition.
- Improved understanding of the fate of micropollutants (both biotic and abiotic) in the source, use, and recycling of water used in agriculture.
- Elucidation of physical and chemical processes occurring at surfaces to understand the interactions of pollutants with soils and soil amendments and enable development of improved separation methods.
- Development of new materials and manufacturing processes for robust, low-cost micro-irrigation systems, including renewable and self-healing polymer materials.
- New analytical tools for real-time monitoring of pollutants, nutrients, water quality, soil moisture, and plant health.



## References

1. D. Molden, T., Oweis, P. Steduto, P. Bindraban, M. A. Hanjra, and J. Kijne. "Improving agricultural water productivity: Between optimism and caution," *Agricultural Water Management, Comprehensive Assessment of Water Management in Agriculture* **97**(4), 528–535 (2010).
2. UNESCO, World Water Assessment Programme (WWAP) 2012.  
<http://www.unesco.org/new/en/natural-sciences/environment/water/wwap/facts-and-figures/>
3. M. W. Rosegrant, X. Cai, and S. A. Cline. "World water and food to 2025: Dealing with scarcity," Intl. Food Policy Res. Inst. (2002).
4. United Nations Water, "Water for Food Fact Sheet," 2013.  
[http://www.unwater.org/fileadmin/user\\_upload/unwater\\_new/docs/water\\_for\\_food.pdf](http://www.unwater.org/fileadmin/user_upload/unwater_new/docs/water_for_food.pdf)
5. C. Burt, D. Howes, and G. Wilson. California Agricultural Water Electrical Energy Requirements: Technical report for California Energy Commission, Sacramento, California, 2003.
6. J. Elliott, D. Deryng, C. Müller, K. Frieler, M. Konzmann, D. Gerten, et al. "Constraints and potentials of future irrigation water availability on agricultural production under climate change," *PNAS*, 201222474 (2013). doi:10.1073/pnas.1222474110.
7. Weather and Climate Extremes in a changing Climate: Regions of Focus: North America, Hawaii, Caribbean, and US Pacific Islands, US Climate Change Science Program, 2008.
8. T. Sato, M. Qadir, S. Yamamoto, T. Endo, and A. Zahoor. "Global, regional, and country level need for data on wastewater generation, treatment, and use," *Agricultural Water Management* **130**, 1–13 (2013).
9. M. Qadir, D. Wichelns, L. Raschid-Sally, P. G. McCornick, P. Drechsel, A. Bahri, and P. S. Minhas. "The challenges of wastewater irrigation in developing countries," *Agricultural Water Management* **97**(4), 561–568 (2010).
10. P. Drechsel, S. Graefe, M. Sonou, and O.O. Cofie. "Informal irrigation in urban West Africa: An overview," in Research Report 102, IWMI, Colombo, Sri Lanka, 2006.
11. S. K. Sharma and R. Sanghi. Wastewater Reuse and Management, Springer, New York, 2013.
12. National Research Council (US) Committee on Advancing Desalination Technology. Desalination: A National Perspective, National Academies Press, Washington, D.C., 2008.
13. M. Elimelech and W. A. Phillip. "The future of seawater desalination: Energy, technology, and the environment," *Science* **333**(6043), 712–717 (2011).
14. A. Kar, R. Guha, N. Dani, D. Velegol, and M. Kumar, "Particle deposition on microporous membranes can be enhanced or reduced by salt gradients," *Langmuir* **30**, 793–799 (2014).
15. J. McDermott, A. Kar, M. Daher, et al., "Self-generated diffusioosmotic flows from calcium carbonate micropumps," *Langmuir* **28**, 15491–15497 (2012).
16. K. N. Knust, D. Hlushkou, R. K. Anand, U. Tallarek, and R. M. Crooks, "Electrochemically mediated seawater desalination," *Angew Chem. Int. Ed.* **52**, 8107–8110 (2013).
17. D. Brogioli. "Extracting renewable energy from a salinity difference using a capacitor," *Phys. Rev. Lett.* **103**, 058501 (2009).
18. F. La Mantia, M. Pasta, H. D. Deshazer, B. E. Logan, and Y. Cui, "Batteries for efficient energy extraction from a water salinity difference," *Nano Lett.* **11**, 1810–1813 (2011).
19. M. C. Hatzell, R. D. Cusick, and B. E. Logan, "Capacitive mixing power production from salinity gradient energy enhanced through exoelectrogen- generated ionic currents," *Energy Environ. Sci.* **7**, 1159–1165 (2014).
20. P. Simon and Y. Gogotsi. "Materials for electrochemical capacitors," *Nature Mater.* **7**, 845–854 (2008).
21. H. Cooley, J. Christian-Smith, and P. H. Gleick. *Sustaining California Agriculture in an Uncertain Future*, Pacific Institute, 2009.
22. R. Bongiovanni and J. Lowenberg-Deboer. "Precision agriculture and sustainability," *Precision Agriculture* **5**(4), 359–387 (2004).
23. B. E. Logan and K. Rabaey, "Conversion of wastes into bioelectricity and chemical by using microbial electrochemical technologies," *Science* **337**, 686–690 (2012).

## 2. Nutrient Life Cycle: Closing the Loop

### Introduction

Trace nutrients, such as phosphorus (P) and nitrogen (N), are essential components of nucleotides and peptides that are the building blocks of all plant and animal life. Modern agriculture depends on applying fertilizers containing these key nutrients to maintain the nutrient fertility of the soil despite high uptake rates from harvested crops. However, the ways in which N and P are used today are far from sustainable [1]. Today virtually all P used in fertilizers is recovered from phosphate-containing rock derived from fossil sources that are in finite supply. Further, major P mines are mainly located outside the United States, presenting a potential supply threat for domestic food production.

Although  $N_2$  is abundant in the atmosphere, it must be supplied in a reduced form, such as  $NH_3$  (ammonia), to be available for plant uptake. The reduction is carried out naturally by soil microorganisms or nitrogen-fixing plants, such as legumes, or can be done synthetically. Today, N for fertilizer is not in short supply because  $NH_3$  can be produced by reacting atmospheric  $N_2$  with  $H_2$  via the Haber-Bosch process. However, this process is very energy intensive; therefore, new catalytic processes are needed to produce reduced N for agricultural use.

Contributing to the sustainability issues surrounding these two nutrients is the fact that most of the P and N applied to crops is lost from the food-production system [2,3]. Only about 16% of the nutrients used contributes directly toward producing human food, and large amounts are lost as runoff from fields, animal manures, and food-processing wastes. The losses cause severe environmental problems: eutrophication from P and N and odors from

$NH_3$ . In turn, these losses also contribute to increased demand for imported P and increased energy use to produce N. Thus these losses lead to higher costs for farmers, animal producers, food producers, and consumers.

The ultimate goal is to close the loop on nutrient use, as this will provide major benefits in each of the sustainability areas [4]. Methods of closing the loop include (1) more efficient application and uptake of P and N in agricultural use; (2) recovery and reuse of p and N in high-strength organic streams from animal operations, food processing, and human waste; and (3) capture and recovery of P and N from agricultural runoff.

*"Quite simply, without phosphorus we cannot produce food."*

*Dr. Dana Cordell,  
University of Technology, Sydney, Australia.*

### More Efficient Application and Uptake of P and N in Crops

Efforts are under way in the plant biology community to create genetically modified plant strains that are more effective at P uptake (e.g., Ref [5]). More efficient uptake should mean that less P can be applied to the soil to meet plant requirements. Higher efficiency should therefore decrease fertilizer demand, lower costs to farmers, and result in significant decreases in nutrient erosion and runoff.

Closely aligned with more efficient nutrient uptake is precise application of fertilizer. Part of the strategy for improved application focuses on new methods to deliver nutrients directly to the plant roots, rather than broadcasting fertilizer indiscriminately throughout the soil. However, precision application depends on effective means of monitoring multiple factors affecting plant health, such as weather conditions, crop

and weed status, and soil fertility, all of which determine the need for and timing of fertilizer application. Therefore, new analytical methods are needed to monitor all aspects of the health of the crop, especially sensors that can monitor specific key indicators in real time. Finally, computational algorithms are needed to assimilate the data and provide guidance to precise application of fertilizers.

### **Recovery and Reuse of P and N from High-Strength Organic Streams**

The entire food system generates many waste streams that are characterized by high water content and high concentrations of organic matter, N, and P [3]. Examples are wastes from confined animal feeding operations, dairies, biofuel production, breweries and other beverage manufacturers, and various food processors. Other high-organic-waste streams include those from fish farms, microalgae ponds, and human sewage treatment facilities.

Although the organic waste streams exhibit considerable variety in terms of concentrations of organic matter (measured as chemical oxygen demand), N, and P, all of them share a common feature that makes them readily amenable to recovery and reuse of N and P. This common feature is that the N and P are associated with organic matter embodying a large amount of energy in its carbon. Capturing the energy value of these waste streams provides a significant economic benefit itself, and it also avoids high pollution impacts to water, air, and soil. An additional benefit is that these high-strength organic streams normally have a high water content (typically >95%). The water content makes them readily amenable to energy capture by anaerobic microbial processes that naturally release the N and P as  $\text{NH}_4^+$  and  $\text{HPO}_4^{2-}$  ions that can be recovered by separation methods. Along with improvements in microbial processing to

capture the energy associated with these wastes, new separation methods are critically needed to recover N and P.

One method of capturing the energy value of organic wastes that exist in water-based slurries is methanogenesis, commonly called anaerobic digestion [6]. Methanogenesis is a mature technology, but it has two drawbacks that have limited its application in the United States. The first drawback is that the energy product— $\text{CH}_4$  or methane, the principal component of natural gas—currently has a low economic value because of the large increase in methane supply from hydraulic fracturing in recent years. The second drawback is that anaerobic digestion normally requires large volumes, which result in substantial capital equipment and land costs. The outcome is that anaerobic digestion of wastes is generally applied today only in large operations and where energy prices are high (e.g., in California and Hawaii).

New approaches are needed to overcome current drawbacks in capturing energy from organic wastes. For example, microbial electrochemical cells have been shown to produce a range of products, including electrical power, hydrogen gas, hydrogen peroxide, and liquid-fuel feedstock [3,7]. Because they exploit bacteria that carry out anode respiration, electrochemical systems could be much smaller than anaerobic digesters and may be able to achieve a higher conversion efficiency of organic matter into energy, N, and P. The valuable output from a microbial electrochemical cell occurs at the cathode; therefore, improved cathode materials, including catalysts, have considerable potential for substantially improving this process.

New, efficient approaches for the recovery of N and P after it is released from the organics would have a major impact on nutrient sustainability because more than 50% of the P applied in fertilizer ends up in these high-strength streams



**Figure 6.** Struvite ( $\text{MgNH}_4\text{PO}_4 \cdot 6\text{H}_2\text{O}$ ) is a source of P and N and can cause blockages in sewer pipes. [After D. Merrill]

[2,3]. A well-established technology for P and N recovery is precipitation of struvite,  $\text{MgNH}_4\text{PO}_4 \cdot 6\text{H}_2\text{O}$ . Struvite is perhaps best known as the source of urinary sediments or kidney stones and is also known to form in animal manure, where it is called “guanite.” It is interesting that the technology to make struvite originally was developed to prevent its precipitation inside anaerobic digesters used within sewage-treatment plants, where it can block pipes (see Figure 6). Struvite’s value as a slow-release fertilizer is now recognized, and several companies market struvite-based materials as fertilizers. Struvite precipitation requires that magnesium, ammonium, and phosphate be present at roughly equal-mole ratios, which means that an element in short supply (often magnesium) must be added, whereas an element in excess (usually N) is only partially captured.

An alternate approach would be to remove phosphate anions and ammonium cations from waste streams by selective separation processes. New highly selective, efficient separation approaches for processing these waste streams would provide a good replacement source for the non-sustainable supplies available currently. However, improvements in selectivity for the phosphate and ammonium ions will be particularly challenging because of the presence of many other salts in the waste streams. These

wastes are extremely complex, and separation approaches must rely on an understanding of the impacts of these other inorganic species, as well as of organics, which may compete for adsorption sites or foul separation media. As with all separation approaches, these highly selective separation media must sorb the target material reversibly and be capable of being regenerated with high efficiency.

Ammonia gas also can be recovered from organic wastes by stripping it from the waste stream at high pH (pKa for the production of ammonia,  $\text{NH}_4^+ \rightleftharpoons \text{NH}_3 + \text{H}^+$ , is  $\sim 9.3$ ). However, current technologies for recovering ammonia gas based on adsorption or condensation are very expensive, limiting their commercial use. New processes are therefore needed to allow cost-effective recovery of ammonia from waste streams.

### **Capture and recovery of P and N from Agricultural Runoff**

The N and P in agricultural runoff are the major causes of eutrophication worldwide (see the photograph of severely eutrophic water in Figure 7), and their capture would have an immensely positive impact on water quality. Because about half of the P applied as fertilizers ends up in runoff [2,3], its recovery would be a large step toward closing the loop for nutrient sustainability. The P and N are in quite different forms in runoff. The P is associated with eroded soil particles, while the N is present primarily as soluble  $\text{NO}_3^-$ . To capture P and N from agricultural runoff will thus require understanding how these materials partition in the environment. Armed with this information, researchers can devise new separation methods for recovering these materials for reuse and protecting the environment. Perhaps the biggest challenge in recovering these nutrients is that runoff is highly periodic and tends to be large in

volume, resulting in large inflows of P and N into surface waters, albeit at low concentrations. Therefore, capture of these nutrients from runoff will require highly efficient, selective, cost-effective separation and recovery methods. This need is critical because, in addition to recovery of P and N, technical and economic realities suggest that removing these nutrients to protect water quality is a major the driver of innovation in this area.



**Figure 7.** Eutrophication from field run-off and agricultural wastes causes excessive plant growth and decreases in water oxygen levels in surface waters. This process is evident in the bright green water in the Potomac River, caused by a dense bloom of cyanobacteria. (Photo by Sasha Trubetskov. Licensed under Creative Commons Attribution-Share Alike 3.0)

## Conclusions

Closing the loop for fertilizer nutrients has immense potential for making the food system more resilient against supply uncertainties, as well as for protecting water quality. However, the technologies for achieving this goal fall far short of what is required. The following areas

have been identified as high priorities for fundamental research required to close the loop on the nutrient life cycle involving P and N:

- Improved understanding of interfacial chemical processes that will lead to improved separation of targeted nutrients with high selectivity and efficiency.
- Fundamental understanding of chemical speciation and mobility of P and N in soils to improve capture for nutrient recycling and minimize runoff into surface waters.
- New catalysts and chemical processes for efficiently producing energy from waste streams, especially in concert with P and N recovery, and for producing ammonia from atmospheric N at lower cost.
- Novel sensors for in-field monitoring of nutrient levels required for optimum plant health.

## References

1. J. J. Elser and E. Bennett. "Phosphorus: A broken biogeochemical cycle," *Nature* **478**, 29–31 (2011).
2. D. Cordell, J. O. Drangert, and S. White. "The story of phosphorus: global food security and food for thought," *Global Environ. Change* **19**, 292–305 (2009).
3. B. E. Rittmann, B. Mayer, P. Westerhoff, and M. Edwards 2011. "Capturing the lost phosphorus," *Chemosphere* **84**, 846–853.
4. D. L. Childers, J. Corman, M. Edwards, and J.J. Elser. "Sustainability challenges of phosphorus and food: Solutions from closing the human phosphorus cycle," *Bioscience* **61**, 117–124 (2011).
5. R. Gaxiola, M. Edwards, and J. J. Elser. "A transgenic approach to enhance phosphorus use efficiency in crops as part of a comprehensive strategy for sustainable agriculture," *Chemosphere* **84**, 840–845 (2011).
6. B. E. Rittmann and P. L. McCarty 2001. *Environmental Biotechnology: Principles and*

Applications, McGraw-Hill Book Co., New York.

7. B. E. Rittmann. 2008. "Opportunities for renewable bioenergy using microorganisms," *Biotechnol. Bioengr.* **100**, 203–212.

### 3. Crop Protection

#### Introduction

Pesticides are defined as chemicals (or mixtures) used by humans to restrict or repel pests such as insects, weeds, fungi, nematodes, mites mollusks, birds, rodents and other organisms that affect food production or human health. The trend in the United States has been to use lesser amounts of pesticides since their use peaked in the early 1980s. This trend reflects a combination of several factors:

- Banning or phase-out of high-use volume synthetics like toxaphene, chlordane, and methyl bromide.
- Development of more efficient application techniques that deliver more chemical to the target and allow less of it to be carried away by the wind or by surface runoff, thus becoming an environmental contaminant.
- Introduction of transgenic modifications in some crops (e.g., cotton, corn, and soybeans), that confer resistance to or tolerance of pests or threats.

Farmers are also using more integrated pest management tools such as intercropping, cover crops, biocontrol, and crop rotation, along with reduced-risk chemicals such as synthetic pyrethroids, avermectins, and spinosads that are generally effective at lower application rates than conventional pesticides. These tools all work to reduce the amount of chemical applied to crops to obtain economically acceptable levels of pest control.

#### Biopesticides

Biopesticides are naturally occurring materials or are derived from natural products by straightforward chemical modification. The US Environmental Protection Agency (EPA) defines

biopesticides as natural compounds or mixtures that manage pests without a toxic mode of action.

The common elements of biopesticides can include some or all of the following characteristics: naturally occurring, little or no toxicity to non-target organisms, not persistent in the environment or in ecological food chains, useable in organic farming, low in mammalian toxicity so as to be safe to handle, and not restricted in use according to EPA and state regulatory agency labeling [1]. Few products will fit all of these criteria, but there is a clean intention to stimulate environmentally benign technologies for sustainable pest management and control. Sulfur, various mineral oils, and some plant materials, such as essential oils (e.g., orange oil for termite control) and corn gluten (for weed control), might be considered within the realm of biopesticides. However, none of the top-use pesticides in the United States, including in California, clearly meets all of the criteria for a “biopesticide” according to the EPA definition [2].

Spinosads are an example that well represents the commercial possibilities for biopesticides. This class of compounds has gained a large market share in recent years for protection of apples, pears, strawberries, and other high-value crops. This is in part because the residues left by spinosads are of low toxicity; the treated produce is considered safe for consumers, including infants and children, when the product is applied in the manner specified on the label. Spinosads are macrocyclic lactones produced by soil-borne fungi (*Saccharopolyspora spinosa*). Similarly, avermectins are macrocyclic lactones produced by fermentation of naturally-occurring soil bacteria (*Streptomyces avermitilis*). These compounds have been found to be effective for crop protection, as well as for parasite treatment and disease control in livestock. EPA has helped to move biopesticide technology forward by

offering a “fast-track” for registration of biopesticides.

The demand for these new pesticides is high because of their inherent low toxicity to mammals. Research is needed to develop new classes of these materials, including fungicides, repellants and attractants (semiochemicals), insecticides, and nematicides. For example, non-synthetic chemical management of weeds in organic culture is a serious problem, slowing wider use of organic farming methods. The few biological or environmentally benign products for weed control use high application rates or multiple applications, and even then their efficacy is somewhat unpredictable. Since the last herbicides with new modes of action were introduced 20 or more years ago, problems with weed resistance have developed. Indeed, the evolution of weeds resistant to glyphosate (Roundup®) may accelerate developments in this area. Therefore research is needed to develop effective, selective bioherbicides. Similarly, new bionematicides for soil application and for use in stored products are critically needed. This is due to the mandated (Montreal Protocol) phase-out of methyl bromide, and off-target movement and exposure issues with other fumigants like methyl isothiocyanate (MITC) and chloropicrin [3].

Semiochemicals, or sensing chemicals, are another promising class of biopesticides that are far along in development for crop production. They include pheromones, allomones, kairomones, and other attractants and repellents for both monitoring and population control of pests. Pheromones or synthetic analogs are widely used to survey for pest populations so that insecticide applications can be timed to be most effective. Mass trapping or confusion approaches have also been used with some success, using pheromones or synthetic or naturally occurring alternatives that disrupt pest insect populations. A good example is a

pheromone and natural alternative found in pear leaves that can aid in control of the codling moth in apple, pear, walnut, almond, and other crops susceptible to economic damage by this pest [4]. Controlling this damaging pest, and other boring insects that affect cotton seed and peanuts, is a critical element in controlling the invasion of *Aspergillus* fungi, which can affect pome fruits (e.g., apples and pears), nuts, or seeds and produce aflatoxins—a group of carcinogenic mold metabolites.

Insect sex pheromones are gaining in interest as they are effective in limiting pest populations and yet are nontoxic and safe for human consumption at the levels used in pest control. Because these naturally occurring chemicals are difficult to isolate from natural sources in required quantities, new synthetic routes to produce these pheromones, as well as other semiochemicals, efficiently could lead to new routes to protect crops and livestock. Recently, a concise synthesis of insect pheromones was reported using Z-selective cross metathesis [5]. Additional research is needed to identify new biopesticides from natural sources and to identify efficient synthesis routes for these and other semiochemicals.

Another innovative approach to pest control was recently illustrated by Pulsifer et al. [6], who used photonic crystal patterning to replicate the unique coloration of the emerald ash borer (*Agrilus planipennis*) in inanimate plastic decoys. This brightly colored green insect is an invasive species that has killed hundreds of millions of ash trees in North America since 2002. The decoys (see Figure 8) are designed to fool male insects, who identify their mates visually. The production of convincing decoys required the development of methods to faithfully replicate the microstructure of the female insect wings using masters made by pattern transfer from flexible poly(dimethylsiloxane) stamps [6]. This study



built on soft lithography methods and photonic crystal design principles that have been developed primarily for applications in microelectronics and optics and applied them to a problem of practical interest in agriculture.



**Figure 8.** Emerald ash borer (left) and a manufactured decoy (right). [After J. Bionic Engr.,10, 129-138 (2013)]

### Gene-based Crop Protection

Chemical control of pests is widely practiced, but major crops (e.g., wheat, rice and other staples) genetically improved to resist pests (insects, disease, nematodes, weeds) are needed to offset chemical usage while protecting valuable food sources. In some cases the resistance genes are engineered into the crop, giving farmers new genetic resources for insect resistance, such as *Bacillus thuringiensis* genes in corn and Roundup Ready cotton. In these genetically modified varieties, little or no external chemical pesticide application may be needed. In the case of Roundup Ready crops, the crop is resistant to the herbicide Roundup, allowing use of the chemical to control a suite of weeds that might lower or destroy the crop quality if present during crop growth and harvesting.

Gene-based technologies, such as RNA interference (RNAi), are underpinning new technologies in pest control (see Figure 9) [7].

RNAi is based on a natural process that affects the activity of genes. Research has successfully led to artificial RNAs that target genes in pest insects, slowing growth or killing them. The development of genetically modified crops that make RNAi harmful to their pests is under active exploration. As with most new technologies, there is a safety concern that RNAi or other gene-based technology might also harm desirable species. Research is needed to address this concern prior to deployment of any gene-based technology to gain public acceptance.

New methods will also be needed to identify early signs that pests are developing resistance to any of these new control approaches. Seemingly, for every technological advance, the target pest evolves a strategy for overcoming the protection, as happened with resistance in insect and fungal pests previously controlled with synthetic pesticides like DDT and parathion. This is possible with the next generation of pest control, whether biopesticides or genetically modified crops.

### Smart Application Systems

It has been estimated that often at least half of a pesticide application does not reach the crop to be protected, but rather bypasses the target and enters the soil, contacts non-target vegetation, or is carried away by wind. As is the case for targeted water and fertilizer application, new materials and approaches are needed for applying pesticides to crops. These improvements would save on the amount of pesticide needed for a particular application and prevent inadvertent residues that can harm unintended crops, waterway quality, or animals and humans. For example, pesticides could be delivered via drip irrigation. In addition, new analytical methods and sensors are needed to identify the presence of threats to crops so pesticide application can be made precisely at

the right time and at the right level of application.



**Figure 9.** RNAi offers a new means of pest-control. For example, corn rootworms can be controlled by using RNAi to kill larvae that feed on corn roots. The RNAi is introduced into the corn plant and is ingested by the worm, disrupting the production of specific proteins. Source: *Science* 341, 732–733, 20130 (2013)

### Conclusions

The need to produce food for a world population expected to exceed 10 billion by the end of the century will require the use of pesticides as primary tools for combating pests in the field and in stored food products, as well as for public health. The field of pest management needs to change from sole reliance on toxic chemicals to bio-based approaches that are effective but pose little risk to animals, humans, and the environment. There is a need to transition from conventional, broad-spectrum chemical control of pests to a more biologically sustainable system of control, one that uses many different, specific biopesticides in a “toolbox” approach. Overall, fundamental research efforts in the following areas have been identified as high priorities for the development of new approaches to crop protection:

- Elucidating the mechanisms of bio-based pesticide and weed control, including semiochemicals and RNAi, to improve selective pest management with minimal impacts to human health and the environment.

- Identifying new biopesticides and create synthesis routes for viable production.
- Understanding the mechanisms of gene-based technologies such as RNAi that will yield plants modified for pest control.
- Developing new analytical tools and sensors for detecting pests and monitoring crop health to allow precise application of pesticides.
- Developing new approaches and materials for precise delivery of pesticides to crops.

### References

1. C. L. Cantrell, F. E. Dayan, and S. O. Duke. “Natural products as sources for new pesticides,” *J. Natl. Products* **75**, 1231–1242 (2012).
2. California Use Report, California Department of Pesticide Regulation, Sacramento, California.
3. Ozone Secretariat. The Montreal Protocol on Substances that Deplete the Ozone Layer, from United Nations Environment Programme, 2000.
4. M. Light and J. J. Beck. “Behavior of codling moth (Lepidoptera: Tortricidae) neonate larvae on surfaces treated with microencapsulated pear ester,” *Environ. Entomol.* **41**(3), 603–611 (2012).
5. M. B. Herbert, V. M. Marx, R. L. Pederson, and R. H. Grubbs. “Concise synthesis of insect pheromones using z-selective cross metathesis,” *Angewante Chemie Int. Ed.* **52**, 310–314 (2013).
6. D. P. Pulsifer, A. Lakhtakia, M. S. Narkhede, M. J. Domingue, B. G. Post, J. Kumar, R. J. Martín-Palma, and T. C. Baker. “Fabrication of polymeric visual decoys for the male emerald ash borer (*Agrilus planipennis*),” *J. Bionic Engr.* **10**, 129–138 (2013).

## 4. Innovation in Processes and Materials to Prevent Waste of Food and Energy

### Introduction

Directly or indirectly, our food is created by the conversion of distributed solar energy to concentrated chemical energy. Energy densities of foods span a wide range, from approximately 1 kJ/ g for fruits and vegetables up to approximately 40 kJ/ g for pure lipids. As a form of energy, food is comparable to fossil fuels, with various coal grades containing 20–30 kJ/ g [1]. The United States population of nearly 315 million people consumes food with a total energy content of  $\sim 1 \times 10^{18}$  J (1 quad) annually, representing about 1% of our national annual energy budget of  $\sim 100$  quads [2]. Of course, even more energy is consumed in producing, transporting, processing, handling, storing, and preparing food. A conservative estimate of the energy required for food intended for domestic consumption amounts to  $\sim 8\%$  of our national energy budget [3]. Using broader criteria for energy requirements, the US Department of Agriculture reports that our food systems account for  $\sim 16\%$  of annual US energy consumption [4], mostly in the food production phase.

Some foods, especially animal proteins, are inherently more energy-intensive than others. For example, producing the 43 million tons of meat, poultry, and fish that Americans consumed in 2004 required  $\sim 800$  TJ of energy ( $1 \text{ TJ} = 10^{12} \text{ J}$ ); whereas only 75 TJ were needed to supply 74 million tons of grains [3]. Consumer choices based on food-miles (i.e., the preference for locally- grown foods, based on their lower transportation energy requirements) are often far less consequential than the types of food we choose to eat [5]. Because of the

magnitude of these energy requirements, combined with the rising share of our national energy budget devoted to food [4], changes in the cost and availability of energy (e.g., via a carbon tax) would have important repercussions upon food prices. The corollary is that wasted food (i.e., food that is produced but not consumed) represents a very significant amount of wasted energy and unnecessary greenhouse gas emissions.

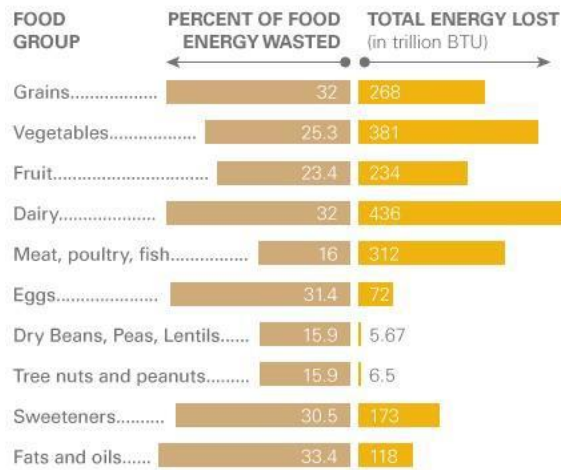
Food is also a water-intensive commodity, and the link between food and freshwater consumption is especially strong. A recent, high-resolution study estimates that 92% of the annual global water footprint is attributable to agriculture [6]. Thus discarded food also represents an enormous amount of wasted water, at a time when water scarcity is a concern in many parts of the United States, particularly in its most valuable food- producing regions, such as California.

Because valuable resources such as energy and freshwater are also wasted when food is discarded, new technologies are needed to minimize waste by protecting food from farm to table. Furthermore, new technologies can be used to recover the energy content of food waste and/or convert it into other useful products.

### Magnitude of the Food Waste Issue

Food is lost from food supply chains (FSCs) when spoilage makes it no longer fit for human consumption. However, food is also wasted when it is discarded for reasons related to consumer preferences [7]. One study estimates that globally, as much as half of all food grown is never consumed [8]; another reports that worldwide, some 30–50% of all edible food is discarded instead of being consumed [9]. In developed countries, the fraction seems to be about one- quarter. For example, Kantor and

Lipton estimate that 27 % of edible food was wasted in the United States in 1995 [7]. Cuéllar and Webber consider this to be a lower bound for contemporary food waste, but nevertheless used it to estimate that the energy loss due to discarded food represents approximately 2% of our national energy budget [3].



**Figure 10.** Food energy and waste in America. ([www.utexas.edu/features/2010/11/20/food\\_waste](http://www.utexas.edu/features/2010/11/20/food_waste))

Waste is concentrated at different places in food supply chains depending on the country [10]. In developing countries, lack of a reliable cold chain and degradation by pests are significant contributors to post-harvest food waste [7]. In contrast, the post-consumer stage accounts for a large fraction of food waste in developed countries. Losses are highest for dairy products (33% discarded) and fruits and vegetables (25% discarded), because of their highly perishable nature (Figure 10). The fraction of wasted food has increased in recent decades because of urbanization (which requires longer food supply chains), increasing consumer choice and increasing affluence (which result in a declining fraction of household budgets dedicated to food, minimizing the penalty for waste), smaller household sizes (since the fraction of wasted is inversely related to household size), and expanding consumer preferences for more perishable foods [7].

## Reducing Food Waste with Enhanced Packaging

In the United States, food is discarded mainly by its distributors and consumers, who do so largely for quality and/or cosmetic reasons. The use of expiration dates on packaging is a very crude way to detect when food is no longer edible and causes considerable amounts of usable food to be wasted. New technologies that enhance supply chain management (such as embedded food labeling) and reduce energy use (such as high-efficiency cool storage systems [7]) could reduce waste during processing, transportation, and storage of food items. In addition, new materials could greatly enhance the preservation of food quality from farm to table. Improved packaging materials, for example, could protect against food spoilage. Clay-polymer and graphene oxide-polymer composite films are reported to provide superior food preservation because of their extremely low gas permeabilities, [11] and antibacterial wrapping paper coated with silver nanoparticles has been shown to prolong shelf-life [12]. Edible coatings could be developed to prevent fresh fruit and vegetables from dehydrating or spoiling, to enhance shelf life, and to reduce the amount of refrigeration required to keep products fresh [13]. Catalysts (including photocatalysts) can be designed to destroy ethylene and thereby delay ripening or prevent over-ripening of fruits and vegetables [14].

In addition to improved food packaging, innovations are needed to provide indicators for spoilage. So-called smart polymers containing TiO<sub>2</sub> nanoparticles and methylene blue have been developed that change color when exposed to oxygen [15]. Further research is needed to develop additional indicators of food integrity, such as temperature-sensitive inks and/or labels to detect even short temperature excursions that may trigger food spoilage. Wrappers might be designed to contain inexpensive sensors that

detect harmful bacteria present in foods. Such sensors could also be self-reporting to assist in inventory control in transit, at the store, or in the home. For both enhanced packaging and sensors, new technologies and strategies must be inexpensive, robust, and sustainable.

### Recovering the Energy Content of Discarded Food

*"If 50% of the food waste generated each year in the U.S. was anaerobically digested, enough electricity would be generated to power over 2.5 million homes for a year."*

<http://www.epa.gov/region9/waste/features/foodtoenergy/>.

Over 30 million tons of food waste ends up in US landfills annually (Figure 11, [16]) not including the millions of tons of waste (manures) associated with meat and dairy production. Although gases are captured from landfills in some places, discarding wasted food in this way represents a lost opportunity for the production of energy. Recovering some of this energy would have the desirable side-benefit of reducing N<sub>2</sub>O and CH<sub>4</sub> emissions to the environment that arise from landfills as well as from poor composting practices.

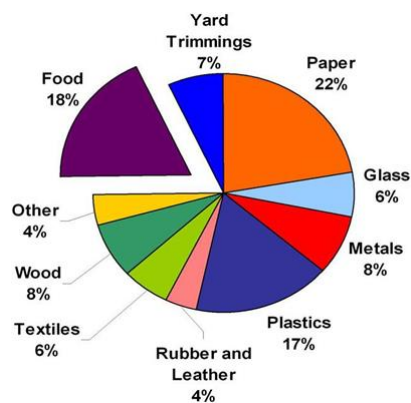
Improved processes are needed to extract energy efficiently from food and animal wastes. A variety of conversion processes can be envisaged, including microbial and catalytic treatments. For example, anaerobic digestion in wastewater treatment plants can be used to generate biogas [17]. Such processes need to be designed to optimize all potential uses of the waste materials—energy, biomass (to be used in chemicals and materials, as described in Section 3), and nutrients (as described in Section 2). This holistic approach will provide the ultimate

recycling of wastes to useful products, including returning carbon to the soil.

### Conclusions

Innovative research in developing new processes and materials for reducing food waste, thereby improving the efficiency of energy and water use in food production, is a high priority. The following areas are examples of potential targets for fundamental research:

- Design of new packaging and coating materials to protect foods from primary degradation processes—such as exposure to oxygen, ethylene, and other chemicals—and extend food shelf-life.
- Development of new sensors that can detect changes in temperature, the presence of microbes and toxins, and other issues that impact food quality.
- Discovery of efficient microbial and/or catalytic processes to recover the energy content of food waste (see Sections 2 and 6 for more detail).
- Integration of these approaches to allow full utilization of food wastes, including energy production, biomass-based chemical and materials, and fertilizers and returning remaining waste material to the soil to enrich it.



**Figure 11.** Annual contributions to US landfills. Source: Municipal solid waste generation, recycling, and disposal in the United States, EPA 2007.

## References

1. Food and Agriculture Organization. *Food Energy—Methods of Analysis and Conversion Factors*, FAO Food and Nutrition Paper 77, Food and Agriculture Organization of the United Nations, Rome, 2003. Available online at: [www.fao.org/docrep/006/y5022e/y5022e00.htm#Contents](http://www.fao.org/docrep/006/y5022e/y5022e00.htm#Contents). Accessed June 18, 2014.
2. Department of Energy. *Annual Energy Review 2007*, DOE/EIA-0384 (2007), Energy Information Administration, Washington, D.C., June 2008.
3. A. D. Cuéllar and M. E. Webber. “Wasted food, wasted energy: The embedded energy in food waste in the United States,” *Environ. Sci. Tech.* **44**(16), 6464–6469 (2010). <http://pubs.acs.org/doi/full/10.1021/es100310>
4. P. Canning, A. Charles, S. Huang, K. R. Polenske, and A. Waters. *Energy Use in the U.S. Food System*, US Department of Agriculture, Economic Research Service, 2010.
5. C. L. Weber and H. S. Matthews. “Food-miles and the relative climate impacts of food choices in the United States,” *Environ. Sci. Tech.* **42**(10), 3508–3513 (2008). DOI: 10.1021/es702969f
6. A. Y. Hoekstra and M. M. Mekonnen. “The water-footprint of humanity,” *PNAS* **109**, 3232–3237 (2012). DOI: 10.1073/pnas.1109936109
7. L. S. Kantor and K. Lipton. “Estimating and addressing America’s food losses,” *Food Review* **20**(1), 2 (1997).
8. Lundqvist, C. de Fraiture and D. Molden. *Saving Water: From Field to Fork—Curbing Losses and Wastage in the Food Chain*, SIWI Policy Brief, SIWI, 2008. Available online at [www.siwi.org/publication/from-field-to-fork-wastage-of-water-in-the-food-chain/](http://www.siwi.org/publication/from-field-to-fork-wastage-of-water-in-the-food-chain/). Accessed June 18, 2014.
9. Institution of Mechanical Engineers. *Global Food: Waste Not, Want Not*, Institution of Mechanical Engineers, London, January 2013. Available online at [www.imeche.org/knowledge/themes/environmental/global-food](http://www.imeche.org/knowledge/themes/environmental/global-food). Accessed June 18, 2014.
10. J. Parfitt, M. Barthel, and S. Macnaughton. “Food waste within food supply chains: Quantification and potential for change to 2050,” *Phil. Trans. R. Soc. B* **365**, 3065–3081 (2010). DOI: 10.1098/rstb.2010.0126
11. Y.-H. Yang, L. Bolling, M. A. Priolo, and J. C. Grunla. “Super gas barrier and selectivity of graphene oxide-polymer multilayer thin films,” *Adv. Mater.* **25**, 503–508 (2013). DOI: 10.1002/adma.201202951
12. R. Gottesman, S. Shukla, N. Perkas, L. A. Solovyov, Ye. Nitzan, and A. Gedanken. “Sonochemical coating of paper by microbiodicidal silver nanoparticles,” *Langmuir* **27**(2), 720–726 (2011). DOI: 10.1021/la103401z
13. A. E. Pavlath and W. Orts. “Edible films and coatings: Why, what, and how?” in *Edible Films and Coatings for Food Applications*, M. E. Embuscado and K. C. Huber, eds., Springer, 2009, pp. 1–23. DOI 10.1007/978-0-387-92824-1\_1
14. N. Keller, M.-N. Ducamp, D. Robert, and V. Keller. “Ethylene removal and fresh product storage: A challenge at the frontiers of chemistry. Toward an approach by photocatalytic oxidation,” *Chem. Rev.* **113**(7), 5029–5070 (2013). <http://pubs.acs.org/doi/abs/10.1021/cr900398v>
15. S.-K. Lee, A. Mills and A. Lepre. “An intelligent ink for oxygen,” *Chem. Commun.*, 1912–1913 (2004). A. Mills, K. Lawrie, J. Bardin, A. Apedaile, G. A. Skinner and C. O’Rourke, “An O<sub>2</sub> smart plastic film for packaging,” *Analyst* **137**, 106–112 (2012). DOI: 10.1039/C1AN15774D
16. Environmental Protection Agency. “Municipal solid waste generation, recycling, and disposal in the United States: Facts and figures for 2008,” US Environmental Protection Agency, November 2009. <http://www.epa.gov/epawaste/nonhaz/municipal/pubs/msw2008rpt.pdf>. Accessed June 17, 2014.
17. J. W. Levis and M. A. Barlaz. “What is the most environmentally beneficial way to treat commercial food waste?” *Environ. Sci. Tec.* **45**(17), 7438–7444 (2011). DOI: 10.1021/es103556m

## 5. Sensors for Food Security and Food Safety

### Introduction

As the world population continues to increase, enhanced food production will become increasingly important. Food safety is also a significant challenge. The Centers for Disease Control and Prevention (CDC) estimates 48 million cases of foodborne illness occur each year and 3,000 of those result in fatalities [1]. These food safety challenges result in substantial economic losses (nearly \$152 billion/year) to the US food industry [2]. Sensor technology can provide needed monitoring of food quality from “farm-to-fork” and assist in enhanced crop yields.

Precision agriculture (PA), as applied to crop production in its most basic form, means collecting data on the performance of sections of fields and then using those data to make decisions about crop planting density and fertilization (Figure 12). However, in the mid-1090s, the ability to produce low-cost geographical positioning systems (GPS) and yield monitors redefined the term to allow studies of large plots of land. Today, a more general definition of PA as applied to crop production is “focusing on sustainable development and taking into account traditional profitability along with environmental and social benefits [3].” Stated in operational terms, the goals of PA are to enable maximum crop yields by using only the necessary amount of fertilizer and pesticides. In full implementation, fertilizer runoff would be eliminated and pesticides would be used only when necessary and at levels that would be well below allowable levels for consumption described by the Food and Drug Administration.

### State-of-the-Art Food Security

Wireless sensor technology for monitoring the complicated interplay between the quality of soil, soil moisture level, nutrient levels (phosphorus, nitrogen and potassium), weather patterns, and crop yield are under development. For example, on-the-go sensors connected to GPS units for monitoring pH, conductivity, salinity, dissolved oxygen, and nutrient concentration have been tested. These devices include electrochemical, electromagnetic, and optical detection concepts. However, ion selective electrodes (ISEs) and ion selective field effect transistor systems have been the most studied to date. Solvent extraction followed by electrochemical detection is currently used to characterize analyte concentrations at the level of mg/L [4].

Sensor networks that can report soil water content and volatile organic molecules are important for precision farming, but they must be inexpensive and reliable and preferably will communicate wirelessly. An interesting development in this field is the molecular design of ethylene sensors based on copper (I) complexes embedded in carbon nanotube networks. Such networks are sensitive to chemically driven swelling of the contact points between nanotubes that changes the electrical resistance of the network. These low-cost sensors are highly selective for ethylene and can detect it at sub-ppm levels from ripening fruit [5]. Such sensor arrays are readily multiplexed to analyze complex gas mixtures via principal component analysis.



**Figure 12.** Real time monitoring of nutrients, water and soil quality. Source: Velez, <http://sdcornblog.org/archives/tag/precision-agriculture>

We have an increasingly sophisticated understanding of the chemical signaling that is the “language” of plants [6],” and of the biochemistry that limits crop yields. Innovations in materials are now beginning to enable low-cost sensing at a scale that is relevant to precision farming and to minimizing food waste along the supply chain.

### Food Safety

Pathogen detection is one area of significant interest for the evaluation of food safety. The gold standard for pathogen detection involves culturing and plating, which typically takes 3–10 days. Methods for rapid, reliable detection of foodborne pathogens are needed to ensure safety. Biosensors involving the use of antibodies or DNA for the detection of pathogens such as *E. coli* and *Bacillus cereus* and *Listeria* have been reported. Detection capabilities requiring from 1 hour to 10 minutes of analysis have been achieved using electrochemical measurements [7, 8]. Optical methods of monitoring pathogens are also under study. However, most of these methods are currently not field-portable, or the sensitivity of

the method is too low for it to be useful. Nano-optical sensors for food safety applications are also under development that can cut the analysis time to 4–8 hours [9]. Other analytical techniques, such as field-portable mass spectrometry, may also provide rapid detection and identification of pathogens.

Real-time detection of trace amounts of herbicides and pesticides is also desirable from PA and food safety applications. As an example, miniature chip-based devices have been developed that can detect atrazine at a level of 100 nM in plant material [10]. However, real-time, in situ methods do not currently exist.

Innovative concepts that would detect trace chemicals and pathogens would greatly enhance food security and safety. For example, 3-dimensional imaging methods were developed recently that allow 3-dimensional sensing and visualization of biological organisms. This technology involves the detection of pathogens in real time using 3-dimensional dynamic holographic microscopy. Although this new technology is currently not field-portable, would it become possible, with continued innovation, for it to provide near-site or in situ analyses [11]? Recent examples using Raman microscopy and Fourier transform infrared imaging of cells and cell components also illustrate the possibility of other spectroscopic techniques that might be valuable in providing pathogen analysis [12].

### Conclusions

The development of robust, highly specific, sensitive detectors for PA would significantly contribute to food security across the world. Innovations in food safety would not only improve human health but also provide considerable economic value. Overall, fundamental research in the following areas has



been identified as representing high priorities for developing a new generation of sensors for food security and food safety:

- Understanding of the combination of sensor technologies that will describe correctly the appropriate soil properties for a diverse range of crop growth conditions
- Improved precision and accuracy of sensors of interest for PA
- Computational analysis to assess sensor data in real time
- New analytical methods with lower detection limits for rapid analysis of pathogens, pesticides, and herbicides and other environmental pollutants
- Real-time monitoring of both biological and chemical toxins either in the field or near the field to allow the removal of contaminated foods from the food chain

## References

1. J. A. Flint et al. "Estimating the burden of acute gastroenteritis, foodborne disease, and pathogens commonly transmitted by food: An international review," *Clin. Infect. Dis.* **41**, 698–704 (2005).
2. R. Scharff. "Health related costs from foodborne illness in the United States," The Product Safety Project at Georgetown University, [www.productsafetyproject.org](http://www.productsafetyproject.org), 2010.
3. A. McBratnew, B. Whelan, and T. Ancev. "Future direction of precision agriculture," *Precision Agriculture* **6**, 7–23 (2005).
4. H. J. Kim, K. A. Sudduth, J. A. Hummel, and S.T. Drummond. "Validation testing of a soil macronutrient sensing system," *Trans. Amer. Soc. Agric. Biol. Eng.* **56**, 23–31 (2013).
5. B. Esser, J. M. Schnorr, and T. M. Swager, "Selective detection of ethylene gas using carbon nanotube-based devices: Utility in determination of fruit ripeness," *Angew. Chem. Int. Ed.* **51**, 5752–5756 (2012).
6. I. T. Baldwin, R. Halitschke, A. Paschold, C. C. von Dahl, and C. A. Preston. "Volatile signaling in plant-plant interactions: 'Talking trees' in the genomics era," *Science* **311**(5762), 812–815 (February 10, 2006).
7. J. Kirsch, C. Siltanen, Q. Zhou, A. Revzin, and A. Simonian. "Biosensor technology: Recent advances in threat agent detection and medicine," *Chem. Soc. Rev.* **43**, 8733–8768 (2013).
8. K. Arshakm, V. Velusamy, O. Korostynska, K. Oliwa-Stasiak, and C. Adley. "Conduction polymers and their applications to biosensors: Emphasizing on foodborne pathogen detection," *IEEE Sensors Journal* **9**, 1942–1951 (2009).
9. E. Bae and A.K. Bhunia, "Nano-optical sensors," Chapter 19 in *Optochemical Nanosensors*, Andrea Cusano, Francisco J. Arregui, Michele Giordano, and Antonello Cutolo, eds., Taylor and Francis, pp. 497–512, 2012.
10. K.-S. Shin, Y. H. Kim, J.-A. Min, S.-M. Kwak, S. K. Kim, E. G. Yang, J.-H. Park, B.-K. T.-S. Kim, and J. Y. Kang. "Miniaturized fluorescence detection chip for capillary electrophoresis immunoassay of agricultural herbicide atrazine," *Anal. Chim. Acta*, **573-574**, 164–171 (2006).
11. Yeom, I. Moon, and B. Javidi. "Real-time 3-D sensing, visualization, and recognition of dynamic biological microorganisms," *Proc. IEEE* **94**, 550–567 (2006).
12. C. Petbois. "Imaging methods for elemental, chemical, molecular and morphological analysis of single cells," *Anal. Bioanal. Chem.* **397**, 2051–2065 (2010).

## 6. Maximizing Biomass Conversion to Fuels, Chemicals, Food, and Materials without Harming Food Production

### Introduction

There is ever-increasing strain on the food supply from the competition in land and water use between food production and biomass production for non-food use. To ease this strain, more efficient processes must be developed for conversion of biomass to fuels and bulk chemicals/materials. Further, the more these processes use only those parts of the crops that are not edible (namely lignocellulosic biomass), the less strain the competition will place on the food supply. While the best use for a large part of this biomass is to put it back into the soil to improve soil quality and nutrient levels, estimates indicate that roughly half can be used more effectively in alternative processes. Therefore basic research is needed that will enable processes for more resource-efficient conversion of lignocellulosic biomass to fuels, bulk chemicals, materials, food, and energy. In addition, more sustainable land-efficient and water-efficient ways are required to produce the biomass needed for these alternative processes to minimize the impact on food supply. Further, the need for a closed-cycle-based economy requires that biomass be efficiently recycled and returned to the market. To realize the full potential of biomass and still protect the food supply will require significant technical advances in catalysis.

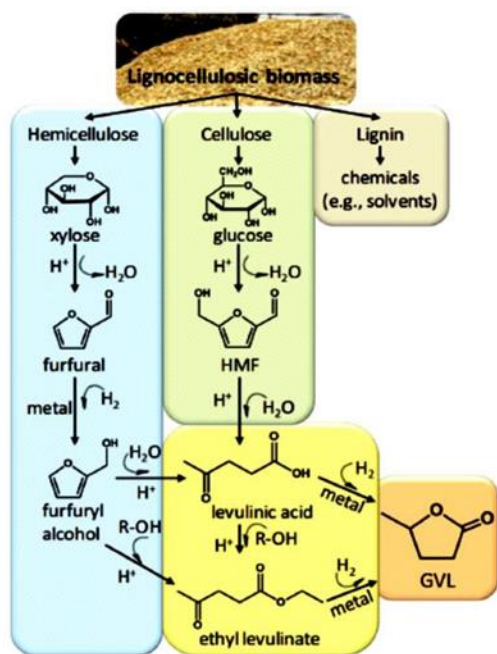
### Catalytic Conversion of Biomass to Fuels and Chemicals

Dumesic recently outlined a roadmap for conversion of lignocellulosic biomass to chemicals and fuels [1,2], as summarized in Figure 13. The lignocellulosic biomass is first fractionated into its main components (hemicellulose, cellulose, and lignin), which allows for processing each fraction at different conditions to achieve high yields of target products (mainly C6 and C5 sugars). These are then further processed at mild conditions to make “platform chemicals”: furfural, hydroxymethylfurfural, and levulinic acid (LA), [3,4] and then gamma-valerolactone (GVL). These platform chemicals are less reactive than the original sugars and therefore more stable, yet they have enough functionality to be used as building blocks to produce a variety of chemicals and fuels depending on market demand. For example, GVL can be produced from C6 and C5 sugars through hydrogenation of LA as an intermediate (Figure 1). GVL is stable in water and air and is nontoxic. It can be used as a solvent and has the functionality/reactivity to be upgraded to a variety of chemicals, fuels additives, and fuels. This is but one example of how biomass can be converted to fuels [5,6].

Alternatively, sugars or platform molecules produced from such biomass can be converted to food ingredients. Some processes for this are already commercialized. For example, CJ Bio America began construction of a \$320 million lysine production facility in Fort Dodge, Iowa, in 2012 that will annually produce more than 100,000 metric tons of amino acids to supplement animal feeds. The plant will convert corn by-products to lysine, an essential amino acid that will be used in hog and poultry feed.

The examples described illustrate the enormous promise for the conversion of biomass to fuels, chemicals, and food. To reach the full potential

of biomass conversion to useful products, new catalysts and chemical processes need to be developed and optimized to make them highly efficient. Further, these processes should be designed to use starting biomass that does not compete with food production or to use byproducts from food production.



**Figure 13.** Fractionation of lignocellulosic biomass and reaction pathways to produce GVL from hemicellulose and cellulose. Source: Alonso, *Green Chemistry* 15, 2013]

### Heterogeneous Catalysis in the Liquid Phase

Essentially everything we know about the state of working heterogeneous catalysts and their surfaces (e.g., structure, oxidation states of metals) comes from years of research and applications using gas-phase reaction conditions. These reveal that catalyst performance depends sensitively on the sizes and even shapes of the nanoparticles, the nature of the support surfaces upon which they sit, and the oxidation states. But biomass conversions require liquid-phase processes instead. The solvents and solvent mixtures that are employed in these reactions can produce a complex

environment with multiple variables that must be understood and controlled to optimize conditions. Such variables include composition, pH, polarity, hydrophobicity, and others. To understand these complex catalytic processes under these conditions, new analytical tools are needed for examining the structures of supported nanoparticles and the surfaces of these nanoparticles and their support materials under liquid solutions. Further, methods are needed to examine reactions occurring at these interfaces in situ and in operando. Especially important will be the use of multiple experimental techniques requiring the use of data analytics to interpret and guide experiments. New approaches are also needed to predict and model these catalytic materials and associated processes to help accelerate the discovery of new catalyst systems.

### Conclusions

Many potential scenarios exist for converting biomass to fuels, chemicals, food, and materials without harming food production. However, for these scenarios to be realized, chemical processing of lignocellulosic biomass needs to be improved so that it is more energy-efficient and the capital equipment is less costly. Basic research in chemistry and physics is needed to provide the understanding needed to guide the development of new and improved processing strategies.

The following areas have been identified as high priorities for fundamental research:

- Enhancement of fundamental understanding of structure–function relationships in catalytic materials
- New analytical tools for studying the structures of catalyst surfaces and reaction dynamics in situ and in operando, especially in liquid phases

- New computational methods to model interfacial reactions on solid surfaces, in both gas and liquid environments, to help interpret and guide experiments
  - New computational and experimental approaches for accelerating the discovery of new heterogeneous catalysis processes in both gas and liquid phases
  - New liquid-phase catalytic processes
    - Understanding of the state of metal nanoparticle catalysts under liquid-phase reaction conditions
    - Understanding of the effects of solvents on reaction kinetics
    - Understanding of how to stabilize catalyst structures in liquid solution under reaction conditions
5. Singh, N. R., W. N. Delgass, F. H. Ribeiro, and R. Agrawal. "Estimation of liquid fuel yields from biomass," *Environ. Sci. & Tech.* **44**, 5298–5305 (2010).
  6. Venkatakrisnan, V. K., J. C. Degenstein, A.D. Smeltz, W. N. Delgass, R. Agrawal, and F. H. Ribeiro. "High-pressure fast-pyrolysis, fast-hydroxylation and catalytic hydrodeoxygenation of cellulose: Production of liquid fuel from biomass," *Green Chem.* **16**, 792–802 (2014).

This basic research in surface chemistry and catalysis has the added benefit that it will help advance many other technologies that impact food systems, such as liquid-phase separations and energy technologies (e.g., fossil fuels conversions, solar energy, and energy storage).

## References

1. Alonso, D. M.; S. G. Wettstein, and J. A. Dumesic. "Gamma-valerolactone, a sustainable platform molecule derived from lignocellulosic biomass," *Green Chem.* **15**, 584–595 (2013).
2. Wettstein, S. G.; D. M. Alonso, E. Gurbuz, and J. A. Dumesic. "A roadmap for conversion of lignocellulosic biomass to chemicals and fuels," *Current Opinion in Chemical Engineering* **1**, 218–224 (2012).
3. T. Werpy and G. Petersen, *Top Value Added Chemicals from Biomass. Volume I: Results of Screening for Potential Candidates from Sugars and Synthesis Gas*, US Department of Energy, Washington, D. C. 2004. Available at <http://www.nrel.gov/docs/fy04osti/35523.pdf>. Accessed June 2014.
4. J. J. Bozell and G. R. Petersen, *Green Chem.* **12**, 539–554 (2010).

## Summary

The need to ensure a secure and affordable food supply is a high priority for the future of humankind. The relationship of food production with water and energy must be considered together, as stresses on one area—due to global population growth, climate change, political environment, or other factors—can profoundly impact the others. This can be seen when shortages of water or energy impact the availability (and price) of food or when land/crops and water are diverted to produce energy. If the three issues are considered together, solutions can be developed to mitigate these stresses.

The technical challenges involved in maximizing, recycling, and reusing resources associated with global food production are daunting—representing scales rarely considered previously. This Mathematics and Physical Sciences Advisory Committee subcommittee, charged to study the role of the National Science Foundation/Mathematics and Physical Sciences Directorate (NSF/MPS) in food systems research, has identified a number of technical bottlenecks that currently exist in the food supply chain, with special consideration of the inextricable roles of water and energy. This led to the identification of six specific research areas for MPS: (1) Ensuring a Sustainable Water Supply for Agriculture; (2) “Closing the Loop” for Nutrient Life Cycles; (3) Crop Protection; (4) Innovations to Prevent Waste of Food and Energy; (5) Sensors for Food Security and Safety; and (6) Maximizing Biomass Conversion to Fuels, Chemicals, Food, and Materials.

In addressing the research needed in these areas, a number of themes emerged as high priorities for research in the mathematical and physical sciences. These cross-cutting themes, described below, are meant to inspire scientists to develop broad fundamental knowledge that will underpin

the development of revolutionary technologies for ensuring a sustainable food supply in the future. Finally, the subcommittee believes that NSF/MPS has a special role in this research, educating and training the next-generation workforce that will develop additional technology breakthroughs and support the entire food production enterprise.

*Separations* play a critical role in the development of future technologies for sustainable food systems. To be widely adopted, new separations methods must have high selectivity and efficiency but must operate at low costs, especially with respect to energy use. The gas and liquid streams generated in food production are large and complex and current separation methods fall far short of what is needed to provide clean water for crops from brackish or salt water sources or from wastewater and runoff. Using these non-conventional sources will reduce global dependence on ever-shrinking freshwater sources for food production. Likewise, new separations methods are needed to recover critical nutrients, such as phosphorus and nitrogen, from runoff and from food and animal wastes. Recovering phosphorus is particularly important because this element is a limiting nutrient, required for plant and animal growth; it has been estimated that global supplies of readily mined, high-grade phosphorus are limited to only a few decades of use. To meet these needs for nutrients, one can envision entirely new strategies for separations, including novel adsorbents based on bio-inspired processes and molecular recognition to provide optimized separation. However, it is first necessary to gain improved understanding of separation processes for applications specific to food sustainability. Complementing experimental studies, computational methods can play an important role in modeling materials transport that occurs during separation, as well

as in designing new materials and processes specifically tailored for optimized separations. With this knowledge, a new generation of highly efficient, selective, and low-energy separation processes can be developed.

**Catalyst materials and catalytic processes** will enable the development of new chemicals and materials for future agriculture systems. Demand for fertilizers will grow rapidly as the demand for food increases globally. New catalytic processes are needed to produce ammonia and other forms of fixed nitrogen from atmospheric nitrogen with far lower energy requirements than current processes have. The development of “green” or renewable energy, or even chemicals and materials derived from plant and animal wastes, has enormous potential to utilize material now discarded in landfills. A new generation of catalysts, especially those that can operate in solution, are critically needed to realize this vision. This will require research focused on obtaining fundamental insight into both the structures of metal nanoparticles and the dynamics of associated reactions in the liquid phase, including understanding the effects of solvation on reaction kinetics. This knowledge will enable the design of a new generation of catalysts that can operate in solution at low temperatures and pressures, thereby reducing energy costs. Computational modeling is needed to help guide these experiments, interpret data, and design highly selective catalytic materials and chemical processes. In addition to conventional heterogeneous catalysts and electrocatalysts, the development of new microbial and bio-inspired catalytic processes is also important, especially for the conversion of food and animal wastes to biogas and energy production.

**Interfaces** between solids and fluids are the basis of functionality in both separation and catalytic processes; however, our understanding of these interfaces is rudimentary at best.

Research must be directed toward the elucidation of fundamental physical and chemical processes occurring at surfaces to allow these processes to be optimized. This information will form the foundation needed to develop new materials and chemical processes required for specific applications in separation processes and the production of fuels, chemicals, and materials from biomass. Understanding interfaces will also assist in designing membranes that can resist fouling when used with complex feed waters. Improved membrane separations can enhance wastewater reuse and lower costs in desalination pretreatment. Further, the interactions of essential plant nutrients, including phosphorus and nitrogen, with the surfaces of soil particulates must be fully understood to design processes for more efficient delivery of these nutrients to root systems and for recovery from field runoff.

**New materials and chemical processes** tailored for specific applications will greatly advance the efficient production of food with low impact on water and energy. For example, as new approaches to field irrigation become more efficient and transition to targeted, on-demand micro-irrigation systems, new polymeric materials that are renewable, robust, and self-healing are needed. To avoid staggering food waste that currently has an enormous impact on both water and energy usage in food production, new materials for packaging and coatings are needed. These materials will be specifically designed with additives or selective membranes to protect foods from primary degradation processes, such as exposure to oxygen, ethylene, and other chemicals, and extend shelf life. Advances in the design of polymers and other materials are also needed to enable the development of sensitive and selective sensors, for use both in the field and in product packaging materials. Many other new chemicals and materials can be envisioned to improve the

production of food from “farm to fork,” such as moisture- retentive and slow-release soil-amendment materials and safe, highly specific anti-microbial and disinfection agents that could be incorporated into food packaging. Finally, new approaches to maintaining the health of crops are necessary that will target pests and diseases selectively without harming human health and the environment. These will require new chemicals and processes, including those inspired by nature.

New materials, especially nanoscale materials, are impacting other relevant technologies that include solar and thermoelectric energy conversion, electrical energy storage, separations, catalysis, and remediation of contaminated water and soil. Advances in computation and high-throughput experimentation are enabling more rapid discovery of new materials with desirable properties.

***New analysis techniques and sensors*** will provide key information to support research in laboratories and real-time information on crop protection, agricultural conditions and food products. To support fundamental studies described previously, new capabilities for studying materials structure and reaction dynamics in situ and in operando are required. This is especially important for the development of new liquid-phase catalytic processes. New field-deployable analytical tools and inexpensive sensors are also required for real-time monitoring of many variables in the field, such as pollutants, nutrients, temperature, water quality, soil moisture, pests, and plant health. Such capabilities will improve our understanding of the specific variables that must be monitored to describe and optimize the appropriate conditions for plant growth over a diverse range of crop growth conditions. New analytical techniques are also needed to assess food quality, including sensors embedded in

packaging materials that can self-report when food is spoiling. To ensure food quality and safety, the detection limits of analysis need to be improved. All of these technologies will require computational methods to collect and assimilate large data sets. In many scenarios, multiple sensing and analysis tools will be required to provide a complete understanding of a crop or system being studied.

***Computational approaches*** are necessary to both analyze and assimilate large data sets as new analytical and sensor technologies are developed. Such capabilities are critical for providing real-time feedback to control agricultural processes—to allow the farmer to make decisions regarding when to apply pest and disease control agents, irrigate, or harvest crops. New computational capabilities are also needed to help guide experimental studies in the laboratory in support of new technology development in separation, catalysis, materials development, among others. New methods are also needed for enabling the computational discovery of new materials for catalysis, separations, and food storage and of new chemicals for crop protection and soil treatment. The properties of new materials can be predicted with increasing accuracy from first-principles calculations when their compositions and structures are known. However, the inverse problem of designing a new material for a given property, and predicting structure for new materials of complex composition, remain persistent grand challenge problems.

***Renewable energy*** is connected to energy needs for water purification and to minimizing the impact of climate change on food production. For example, as irrigation demands increase, the energy needed (and associated costs) to move water will also increase; however renewable energy could help offset this increased demand. Technologies for renewable electrical energy production—especially solar photovoltaics and

wind power—are maturing and becoming cost-competitive with conventional electric power generation from coal, natural gas, and nuclear fission. The manufacturing cost of silicon and thin film photovoltaics is now below \$1/peak watt, and both solar cell and module costs are dropping annually by about 15%. Consequently, solar photovoltaics are expected to reach grid parity within the next decade. However, electricity accounts for only 1/5 of global energy use, with fuels making up the other 4/5, and no economically competitive solar fuel technology exists on the horizon. The electrification of the transportation sector, which is important to shifting the balance of energy use, and the grid-scale deployment of intermittent resources (such as solar and wind), are both dependent on the development of lower-cost and higher-density electrical energy storage technologies [1]. Lithium ion batteries are being aggressively developed for hybrid and electric vehicles, as well as portable power, but they remain too expensive for grid-level storage [2,3]. Other renewable energy resources that are non-intermittent, such as electrical energy from salinity gradients [4] and thermoelectric conversion of waste heat, are in early stages of development.

***Education and training***, along with its broad research community in the mathematical and physical sciences, gives NSF a unique role to play in conducting research directed toward ensuring a secure, sustainable food supply. By participating in the research areas outlined above, the next generation of students will be trained in the issues central to food security, providing them with the necessary enabling foundation to create additional innovative solutions in the future. These students will provide a trained workforce that is cognizant of the importance of integrated efforts between scientists, farmers, food processors, and consumers in all aspects of food security—from

farm to fork. In addition, these students will support a new generation of innovative techniques for efficiently and sustainably converting biomass, including wastes, into fuels, chemicals, and materials.

To achieve a sustainable food supply, the Subcommittee concluded that the technical challenges within all six of the research areas highlighted in this report must be addressed. These research areas considered all aspects of food production, “farm to fork”, as well as wastes. In assessing these research areas, the Subcommittee realized that incremental advances in today’s technologies simply will not be sufficient for meeting these formidable challenges. Rather, fundamental research is needed to provide the foundation for achieving technology breakthroughs required to provide safe, secure, and affordable food supplies globally. Further, this fundamental research will yield concepts that can be developed into a broad range of technologies that could be tailored to meet specific needs for a particular crop, ecosystem, and/or local resources. This Subcommittee was confident that the NSF Mathematical and Physical Sciences Directorate and its scientific community can address these six research areas, especially the identified cross-cutting themes of separations, catalyst materials and catalytic processes, interfaces, new materials and chemical processes, new analysis techniques and sensors, computation, renewable energy, and education and training.



# APPENDIX A. Charge to MPSAC Subcommittee

## National Science Foundation Directorate for Mathematical and Physical Sciences Charge to MPSAC Subcommittee for Studying the Role of NSF/MPS in Food Systems

### Background

Productive, modern agriculture is based inter alia on nitrogen- and phosphorus-derived fertilizer [1,2] and fresh water. Manufacturing nitrogen-based fertilizer (ammonia) is energy intensive, as is the purification of sea water [3] and of water denatured by industrial processes. The latter issue is of particular concern because future supplies of fresh water may be inadequate as a result of climate change, overuse of groundwater aquifers, and competing use of water in energy production [4]. Another concern is that production of phosphorus-based fertilizer may fail to meet world demand by mid-century [2]. Thus, there is an urgent need to discover new science and engineering that will allow large-scale, low-energy water purification, and similar production and recycling of key chemicals. Furthermore, most synthetic chemicals applied to farms wash into streams and rivers, and the small percentage of chemical fertilizer consumed by humans and animals in food eventually ends up as waste that also collects in coastal waters. The resulting nutrient pollution [5] spurs the growth of algae and subsequently of bacteria that feed on algae. The growth of bacteria depletes coastal waters of oxygen which leads to widespread loss of aquatic life. There are prominent “dead zones” as a result in the Mediterranean Sea, the Chesapeake Bay, the Gulf of California, and the Gulf of Mexico. Algal blooms and hypoxic waters have led to severe economic losses in the commercial fishing and tourism industries.

This document charges a subcommittee of the MPSAC to identify fundamental science drivers critical to achieving a sustainable world in the specific areas outlined above. These issues are tightly coupled because energy is expended to produce chemical fertilizer and fresh water, and increasingly society is forced to choose between using land and fertilizer for food or bio- renewable energy production, and between using fresh water for energy production (e.g., hydraulic fracturing) or agriculture.

### Charge to the Subcommittee

The Subcommittee on Food Systems will:

1. Envision an expansive path to breakthroughs in catalysis chemistry that would transform chemical manufacturing by using less energy than current practice. An example could be the articulation of a vision for new catalysis science that will allow a low-energy alternative to the Haber-Bosch process for generation of ammonia-based fertilizers.
2. Develop a vision for enabling the discovery of new fundamental science needed to advance scalable, low-energy purification of seawater and industrial wastewater to provide a secure and sustainable supply of fresh water for human consumption and food and energy production.
3. Develop a vision for enabling new scalable separation science that will allow the sequestration of chemicals used in agriculture and their eventual reuse and recycling, to prevent and/or mitigate nutrient pollution and to ensure future US phosphate security.

### Timeline

Charge to Committee—April 2013

Interim reports to MPSAC will be due quarterly. These will report on the progress being made and bring to the attention of the MPSAC any major issues. The reports can be delivered via Web-Ex or similar meeting tool. These will be coordinated by MPSAC.

A final report will be due in July 2014 with a presentation to the MPSAC at its Summer 2014 meeting. This presentation may be delivered remotely or in person.

### **Resources**

The NSF will arrange for and host Web-Ex meetings as needed by the subcommittee and cover associated costs. NSF/Division of Chemistry will provide financial support for a workshop on the topic, which will be timed to inform the subcommittee.

### **Points of Contact at Federal Agencies:**

- Kelsey Cook. Staff Associate, Office of the Assistant Director, MPS, NSF. [kcook@nsf.gov](mailto:kcook@nsf.gov) (703-292-7490).
- Lin He. Program Director, Chemical Measurement and Imaging, CHE. [lhe@nsf.gov](mailto:lhe@nsf.gov) (703-292-4336).
- DOE representative. TBD.
- USDA representative. TBD.
- Other representatives (NOAA, Gates Foundation, etc.). TBD.

### **References**

1. T. Hager. *The Alchemy of Air*, Three Rivers Press, New York, NY (2008).
2. D. Cordell and S. White. "Peak phosphorus: Clarifying the key issues of a vigorous debate about long-term phosphorus security," *Sustainability* **3**, 2027–2049 (2011).
3. (a) J. E. Drinan and F. Spellman. *Water and Wastewater Treatment: A Guide for the Nonengineering Professional*, Second Edition, CRC Press, Boca Raton, FL (2012). (b) J-F Rischard. *High Noon: 20 Global Problems, 20 Years to Solve Them*, Perseus Books, New York (2002).
4. D. Yergin. *The Quest: Energy, Security, and the Remaking of the Modern World*, Penguin Group, New York (2012).
5. "The facts about nutrient pollution," US Environmental Protection Agency, Washington, D.C. [www.water.epa.gov/polwaste/upload/nutrient\\_pollution\\_factsheet.pdf](http://www.water.epa.gov/polwaste/upload/nutrient_pollution_factsheet.pdf). Accessed June 18, 2014.

## **APPENDIX B. Members of the MPSAC Subcommittee for Studying the Role of NSF/MPS in Food Systems (SFS)**

### **Michelle V. Buchanan (Chair)**

Associate Laboratory Director for Physical Sciences  
Oak Ridge National Laboratory  
P.O. Box 2008  
Oak Ridge, TN 37830

### **Charles T. Campbell**

Professor and B. Seymour Rabinovitch Endowed Chair  
Department of Chemistry  
University of Washington  
Box 35-1700  
Seattle WA 98195-1700

### **Frank J. DiSalvo (MPSAC Liaison)**

John A. Newman Professor  
Department of Chemistry  
Cornell University  
Ithaca, NY 14853

### **Paul L. Edmiston**

Theron L. Peterson and  
Dorothy R. Peterson Professor of Chemistry  
Analytical Department of Chemistry  
The College of Wooster  
213 Severance  
Wooster, OH 44691

### **Thomas E. Mallouk**

Evan Pugh Professor  
Pennsylvania State University  
224 Chemistry Building  
University Park, PA 16801

### **Susan Olesik**

Dow Professor  
Department of Chemistry and Biochemistry  
Ohio State University  
100 West 18th Avenue  
Columbus, OH 43210-1173

### **Bruce Rittmann Regents**

Professor  
Department of Civil and Environmental Engineering  
Arizona State University  
P.O. Box 875701  
Tempe, AZ 85287-5701

### **Susannah Scott**

Professor  
Department of Chemical Engineering  
University of California–Santa Barbara  
10 Mesa Road  
Engineering II, Rm. 3325  
Santa Barbara, CA 93106-5080

### **James N. Seiber**

Department of Environmental Toxicology  
University of California–Davis  
1 Shields Avenue  
Davis, CA 95616-8598

### **Kim R. Williams**

Professor  
Department of Chemistry and Geochemistry  
Colorado School of Mines  
304 Coolbaugh Hall  
1012 14th Street  
Golden, CO 80401

## APPENDIX C. List of Teleconference Speakers

| <b>Speaker</b>            | <b>Affiliation</b>   | <b>Title of Presentation</b>  |
|---------------------------|--|---|
| <b>Mary Ann Dickinson</b> | Alliance for Water Efficiency  | Urban Water Efficiency: Trends and Issues   |
| <b>Sir David King</b>     | Director of Research in Physical Chemistry, Cambridge; Director, Collegio Carlo Alberto; Chancellor, University of Liverpool; Senior Scientific Adviser to UBS | King's Comment—Waste Not, Want Not in Emerging Technologies (no presentation; newsletter article)   |
| <b>James J. Elser</b>     | Arizona State University   | Phosphorus, Food, and Our Future  |
| <b>Bruce A. Moyer</b>     | Oak Ridge National Laboratory  | Approaches to Selective Chemical Separations Applicable to Food and Agriculture                     |
| <b>Jerald L. Schnoor</b>  | University of Iowa   | Water Sustainability: Impacts of climate change on agriculture                                      |
| <b>John W. Finley</b>     | Louisiana State University   | Food, Energy and Water—Can we meet our future needs?  |
| <b>James A. Dumesic</b>   | University of Wisconsin—Madison  | Challenges for Conversion of Lignocellulosic Biomass to Fuels and Chemicals: Liquid-phase catalysis |
| <b>Brooke Mayer</b>       | Marquette University   | Phosphorous Recovery Technology   |
| <b>Michael E. Webber</b>  | University of Texas—Austin   | The Nexus of Food and Energy  |
| <b>Menachem Elimelech</b> | Yale University  | Membrane Technologies for Desalination and Wastewater Reuse for Augmenting Water Supply             |
| <b>William T. Cooper</b>  | Florida State University   | Phosphorus: So Simple, So Necessary   |



