BASIC RESEARCH NEEDS
TO ASSURE
A SECURE ENERGY FUTURE

A Report from the
Basic Energy Sciences Advisory Committee

Basic Research Needs To Assure A Secure Energy Future

Chair: John Stringer, Electric Power Research Institute
Co-Chair: Linda Horton, Oak Ridge National Laboratory

Workshop leaders:
Fossil Energy – Marvin Singer, DOE Office of Fossil Energy
Nuclear Fission Energy – John Ahearne, Sigma Xi
Renewable and Solar Energy – George Crabtree, Argonne National Laboratory
Fusion Energy – Charles Baker, University of California, San Diego
Distributed Energy, Fuel Cells, and Hydrogen – Lutgard DeJonghe, University of California, Berkeley
Transportation Energy Consumption – Jan Herbst, General Motors R&D Center
Residential, Commercial, and Industrial Energy Consumption – Mildred Dresselhaus, Massachusetts Institute of Technology
Cross-Cutting Research and Education – Rick Smalley, Rice University

Factual Document Team – Roger Stoller, Claudette McKamey, Stan Hadley, Tom Rosseel, Barbara Ashdown

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Prepared by
OAK RIDGE NATIONAL LABORATORY
Oak Ridge, Tennessee 37831-6285
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DEDICATION

This report is dedicated to the memory of Dr. Iran L. Thomas, Director, Division of Materials Sciences and Engineering, and Deputy Director for Basic Energy Sciences, Office of Science, United States Department of Energy. Iran passed away on February 28, 2003.

For many years, Iran was a major contributor to the design of the materials science program supported by the Office of Basic Energy Sciences. Throughout, he was always careful to emphasize that a primary responsibility of the program was to support first-class science. He was a strong advocate of the Basic Energy Sciences Advisory Committee, and he often commented on the valuable contributions that BESAC has made to the program.

His vision was a guiding force in the creation of the BESAC subpanel whose work is contained in this report. Without his contributions, and his leadership, it is doubtful that this report could have been produced. We are grateful that he had the opportunity to review the report before his death, and that he was so pleased with the result for which he had worked so hard.

Throughout his career, Iran's leadership and personal contributions helped to shape the basic materials research program in the United States. He will be sorely missed.

Iran Thomas, in his weekend working garb, is shown with the reports on the status and future of x-ray and neutron scattering research facilities. Iran's leadership fostered many of these reports through both BES and BESAC.

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REPORT OF THE BESAC SUBPANEL ON BASIC RESEARCH NEEDS TO ASSURE A SECURE ENERGY FUTURE

EXECUTIVE SUMMARY

Current projections estimate that the energy needs of the world will more than double by the year 2050. This is coupled with increasing demands for “clean” energy – sources of energy that do not add to the already high levels of carbon dioxide and other pollutants in the environment. These coupled challenges simply cannot be met by existing technologies. Major scientific breakthroughs will be required to provide reliable, economic solutions.

In October 2002, a workshop was held to assess the basic research directions that will assure a secure energy future. Over 100 scientists and engineers from academia (27%), industry (16%), and federal laboratories (39%) and agencies (18%) participated in the workshop. As a resource for the workshop participants, a factual document was compiled that summarized the state of energy sources and use at a national and international level. The discussion groups, or topical teams, at the workshop were organized by energy source and energy use. From the Department of Energy (DOE), both basic and applied mission representatives were included in each of the teams.

The results of the workshop are a compilation of 37 proposed research directions (PRDs). At a higher level, these fell into ten general research areas, all of which are multidisciplinary in nature:

- Materials Science to Transcend Energy Barriers
- Energy Biosciences
- Basic Research Towards the Hydrogen Economy
- Innovative Energy Storage
- Novel Membrane Assemblies
- Heterogeneous Catalysis
- Fundamental Approaches to Energy Conversion
- Basic Research for Energy Utilization Efficiency
- Actinide Chemistry and Nuclear Fuel Cycles
- Geosciences

Nanoscale science, engineering, and technology were identified as cross-cutting areas where research may provide solutions and insights to long-standing technical problems and scientific questions. The need for developing quantitative predictive models was also identified in many cases, and this requires better understanding of the underlying fundamental mechanisms of the relevant processes. Often this in turn requires characterization with very high physical, chemical, structural, and temporal precision: DOE’s existing world-leading user facilities currently provide these capabilities, and these capabilities must be continuously enhanced and new ones developed. In addition, requirements for theory, modeling, and simulation will demand advanced computational tools, including high-end computer user facilities. All the participants agreed that the education of the next generation of research scientists is of crucial importance; and this should include making the importance of the energy security issue clear to everyone.

It is clear that assuring the security of the energy supply for the U.S. over the next few decades will present major problems. There are a number of reasons for this. The most important of these is the current reliance on fossil fuels for a high proportion of the energy, of which a significant fraction is imported. The Developing World countries will have greatly increased needs for energy, in part because of the expected population increase, and in part because of the increase in their presently very low standards of living. A second problem is related to concerns over the environmental effects of the use of fossil fuels. Third, the peaking of the production of fossil fuels is likely within the next several decades. For these reasons, it is very important that the U.S. undertakes a vigorous research and development program to address the issues identified in this report.

There are a number of actions that can help in the nearer term: increased efficiency in the conversion and use of energy; increased conservation; and aggressive environmental control requirements. However, while these may delay the major impact, they will not in the longer run provide the assured energy future that the U.S. requires. It is also clear that there is no single answer to this problem. There are several options that are available at the moment, and many – or indeed all – of them must be pursued.

Basic research will make an important contribution to the solution to this problem by providing the basis on which entities which include DOE's applied missions programs will develop new technological approaches; and by leading to the discovery of new concepts. The time between the basic research and its contribution to new or significantly improved technical solutions that can make major contributions to the future energy supply is often measured in decades. Major new discoveries are needed, and these will largely come from basic research programs.

It is clear from the analysis presented in this report that there are a number of opportunities. Essentially all of these are interdisciplinary in character. The Office of Basic Energy Sciences (BES) should review its current research portfolio to assess how it is contributing to the research directions proposed by this study.

The BES Advisory Committee (BESAC) expects, however, that a much larger effort will be needed than the current BES program. The magnitude of the energy challenge should not be underestimated. With major scientific discoveries and development of the underlying knowledge base, we must enable vast technological changes in the largest industry in the world (energy), and we must do it quickly. If we are successful, we will both assure energy security at home and promote peace and prosperity worldwide.

RECOMMENDATION: Considering the urgency of the energy problem, the magnitude of the needed scientific breakthroughs, and the historic rate of scientific discovery, current efforts will likely be too little, too late. Accordingly, BESAC believes that a new national energy research program is essential and must be initiated with the intensity and commitment of the Manhattan Project, and sustained until this problem is solved.

BESAC recommends that BES review its research activities and user facilities to make sure they are optimized for the energy challenge, and develop a strategy for a much more aggressive program in the future.

INTRODUCTION

The world is at a transition in the use of energy. Over the next 50 years, it is expected that energy use will double. The factual document included as Appendix B in this report includes a wealth of statistics and other information on the status of energy use, resources, research needs by energy sector, etc. A brief summary of some of these data follows.

There is a close link between energy usage and Gross Domestic Product (GDP), and thus standard of living. With some variation, this is generally true for all the nations in the world. The per capita energy use in the U.S. is very high. The primary energy resource consumption in 1999 was 102 EJ (97 Quads),* yielding an annual per capita energy use of 100,000 kWh (or 3.4 x 10^8 Btu).

Of these 102 EJ, 86% was generated from fossil fuels, with nearly one third of this being imported petroleum and natural gas. Nuclear power was about 8%; hydroelectric was 3%, and biomass and other sources was 4%. Electricity generation consumed 36 EJ of this total (35%) and transportation consumed 27 EJ (27%). Two other areas of energy consumption are Residential/Commercial, which consumes 19 EJ (19%), and Industrial which consumes 24 EJ (23%).

Also, about 60% of the 96 EJ used in energy production is rejected energy; that is, energy that is currently lost as heat or through other inefficiencies. The overall efficiency is thus about 40%. Considering energy sectors, the overall efficiency of the transportation sector is about 20%, the electricity sector is about 32%, the residential/commercial sector is about 75%; and the industrial sector is 83% ["U. S. Energy Flow – 1999," Gina V. Kalper, UCRL-ID-129990-99 (March 2001)].

From the point of view of energy security, there are two ways of looking at this information. First, of the 102 EJ of primary resource, 27 EJ were imported; essentially all of which was petroleum, natural gas, and related products. Second, 86 EJ are fossil fuels. While there is argument about the resource base for these, there is no argument that they are finite resources, and thus at some point will be exhausted; well before that, the cost of winning and transporting them will increase.

In the broader context, the energy demand in the rest of the world will increase markedly in the next few years for two reasons. First, the energy availability and use per capita in much of the world is very significantly less than in the U.S. In addition, the GDP and thus the standard of living are also much less. It can be expected that the standard of living will rise in other parts of the world; and particularly in the developing world where the standards of living are very low. Second, current models predict a large increase in world population over the next few decades, from its present level of 6 billion to 10 billion by the year 2050. Most of this expansion will take place in the developing countries. For example, in the specific case of electricity use, it is predicted that over this same time period the per capita demand will increase from its present level of 1,000 kWh per annum, to 3,000 kWh per annum. This is still far below the U.S. current demand for electricity, which is 13,600 kWh per annum; but when multiplied by the population increase it still represents an enormous growth in the required generation capacity. For the case of energy requirements for personal transportation, the current indications are that demand will also in-

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* An exajoule (EJ) is 10^{18} joules (J). The equivalent engineering unit is a Quad, 10^{15} Btu. 1 Btu = 1,055.06 J, so 1 Quad = 1.055 EJ. Also, 1 Kilowatt-hour (kWh) is 3,412 Btu; so 1 Quad is 2.93 x 10^{11} kWh. A large electricity generating station typically has a capacity of 1 Gigawatt; approximately 33 of these stations running continuously for a year will generate 1 Quad of energy as electricity.

crease greatly over the next few years in the developing world: China is a case where this is beginning to be apparent now.

Further energy-related questions that need to be addressed include environmental issues, notably those related to global warming and the availability of water. Environmental issues also vary with energy source and energy utilization technology.

There are several possible directions to go to address the problem of energy security for the U.S. in the relatively near term, the next 25 to 35 years. It is important to recognize that energy security is not the goal in itself: the goal is to maintain and improve standards of living. Thus, an increase in the GDP/energy ratio is important. This ratio has been increasing over the last several years, but the rate of increase needs to accelerate. This requires a number of steps. First, the efficiency of energy conversion must increase. Next, the efficiency of the end-use of energy must increase. Third, the overall cost of the processes involved in primary resource collection, transportation, and conversion must be reduced.

In the longer term, it is important to address the issue of the finite fossil fuel resources; this is likely to impact petroleum first, and longer-range research needs to address the issue of substitution of other primary sources.

It makes sense to use longer-term research to develop renewable energy sources. While the carbon-to-hydrogen ratio in primary fuels has been progressively decreasing for many years, the potential link between 'green-house gases' and global warming may require this to be greatly accelerated. From the U.S. point of view, energy security is favored by decreasing use of imported primary sources, and this would also argue for the development of renewable sources.

Historically, the approach to these issues has been largely evolutionary: the improvement in the efficiency of the generation of electricity by systems involving large coal-fired boilers by moving towards higher steam temperatures and pressures, for example; or the recent developments in large wind turbines. This research is necessary and important, and is being supported with the DOE by the applied research offices – in particular, Fossil Energy; Energy Efficiency and Renewable Energy; and Nuclear Energy, Science, and Technology.

One of the energy components of the DOE's mission that relates to the Office of Science is best described by the following element of the BES program description (SC-4) appearing in the DOE Annual Performance Plan for FY 2004:

"The mission of the Basic Energy Sciences (BES) program -- a multipurpose, scientific research effort -- is to foster and support fundamental research to expand the scientific foundations for new and improved energy technologies and for understanding and mitigating the environmental impacts of energy use."

The object of this report is therefore to propose basic research directions appropriate for the Office of Basic Energy Sciences (BES) that will deliver scientific knowledge and discoveries related to the applied energy missions. It follows that these research directions will be different and generally concerned with much longer-range objectives than those of the applied mission offices themselves.

PROPOSED RESEARCH DIRECTIONS

The workshop held in October 2002 assessed the basic research needs for energy technologies to assure a reliable, economic, and environmentally sound energy supply for the future. A subsequent activity to discuss Energy Biosciences in particular was held in January 2003. Over 100 people from academia, industry, the national laboratories, and federal agencies participated in these workshops and related activities. (The details on the charge, organization, program, schedule, membership/attendees, and related information can be found in Appendix C. The introductory presentations from the workshop are in Appendix D.)

The leaders of the workshop and the lead authors for the summaries of the discussion were:

- Marvin Singer (DOE Office of Fossil Energy), Fossil Energy;
- John Ahearne (Sigma Xi), Nuclear Fission Energy;
- George Crabtree (Argonne National Laboratory), Renewable and Solar Energy;
- Charles Baker (University of California San Diego), Fusion Energy;
- Lutgard C. DeJonghe (University of California Berkeley), Distributed Energy, Fuel Cells, and Hydrogen;
- Jan Herbst (General Motors R&D Center), Transportation Energy Consumption;
- Mildred Dresselhaus (Massachusetts Institute of Technology), Residential, Commercial and Industrial Energy Consumption;
- Rick Smalley (Rice University), Cross-Cutting Research and Education; and
- John Stringer (EPRI), Energy Biosciences Research.

The discussions at the workshop presented a sense of urgency for the need for basic research to assure the energy supply for the nation and the world. An underlying theme in the discussions was the need for low-carbon energy while adding 13 TW (13 TJ/s) of world-wide energy generation capability (a true grand challenge that was compared to the race for the moon in the 1960s), perhaps more critical in terms of security of the U.S.

There were many scientific and technological challenges across the energy spectrum. Currently there are no viable ways of meeting these challenges. Non-carbon energy sources have daunting difficulties that need innovative solutions for these to become a high percentage of the energy pool. Fossil fuels have equal challenges relative to environmental concerns, as well as the ability to use non-traditional reserves.

The workshop discussions produced a total of 37 proposed research directions, Table 1. The full text of the supporting statements is contained in Appendix A. The summary presentations given by each of the workshop leaders can be found in Appendix E.

These research directions can be aggregated into the following list of general recommendations for basic research directions. The balance of this section is devoted to a detailed discussion of each of these.

- Materials Science to Transcend Energy Barriers
- Energy Biosciences
- Basic Research Towards the Hydrogen Economy

Table 1. Proposed Research Directions (PRDs)

Fossil Energy
- Reaction Pathways of Inorganic Solid Materials: Synthesis, Reactivity, Stability
- Advanced Subsurface Imaging and Alteration of Fluid-Rock Interactions
- Development of an Atomistic Understanding of High-Temperature Hydrogen Conductors
- Fundamental Combustion Science Towards Predictive Modeling of Combustion Technologies

Nuclear Fission Energy
- Materials Degradation
- Advanced Actinide and Fission Product Separations and Extraction
- Fuels Research
- Fundamental Research in Heat Transfer and Fluid Flow

Renewable and Solar Energy
- To Displace Imported Petroleum by Increasing the Cost-Competitive Production of Fuels and Chemicals from Renewable Biomass by a Hundred Fold
- Develop Methods for Solar Energy Conversion that Result in a Ten-to-Fifty Fold Decrease in the Cost-to-Efficiency Ratio for the Production of Fuels and Electricity
- Develop the Knowledge Base to Enable Widespread Creation of Geothermal Reservoirs
- Conversion of Solar, Wind, or Geothermal Energy Into Stored Chemical Fuels
- Advanced Materials for Renewable Energy Applications

Fusion Energy
- Multiscale Modeling of Microstructural Stability of Irradiated Materials
- Deformation and Fracture Modeling
- Plasma-Surface Interactions
- Thermofluids and “Smart Liquids”
- Plasma Aerodynamics

Distributed Energy, Fuel Cells, and Hydrogen
- Advanced Hydrogen Synthesis
- High-Capacity Hydrogen Storage for Distributed Energy of the Future
- Novel Membrane Assemblies
- Designed Interfaces

Transportation Energy Consumption
- Integrated Quantitative Knowledge Base for Joining of Lightweight Structural Materials for Transportation Applications
- Vehicular Energy Storage
- Fundamental Challenges in Fuel Cell Stack Materials
- Integrated Heterogeneous Catalysis
- Thermoelectric Materials and Energy Conversion Cycles for Mobile Applications
- Complex Systems Science for Sustainable Transportation

Residential, Commercial, and Industrial Energy Consumption
- Sensors
- Solid State Lighting
- Innovative Materials for New Energy Technologies
- Multilayer Thin Film Materials and Deposition Processes

Cross-Cutting Research and Education
- Nanomaterials
- Preparing Tomorrow’s Workforce for the Energy Challenge and Heightening the Public’s Awareness

Energy Biosciences Research
- Energy Biotechnology: Metabolic Engineering of Plants and Microbes for Renewable Production of Fuels and Chemicals
- Genomic Tools for the Development of Designer Energy and Chemical Crops
- Nanoscale Hybrid Assemblies for the Photo-Induced Generation of Fuels and Chemicals

- Innovative Energy Storage
- Novel Membrane Assemblies
- Heterogeneous Catalysis
- Fundamental Approaches to Energy Conversion
- Basic Research for Energy Utilization Efficiency
- Actinide Chemistry and Nuclear Fuel Cycles
- Geosciences

Materials Science to Transcend Energy Barriers

Many of the current technological barriers related to energy hinge on improved materials. Thus, materials research is an area in which scientific advances could have a key impact on future energy security. Examples range from high-efficiency lighting to vastly improved solar cells to materials that last longer and function under more severe conditions. Nanomaterials offer the possibility of revolutionary advances while advanced characterization tools, coupled with modeling using parallel computers, may provide the fundamental understanding to improve materials properties for the challenges of the next decades.

The materials theme appeared in nearly half of the proposed research directions. Within these, there are a number of subthemes:

- Nanomaterials
- Materials Degradation
- Composite Materials
- Materials Fabrication Issues
- Advanced Materials and New Materials Opportunities

Nanomaterials. Possible roles for nanomaterials include new approaches to photovoltaics; thermoelectric materials with significantly improved figures of merit based on quantum dots, quantum wires and quantum well geometries; smart sensors of very small size with a wide range of capabilities, including wireless, self-powered, with on-board signal processing, networking, and communications capabilities. A specific need for basic research is the underlying science that will enable advanced robust wireless sensors with multifunctional detection capabilities in terms of variables, including chemistry, temperature, pressure, and other physical parameters, coupled with the ability to transmit the information and to be ‘smart’ in the sense of acting both as an active remediator and as a part of an interactive system.

Nanocomposites are also proposed as, for example, new battery concepts with significantly improved capacities and semiconductor/polymer nanocomposite photocells.

Another proposed research direction is inorganic, organic, and inorganic/organic hybrid porous materials with pores in the 1-30 nm range as biomimetic materials with the efficiency and specificity of natural systems in light-harvesting, charge separation, and chemical transformation. Nano-scale self-assembly is a related research area with potential revolutionary impact. Related to solar energy, research leading to storage of light energy in the form of high-energy chemicals was discussed as a possible solution. Also as part of this area, there were research directions related to multi-layer thin film assemblies, including creation of explicit mechanistic models that allow precise control and prediction of properties based on deposition conditions and film-growth chemistry. Research is also needed for the development of the next-generation of thin-film deposition techniques and in-situ characterization tools.

Materials Degradation. In systems that generate and use energy, there are pervasive problems with corrosion, high-temperature effects, and radiation-induced damage. These result in degradation of the materials properties, frequently leading to deformation and fracture. Further, there is a critical need to be able to make very confident predictions of lifetimes over very long times – from tens of years for components inside nuclear power reactors to as much as 10,000 years for radioactive waste containment systems. For corrosion processes, the complex chemistries coupled with the effects of radiation make this a very challenging problem. All of the proposed research directions related to degradation issues emphasize the need to develop fundamental understanding of the mechanisms and the increased importance of modeling in future research. These issues are not confined to metallic materials: ceramics, composite materials, polymers, and glasses are among materials that suffer degradation. The degradation issues for nanomaterials, and particularly nanocomposites, were not explicitly considered; but the high surface-area-to-volume ratios and the non-equilibrium nature of many of the composites is likely to lead to degradation in the future applications.

Composite Materials. A composite material behaves in ways that are different, sometimes very different, from materials that are essentially homogeneous. Composite materials for energy applications include not only the well-known polymer matrix-fiber reinforced materials, or metal matrix-oxide particle dispersion-strengthened materials, but also new and innovative materials and structures. Research on novel inorganic/organic hybrid porous materials for advanced light harvesting; advanced, small, dispersed smart sensors; thin-film multilayer concepts; and various nanocomposite materials is recommended. Characterization and modeling of the fundamental phenomena that control structure-property relationships will be of critical importance in realizing the potential benefits of this class of materials.

Materials Fabrication Issues. In the development of truly novel materials, the fabrication often requires specific research in its own right. Joining processes, for example, represent extreme conditions for the materials being joined, and there are generally both spatial and temporal gradients of temperature, composition, and structure. With the new strong lightweight alloys and composites that will be required for more economical fuel consumption, the issues related to assembling these components into a viable structure become very important. Joining of lightweight materials, while retaining their desirable properties, is one particularly challenging research direction. Non-destructive evaluation of joined materials is another. Once again, the path forward will depend on the ability to develop models and evaluation techniques capable of handling these extraordinarily complex problems.

Another proposed challenging research area is the fabrication of thin-film multilayers. This will require the creation of explicit mechanistic models that allow precise control and prediction of properties based on deposition conditions and film-growth chemistry. On the basis of these models, the next generation of thin-film deposition techniques, and the *in situ* characterization tools that will be required by the process control system can be developed.

While these were the specific items related to materials fabrication, it is obvious that many of the other systems described, particularly those based on nanostructures of various kinds, will require substantial research on the fabrication methods including self-assembly. These developments will require a considerable knowledge of the fundamentals of the processes and the evolution of models and characterization tools capable of leading to the design and realization of the necessary procedures.

Advanced Materials and New Materials Opportunities. There are opportunities for innovative materials research that fall outside of the above areas. Examples include materials for solid state lighting, advanced thermoelectric materials, advanced membranes, hybrid solar cells – porous wide bandgap semiconductors with a light-sensitive dye, organic semiconductors, new hydrogen storage materials, and new materials for fuel cell stacks. Development of more efficient and durable building materials – so called smart materials whose properties change with changing environmental conditions – is an interesting area for fundamental materials science.

Energy Biosciences

The use and understanding of biological processes has been a growing area of research. There are reasons to believe that there is a potential for biologically-inspired research to provide solutions to energy issues that we cannot presently imagine. This area was felt to be so exciting that the original workshop group suggested a follow-up workshop specifically to examine these research possibilities. Recommended research areas include biomimetic approaches to solar energy capture and generation of fuels and chemicals. Very exciting is the possibility of using emerging knowledge in functional genomics and molecular technologies to develop plants that are optimized to produce fuels and chemicals. This renewable biomass-generated fuel could eventually replace imported petroleum. The use of biomass could be enhanced if these plants could be made more tolerant of adverse environments, and optimized in terms of nutrient, water, and land use, so that they are not competing with food crops for available land, for example. Another promising research area is the development of biocatalysts to aid in the fractionation of the biomass. An interesting concept was to design-in properties of the plants that would have the effect of addressing the downstream processing of the biomass – a kind of driver for evolution that is totally different from that in a natural system. The development process would be faster with successful research on tools for directed genetic engineering of critical crop properties.

Basic Research Towards the Hydrogen Economy

The development of hydrogen as a substitute to current fossil fuels is a promising area for future energy generation. Consequently, methods of producing and using hydrogen received considerable attention in the workshop discussions. In connection with this, the importance of membranes, not only for separation of gaseous or liquid species, but as components in a fuel cell stack, was discussed extensively. Basic research opportunities recommended here, as in many of the other topic areas, lie not in duplicating applied research, but in fundamental science with the objective of developing appropriate understanding of underlying phenomena and the development of predictive models to guide research to new concepts.

The issue of the production of hydrogen is addressed, noting that some 9 million tons of hydrogen are produced per year in the U.S., primarily through the steam reforming of natural gas. In the future, other production technologies using sustainable feedstocks will be required that do not result in a net production of CO_2. Some of the most daunting research challenges are associated with hydrogen generation through the thermal splitting of water at high temperatures, with the source of the heat being solar collectors or high-temperature nuclear reactors. In thermochemical water splitting, a chemical step is introduced to reduce the temperature needed; however, the chemicals combined with high temperatures and gas production gave rise to very demanding materials problems. The photon energies in visible light are sufficient to split a water molecule, so that low-temperature water splitting using light is possible; the problem is to harvest the light in a way that allows the energy to be directed to a catalytic water splitting reaction. Basic research on fundamental mechanisms would underpin demonstration projects on advanced hydrogen production and help resolve the technological issues that will evolve during this development.

For fuel cell development, an atomistic understanding of high-temperature hydrogen conductors would allow the development of very highly selective membranes capable of operating at temperatures as high as 700°C, using the integration of theory, modeling, and experimentation for new classes of oxide and amorphous metallic proton conductors. Understanding of the interaction of hydrogen with the atomic structure could be enabled with neutron characterization to study both the migration and the storage of hydrogen in various materials. Another approach to this same problem is to study nanocomposite membranes where the transport takes place along their internal interfaces.

The technological issues associated with hydrogen storage are well known. High-pressure storage of hydrogen presents risks that may not be acceptable; liquefaction is unacceptable because of the losses associated with the liquefaction itself, of the order of 30%. Recently, there have been some interesting studies of hydrogen storage using complex hydrides, such as the alanates, $Al(AlH_4)_3$, and others. Basic research efforts to explore the hydrogen storage properties of these materials are virtually nonexistent and is therefore a recommended research direction for the future. A particular issue is the high pressures that are needed to hydrogenate these materials; often the kinetics of the hydrogenation and the dehydrogenation are limiting steps.

Innovative Energy Storage

Energy storage – from traditional battery concepts to non-traditional methods, including hydrogen storage – has research challenges relating to long-term storage and distribution of energy. Use of transient renewable energy sources, such as solar photovoltaic and wind, would be greatly enhanced by improved energy storage. One research area recommended was the study of photoconversion of renewable substrates, such as water, CO_2, and N_2, to produce storable liquid or gaseous fuels. Other basic research directions include catalysis and research leading to inexpensive photoconversion systems. The use of phase transitions in materials as a means for energy storage was also discussed.

Novel Membrane Assemblies

Membranes appear in both new and traditional energy systems including hydrogen separation, fuel cells, environmental applications, etc. Improvements in membranes could lead to more efficient gas separation enabling lower-cost fossil-based hydrogen production processes. The materials problems associated with thermochemical water-splitting cycles for the generation of hydrogen could be reduced by advanced membranes that reduce the temperatures required. Fuel cell operation in the critical 200-600°C range would be greatly beneficial, but it is specifically in this range that functionally useful membranes are yet to be discovered. Fuel cell stack materials, and particularly proton exchange membranes, require significant advances, and these can only be achieved with an improvement in basic understanding of how these membrane materials function. Membranes for fuel cell stacks and for chemical separations using nanotechnology and the development of highly specific membranes to enable economic recovery of elements from sea water, particularly uranium, are future technological needs. Basic research is recommended that will support the establishment of a fundamental understanding of the relationship between membrane structure and functionality.

Heterogeneous Catalysis

Catalysis is of large economic importance to the U.S. economy in a range of energy related areas, especially in the transportation and industrial sectors. Heterogeneous catalysis underlies a number of the concepts proposed for new directions in energy production and utilization. The development of new catalysts is hampered by the lack of detailed structure-function relationships that are essential to the development of a predictive capability for new process concepts and materials design. It is recommended that such research be pursued. In addition, further development of emerging and of wholly new local structural tools that can probe to length scales in the range 0.1-2 nm are required. Other critical research areas include the development of computational models of the governing catalytic reactions and approaches to integration of structural and spectroscopic data to yield self-consistent models of catalyst active sites, gas conversion and particulate oxidation.

Fundamental Approaches to Energy Conversion

Energy conversion, ranging from traditional combustion processes to fuel cells to the conversion of solar and other renewable energy supplies, are key to energy generation, transportation and many industrial processes. Fundamental combustion science to develop predictive modeling of combustion technologies is difficult due to turbulence of the chemically reacting systems. This is particularly true when one considers the very large scale of the combustors in energy generation systems and the complexities presented by the mixing and combustion propagation in internal combustion engines. Basic research to support advances in diagnostic tools, particularly laser-based, and high-performance computing capabilities is recommended as these present real opportunities to advance combustion science and to lead to the development of predictive models to allow improved design of combustors and real-time operation control algorithms. Only by developments of this kind can the environmental standards expected by the year 2012 be attained. Other fruitful proposed research areas are the related topics of heat transfer and fluid flow. These issues include heat transfer in solid-state devices, cooling systems, and heat exchangers. The key concerns are multiphase fluid flow and heat transfer. Recently the introduction of nanophase dispersions in fluids has been shown to produce potentially interesting effects in both fluid flow and heat transfer. However, characterization systems capable of generating data on the behavior of these systems with sufficient spatial and temporal resolution to allow the development of a fundamental understanding are only now becoming available, and this understanding will be essential to develop predictive models.

Improvements in the conversion efficiency of solar devices are critical to the expanded use of solar energy. The issues here include the rapid decay of the photogenerated carriers as they traverse the cells from the generation site to the conversion site. Proposed research areas include the development of interpenetrating network geometries. A related topic is the thermalization of the carriers at high energy levels. There may be potential advantages in utilizing nanostructured materials in circumventing some of the limitations.

Another recommended research area is innovative approaches to convert solar, wind, or geothermal energy into stored chemical fuels. The approaches suggested are: new catalysts to facilitate multi-electron transformations such as those required to produce hydrogen and oxygen from water, or reducing CO_2 to methanol, ethanol, or other carbon based-fuels. Direct solar photoconversion is also a possibility, with the development of photoactive organic, inorganic, or biological molecules or species, which can absorb a large fraction of the solar irradiance and drive the chemical reactions that produce the fuels of interest.

Fuel cells represent possible energy sources for transportation and for distributed power generation. Basic research to make fuel cells feasible for large-scale uses is recommended, including high selectivity membranes and low-cost, high-efficiency catalysts. In addition, utilization of hydrogen or carbon-containing fuels in electrochemical systems depends critically on the properties of interfaces that need to fulfill specific and often conflicting functions. The complexity of the problem requires novel approaches to interface design and modeling.

Extended use of thermoelectric energy conversion requires realization of a significantly improved figure of merit in thermoelectric materials; basic research on quantum well and other low dimensional systems offer this possibility. Possible uses of thermoelectric material systems include improvement in the use of otherwise waste energy in automotive systems.

Basic Research for Energy Utilization Efficiency

Fuel utilization and efficiency are not only important in energy consumption, but also in energy generation – and is an important issue in the use of nuclear fission energy. The research opportunities for improved energy efficiency in the residential and industrial areas are very interesting. Although the actual efficiency of end-use in the residential/commercial sector is quite high, about 75%, it is generally believed that the total amount of energy used in these applications can be significantly reduced. The most important system identified at the workshop was lighting. About 20% of electricity consumption is attributed to lighting. Incandescent and fluorescent bulbs currently provide the majority of that. Incandescent lighting is quite inefficient, with only 5-6% of the electricity consumption being converted to visible light. Fluorescent lighting is more efficient, at approximately 25%. Solid-state lighting, including light-emitting diodes (LEDs), has the potential to exceed these efficiencies. At the moment, white light emitting LEDs are close to twice as efficient as incandescent lights. Future research may result in perhaps an eight-fold improvement over the next 10-20 years. The fundamental physics of the solid-state light emitters is a recommended research area. In terms of new materials opportunities, proposed research directions include nitride-based wide bandgap semiconductors and polymer-based organic electronic materials that have the promise of significant lighting improvements.

Other proposed research areas related to energy generation include catalysis research for improvements in the utilization of fossil fuels. For biomass energy to be viable on a large scale, research is needed that would allow the utilization of marginal land, limited water supplies, and low fertilizer use.

Actinide Chemistry and Nuclear Fuel Cycles

There are a number of concepts currently being discussed for future generations of nuclear reactors in electricity generating systems. For some of these, present roadmaps for future nuclear fuel cycles suggest that fuel reprocessing will be important, and molten salt media may play an important part in improving the efficiency of the recycling process. Fundamental research is recommended that will establish the necessary understanding of the fuel cycle and the chemistry of the associated radionuclides in order to develop efficient processes and to insure the safety and public acceptance of these technologies.

In terms of long-term fuel availability for nuclear fission reactors, it is projected that extraction of uranium from seawater will become economic if the price of uranium increases by a factor of ten. If uranium from seawater is not included, there is sufficient uranium available for 65 years at current consumption rates. While there are additional known amounts of uranium in ore bodies, it will be difficult to recover those. Recycle of nuclear fuels will be critical as the availability of uranium diminishes.

Geoscience

Geosciences underpin discovery of new fossil resources, utilization of hard-to-access reserves and the storage of carbon dioxide in subsurface regions. Locating and extracting technically recoverable reserves of oil and natural gas, particularly in the U.S., is difficult and offers opportunities for high impact research. The two primary directions for recommended research are subsurface imaging and in-situ alteration of fluid/rock interactions. The latter topic is aimed at increasing the mobility of oil and gas phases, thereby increasing the amount of extracted resources. These advanced geoscience technologies will require the development of new fundamental understanding of geophysical, geohydrological, and geochemical processes. Specifically, fundamental research in wave propagation in complex media will provide the understanding needed to make advances in imaging. Rock is a very complex and heterogeneous medium, and the analysis of the propagation and scattering of acoustical waves is a very difficult problem. Furthermore, translating the scattered signals into an image of the geological configuration is also a very difficult computer problem, for which more basic study is recommended.

SUMMARY

This report has highlighted many of the possible fundamental research areas that will help our country avoid a future energy crisis. The report may not have adequately captured the atmosphere of concern that permeated the discussions at the workshop. The difficulties facing our nation and the world in meeting our energy needs over the next several decades are very challenging. It was generally felt that traditional solutions and approaches will not solve the total energy problem. Knowledge that does not exist must be obtained to address both the quantity of energy needed to increase the standard of living world-wide and the quality of energy generation needed to preserve the environment.

In terms of investments, it was clear that there is no single research area that will secure the future energy supply. A diverse range of economic energy sources will be required – and a broad range of fundamental research is needed to enable these. Many of the issues fall into the traditional materials and chemical sciences research areas, but with specific emphasis on understanding mechanisms, energy related phenomena, and pursuing novel directions in, for example, nanoscience and integrated modeling.

An important result from the discussions, which is hopefully apparent from the brief presentations above, is that the problems that must be dealt with are truly multidisciplinary. This means that they require the participation of investigators with different skill sets. Basic science skills have to be complemented by awareness of the overall nature of the problem in a national and world context, and with knowledge of the engineering, design, and control issues in any eventual solution. It is necessary to find ways in which this can be done while still preserving the ability to do first-class basic science. The traditional structure of research, with specific disciplinary groupings, will not be sufficient. This presents great challenges and opportunities for the funders of the research that must be done. For example, the applied research programs in the DOE need a greater awareness of the user facilities and an understanding of how to use them to solve their unique problems.

The discussions reinforced what all of the participants already knew: the issue of energy security is of major importance both for the U.S. and for the world. Furthermore, it is clear that major changes in the primary energy sources, in energy conversion, and in energy use, must be achieved within the next fifty years. This time scale is determined by two drivers: increasing world population and increasing expectations of that population. Much of the research and development currently being done are concerned with incremental improvements in what has been done in the immediate past; and it is necessary to take this path because improvements will be needed across the board. These advances extend the period before the radical changes have to be made; however, they will not solve the underlying, long-range problem.

The Subpanel recommends that a major program be funded to conduct a multidisciplinary research program to address the issues to ensure a secure energy future for the U.S. It is necessary to recognize that this program must be ensured of a long-term stability. It is also necessary that a management and funding structure appropriate for such an approach be developed. The Department of Energy's Office of Basic Energy Sciences is well positioned to support this initiative by enhancement of their already world-class scientific research programs and user facilities.

APPENDIX A

PROPOSED RESEARCH DIRECTIONS

Fossil Energy

Reaction Pathways of Inorganic Solid Materials: Synthesis, Reactivity, Stability

Advanced Subsurface Imaging and Alteration of Fluid-Rock Interactions

Development of an Atomistic Understanding of High-Temperature Hydrogen Conductors

Fundamental Combustion Science Towards Predictive Modeling of Combustion Technologies

REACTION PATHWAYS OF INORGANIC SOLID MATERIALS: SYNTHESIS, REACTIVITY, AND STABILITY

EXECUTIVE SUMMARY

Inorganic materials science today is critically lacking in the knowledge of predictive reaction pathway mechanisms that would allow the design and synthesis of materials with specified reactivity and properties. This is a complex and fundamental problem that affects all aspects of inorganic chemistry and materials science such as oxides, metals, alloys, catalysts, corrosion, degradation and thermal stability. Because the problem is so immense and affects such a wide range of materials, a truly integrated basic research approach of theory, modeling, synthesis, validation and testing is required. Success in merging these methods will allow for unprecedented control and predictability of properties and reactivity of technically relevant materials. It is proposed that the Office of Basic Energy Sciences (BES) invest in research programs that seek to determine the fundamental parameters necessary for predicting the reaction pathways of inorganic solid materials. The combined capabilities of the Department of Energy (DOE) national laboratories and the Nation's research universities will allow for the determination of a new set of principles by which inorganic solids research can be governed. The reliable prediction of the reactivity and properties of materials will foster a new fundamental science, while significantly contributing to applications that improve U.S. energy security.

Current understanding of chemical bonding provides a set of "governing rules" that correctly predict the reaction mechanisms and products for organic chemistry. Such is not the case for solid inorganic chemistry/material science due in part to the complexity of the systems being studied (i.e., compositional variability, defects, electromagnetic interactions, metastability, and cooperative interactions). Illustrative examples of the sensitivity of materials performance to compositional/defect variability include: (1) a chromia-forming heat-resisting alloy with a variation of only 0.5 wt% Si doubling its life span for protective-scale formation under thermal-cycling conditions, and (2) small variation of elemental composition and defect structure of ionic conducting perovskites increasing performance.

Recent advances in materials modeling, synthesis and analytical capabilities provide a strong foundation for significantly advancing understanding of reaction pathways of inorganic solid materials. For example, density functional theory (DFT) allows us to study complex heterogeneous systems and reveal energetically favorable structures, embedding techniques and hybrid methods that capture dynamics allow study of extended systems, and cluster variation method (CVM) calculations allow for predicting the phase equilibria in multicomponent alloys. Synthesis methods have progressed substantially beyond "ball- milling and heating" to procedures that take advantage of new breakthroughs in nanoscience, such as low-temperature synthesis of metastable phases, self-assembly and epitaxial growth of thin films that access previously unachievable phases. Analytical capabilities such as calorimetry of transition metal oxides and neutron science (inelastic neutron scattering of metastable phases and reactions in-situ) allow for fundamental probes of phase formation and kinetic interactions in reactions. Microspectroscopic methods such as X-ray emission and scanning probe microscopies, together with more recent techniques such as 3-dimensional atom probe, will allow study of individual sites with unprecedented energy and temporal resolution.

The knowledge gained through this coordinated technical approach will have significant impacts on fossil energy science and beyond. Understanding the rules that control the synthesis, reactivity and stability of inorganic materials will allow substantial improvements in a wide variety of fossil energy applications including sensors, reliable and durable structural materials for high-temperature applications, membranes, and catalysts. Additional impacts will include energy sources (hydrogen) of the future, legacy clean-up and long-term waste storage and actinide science relevant to the DOE-Defense Program's (DP's) mission.

Summary of Research Direction

Inorganic materials science today is critically lacking in the knowledge of predictive reaction pathway mechanisms that would allow us to design and synthesize materials with specified reactivity and properties. Currently, an "Edisonian" approach is the most common method for directing materials synthesis toward an intended bulk property, with structure/property relationships usually being determined in the post-analysis. This is a non-optimized approach without much predictive capability. Furthermore, this is a complex and fundamental problem that affects all aspects of inorganic chemistry and materials science such as oxides, metals, alloys, catalysts, corrosion, degradation and thermal stability. An integrated basic research effort by academics and national laboratory scientists will combine theory and experiment, using state-of-the-art DOE user facilities to address the following questions:

- What chemical forces drive the operative reactions (e.g., crystallization of unique phases) and can, with the understanding these forces, lead to the synthesis of other classes of materials?
- What chemical mechanisms are responsible for observed bulk properties (e.g., ionic conduction, multicomponent diffusion, or catalytic selectivity)? What are the atomic-scale origins of reactivity in these materials?
- How will understanding atomic-scale properties/phenomena, such as atom-atom and atom-defect binding energies, nearest-neighbor interactions, site selectivity and changes in crystal structure, lead to the synthesis of new classes of tailored inorganic phases?
- How will understanding 1-dimensional and 2-dimensional structural defects in materials lead to the synthesis of materials with tailored properties?
- How can the thermodynamics of systems with stress-mediated interactions and consequential non-equilibrium effects at the interface be properly treated?
- Can interface mobility, as a function of its structure, orientation, composition, and strain field, be accurately modeled? Included here is the growth of a faceted interface (dynamics of step propagation).
- What nontraditional transformation pathway processes need to be established to describe the selection of stable or metastable phase(s) and the advancement of corresponding laws of phase transformations?

The goal of this type of program is detailed understanding of the atomic mechanisms (or reaction pathways) responsible for the formation of inorganic phases and the ability to predict the bulk properties of those formed materials. This general approach is a necessary goal for all areas of inorganic chemical research, including solid inorganic oxide, and metal and alloy chemistry/material science. Examples of areas of need include:

- In the area of ionic conducting perovskites, variation of elemental composition and defect structure increases performance. Existing methods for synthesizing perovskites, and those with high dielectric constants and/or ionic conductivity include ball milling and heating, ball milling to release an exotherm plus heating, solgel synthesis and thin film applications, solgel plus organic addition synthesis (for high surface area materials), and metalorganic chemical vapor deposition. All these methods involve high-temperature heating, necessary for perovskite crystallization. This is not only costly in heating costs, but also adversely affects the final material. Research into low-temperature perovskites derived from stoichiometrically predetermined metastable phases (i.e., solgels, molecular sieves) are different energetically, and probably show more ionic disorder (i.e., metastable which is desirable for properties such as ionic conductivity and high dielectric constant) compared to materials synthesized directly at high temperature. This gives the ability to "tune" the resultant perovskite into novel compositions.

- In the area of synthesizing materials with tailored properties, it is well established that properties are inextricably linked to the micro- and/or nano-structure of a given material. The evolution of a micro- and/or nano-structure often involves self-organized phenomena, which can result in highly regular structures of controllable geometry and size. Although there are multiple routes to self-organization, involving different driving forces, length scales and system dimensionality (i.e., whether 2-d or 3-d), it is important to understand the underlying principles, which universally describe self-organization, irrespective of the specific details of the system.

- In the area of heat-resisting alloys, slight variations in alloy composition can significantly affect resistance to high-temperature degradation and, hence, performance. This is true even for composition variations within the specifications of a commercial alloy. Such a sensitivity to composition reflects the complex interactions of alloying elements on scaling behavior, scale adherence and cracking/spallation behavior, and subsurface diffusion behavior. A holistic approach that addresses all these aspects of high-temperature degradation needs to be taken if there are to be any leap-frog advances in improving the reliability, durability and predictability of alloys and coatings for high-temperature applications.

New Scientific Opportunities

New scientific opportunities exist in the combination of basic synthetic research methods, plus analytical abilities to understand from the reaction pathway level of interactions of reactants to their effect on bulk properties. This is the opportunity for modeling experts to use expanded modeling/simulation codes on ever more powerful computers to predict the true events in these complex materials systems (e.g., see Figure 1-1), and to utilize embedding techniques and hybrid methods that capture dynamics for the study of extended systems.

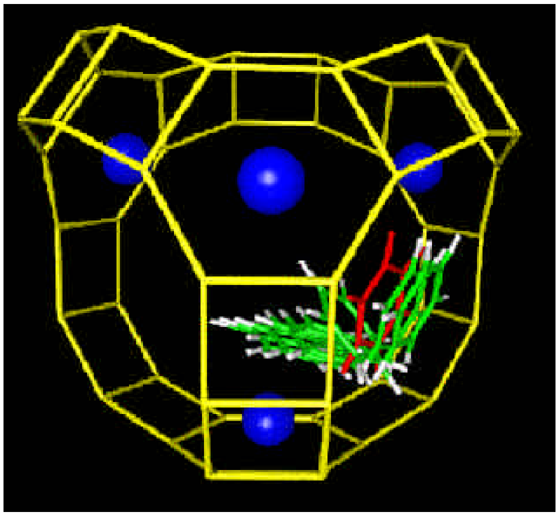

Figure 1-1. Minimum Energy Path for Benzene in NaY Zeolite (between a cation site and the window site). [Auerbach, *Int. Rev.Phys.Chem*. 2000, 19, 155].

Recent progress in synthetic methods allows for the exploration of new phase space areas, particularly in low-temperature synthesis of metastable phases by hydrothermal and chemie douce methods, self-assembly of inorganic oxides and III/V semiconductors through organic molecule capping techniques, and epitaxially growth of thin films. Studies of the synthesis, its optimization and the mechanism of formation will need the combined efforts of X-ray (i.e., synchrotron) and neutron scattering technologies. An excellent example is the use of time-resolved studies at the National Synchrotron Light Source (NSLS) and Advanced Photon Source (APS). Time-resolved studies would allow us to study structure transformation between metastable phases through to thermodynamically stable phases. Fundamental issues to be studied include structure, mechanisms for transformation (i.e., bond breaking), and microporosity durability versus structure densification, through the observation of the reaction from gelation to crystallization using time-resolved scattering. The ability to observe metastable intermediates directly, some of them existing for just a short time, is a distinct advantage and an excellent complement to the exploratory synthesis efforts.

Relevance and Potential Impact

This proposed research direction is of direct relevance to all energy programs (e.g., Fossil, Nuclear, Energy Efficiency, Renewable, Fusion).

The knowledge gained through this coordinated technical effort will have significant impacts on fossil energy science and beyond. Understanding the rules that control the synthesis, reactivity and stability of inorganic materials will allow substantial improvements in a wide variety of fossil energy applications, including sensors for monitoring in high-temperature and caustic environments, reliable and durable structural materials for high-temperature applications in advanced power generation systems, materials and coatings for supercritical reactors, membranes for ionic/proton conduction and hydrocarbon feedstock separations (allowing for the removal of costly distillation units), and catalysts for vastly increased energy and economic efficiency plus reduced environmental impact.

Additional impacts will include energy sources (hydrogen) of the future, legacy clean-up and long-term waste storage and actinide science relevant to the DOE-DP mission. In particular, the fields of proton and ionic conductors have been hampered by “Edisonian” approaches for synthesizing better conducting materials. Instead of traditional human combinatorial approaches, the employment of defined reaction pathways will be used in the design and tuning of high-conducting oxides with built-in thermal, mechanical and chemical stability. Furthermore, the resultant reaction pathway rules will be employed in the synthesis of materials for waste legacy clean-up and long-term waste storage of radioactive solvated nuclei found today in temporary waste storage facilities around the country. Finally, the application of this predictive knowledge to actinide science allows for safe, non-repetitive synthetic laboratory procedures, resulting in minimized exposure to workers.

Estimated Time Scale

The determination of the fundamental parameters of the reaction pathways for inorganic solid materials resulting in predictive synthesis, reactivity and stability is a long-term goal of the basic research community. Achieving this goal has yet to be accomplished due to the significant complexity of the problem. The full cooperation of basic research scientists from national laboratories and academic communities, plus full use of the DOE’s user facilities, will be needed to make any notable headway. We believe that with full cooperation and funding in 3-5 year increments, this will be a 10-20 year investment for BES.

ADVANCED SUBSURFACE IMAGING AND ALTERATION OF FLUID-ROCK INTERACTIONS

EXECUTIVE SUMMARY

Fossil energy resources are currently the backbone of the U.S. energy system, and their continued availability in the short term is critical for maintaining U.S. economic security. The technically recoverable reserves of oil and natural gas are many times those of current proved reserves. Advanced geoscience technologies will enable industry to meet the challenges of locating and extracting these additional reserves in an environmentally acceptable and cost-effective manner. Two research areas that would have major impacts are subsurface imaging and in-situ alteration of fluid/rock interactions. Subsurface imaging will delineate deep geologic structure and the properties, composition, and spatial distribution of rocks and fluids. Research supporting imaging would have application to hazard prediction, resource quantification and reservoir process monitoring. Purposeful in-situ alteration of rock/fluid interaction deals with technologies for increasing the mobility of oil and gas phases, thereby increasing the amount of extracted resources. It also deals with development of technologies which will ultimately enable in-situ processing of hydrocarbons, replacing processing steps that are currently carried out on the surface.

These advanced geoscience technologies will require development of new fundamental understanding of geophysical, geohydrologic, and geochemical processes. Fundamental research in wave propagation and new mathematical methods for inversion of geophysical, geohydrologic, and geochemical data will provide part of the basis for major advances in imaging. Other basic research is needed to understand how to predict processes from measurements at different scales. Exotic physical phenomena such as electrokinetic and seismoelectric effects need to be assessed through basic research to identify technological applications. The basic processes controlling the mobility of one fluid phase relative to another need to be understood. Finally, the possibility of using nanoparticles to alter rock/fluid interactions, thereby either increasing mobility of oil or releasing more easily extractable volatile gas, opens the door for revolutionary new hydrocarbon extraction technology.

Successful application of this basic research will have major scientific payoffs within the next two decades as well as potential financial impacts in the energy industry of billions of dollars per year.

Summary of Research Direction

Advanced geoscience technologies are necessary in order to meet the challenges of environmentally acceptable and cost-effective extraction of remaining domestic reserves of oil and gas and to enable development of unconventional reserves. Two areas that would have a major impact on reserve extraction are subsurface imaging and in-situ alteration of fluid/rock interactions. Major advances in these technologies will require development of new fundamental understanding of geophysical, geohydrologic, and geochemical processes.

Subsurface imaging will delineate subsurface geologic structure and the properties, composition, and spatial distribution of rocks and fluids. By repeating measurements over time, hydrodynamic, geochemical, and geomechanical processes can be monitored. Research supporting imaging technologies would have application in at least three major areas: (1) hazards prediction, (2) resource quantification, and (3) monitoring of reservoir processes.

Improved imaging will reduce the risk of siting and drilling wells. Hazards include overpressure; weak unstable materials, such as shallow water flows; and salt, which creeps. Imaging research needs to focus on providing quantitative information on the physical properties of hazards as well as location and spatial extent.

Subsurface geophysical imaging has been used for decades to identify the location and quantity of oil and gas resources. In conventional oil and gas fields the challenge is now to locate smaller pools which have been missed during original exploration. Unconventional gas resources such as coal bed methane and methane hydrates present new challenges. In neither case are conventional oil and gas imaging technologies adequate to quantitatively evaluate the amount and distribution of the resource.

Monitoring of reservoir processes will enable more cost-effective production as well as provide information on additional reserves. Information is needed on the changes over time in the distribution and pressure of oil, gas, and water during primary, secondary, and tertiary production. Injection of chemically reactive substances, such as CO_2, necessitates geochemical monitoring as well. Imaging for monitoring requires the combination of direct measurement of quantities, such as chemical composition, pressure and fluid flux with indirect geophysical measurements. Research is needed to develop methods that integrate the various types of data in developing an image, as well as to improve resolution and quantitative interpretation of imaging results.

Purposeful in-situ alteration of rock/fluid interactions is the second research area that could have major impacts on oil and gas recovery. Primary production of oil and gas is carried out utilizing natural forces such as differential fluid pressure, gravity, and reservoir compaction. Injection of water, steam, CO_2, or other chemicals are used for secondary and tertiary recovery of oil, and are examples of purposeful alteration of rock/fluid interactions.

Most secondary and tertiary methods involve modification of the mobility of one phase relative to another. Wettability describes the relationship among mineral surfaces and the immiscible fluid phases. It strongly influences the location and distribution of fluids and fluid relative permeabilities and is one of the main design parameters for selecting the best recovery strategy. Nonetheless, the complex mechanisms controlling wettability and its effect on oil recovery are not well understood.

It has been suggested that phase mobility can be modified by low-frequency seismic energy, diffusive pressure waves, and electrokinetic and seismoelectric phenomena. Research is needed to evaluate fundamental mechanical, hydrodynamic, and electrochemical processes that may change the mobility of one fluid phase relative to another.

The possibility of using nanoparticles to alter rock/fluid interactions, and, in particular, increase oil mobility, represents a new, potentially significant research direction. For example, oil might be sorbed onto nanoparticles which would have lower capillary forces than the unmodified oil. Another technique might be to use nanoparticles that would adhere to pore surfaces but present hydrophilic surfaces to the oil. Finally, tailoring electronic properties of nanoparticles opens the door for developing materials, and perhaps slight variants of natural minerals, that would have unique catalytic properties. It may then be possible to break long-chain hydrocarbons in place, releasing more easily extracted volatiles.

New Scientific Opportunities

Research directed toward subsurface imaging and alteration of fluid rock interactions will provide opportunities for broadening and developing new areas of fundamental science in geophysics, geohydrology, and geochemistry.

Fundamental research in wave propagation in complex media will provide understanding needed to make advances in imaging. The complexity of rock masses arises from the existence of discontinuities such as fractures and faults, which exist at all scales, heterogeneity in lithology arising from natural geologic processes such as deposition, intrusion, and hydrothermal alteration, and the presence of fluids of different phases and properties that are heterogeneously distributed at all scales. For such media, the relative contribution of scattering and intrinsic attenuation to frequency dependent changes in amplitude needs to be better understood. New rock physic models are needed that quantitatively describe intrinsic attenuation in porous rock containing heterogeneous distribution of fluids of multiple phases. New models for wave propagation at a macroscopic scale that accurately capture effects of different loss mechanism, need to be developed. Differences in the models for different geologic environments need to be understood. Factors affecting wave-propagation are expected to be very different in sand, shale, soil (unconsolidated sediments), coal, and granite.

Electrokinetic phenomena, and in particular, seismic-electric, and electro-seismic coupling are not well understood. Prediction of behavior at the macroscopic, or field scale, is particularly uncertain. Diffuse pressure waves, which travel primarily in the fluid phase, are also not well modeled and characterized. Further fundamental work on these phenomena could lead to new imaging methods. These same phenomena may also have effects on phase mobility which could lead to breakthrough technologies for enhanced recovery of oil and gas resources.

The non-uniqueness of inversion is a fundamental problem in imaging. Joint inversion of various types of data is one approach to the problem of non-uniqueness, but joint inversion is computationally intensive. New mathematical approaches, including support vectors and other new algebras, need to be explored.

Fundamental research needs to be focused in geophysics, geohydrology and geochemistry on issues of scale in complex media. It is not clear how to scale geophysical measurements from the laboratory scale to field scale. It is not clear how to combine hydrologic models of processes at the microscale in pores and fractures to generate effective media models applicable at field scale. It is not well understood why fluid/rock reaction rates determined at laboratory scale experiments are up to several orders of magnitude faster than similar reaction rates measured at field scale.

Advancements in purposeful alteration of rock/fluid interaction requires new fundamental understanding of the mechanisms controlling wettability in reservoirs. Scientific opportunities include: (1) understanding influence of asphaltenes and oil composition on wettability, (2) studies of effects of brine composition, (3) studies of clay and colloid particle content and composition, and (4) understanding influences of colloid-interface associations.

Finally, the potential for development of new approaches to alter fluid/rock interactions using nanoparticles provides a whole new area of nanoscience research opportunities. Very little is known about the properties of mineral nanoparticles that would be most applicable, although several expectations arise from what is known about semiconductor nanoparticles and crystals. The electronic properties of nanominerals are size dependent and not the same as the bulk structure of the same material. Surface properties such as surface tension and hydropholicity/hydrophilicity are also size dependent. Chemical modification of nanoparticle surfaces may be possible that would enable unique collective phenomena such as aggregation. All of these properties may be tailored for enhanced recovery applications.

Relevance and Potential Impact

Fossil energy resources are currently the backbone of the U.S. energy system and their continued availability in the short term is critical for maintaining U.S. economic security. It is well known that domestic oil reserves and oil production are declining. Conventional production of natural gas in the U.S. may peak as early as the year 2015, though natural gas consumption is increasing faster than any other fossil fuel. Though the current proved domestic reserves of crude oil and natural gas are 22 BBO (billion barrels oil) and 177 TCF (trillion cubic feet), the technically recoverable reserves are 175 BBO and 1431 TCF, respectively. In 1995, the United States Geological Survey (USGS) estimated that over 50% of the technically recoverable oil reserves is oil in known fields that could be added through field extension, additions of new pools and application of new recovery techniques. Even 90 BBO is a large increase in oil reserves. Major breakthroughs in imaging and new advances in purposeful alteration of rock/fluid interactions will provide the technology needed to cost effectively locate and extract much larger percentages of the technically recoverable resources. Financial impacts of technology breakthroughs in the energy industry are measurable in terms of billions of dollars per year.

Estimated Time Scale

It is extremely difficult to forecast technology breakthroughs. It is envisioned that research will be continuing in each of the areas discussed for decades. At the same time, useful results will be generated over the course of continuing research efforts. Whether by incremental advancement of knowledge or major breakthroughs, major payoffs would be anticipated during the next two decades.

DEVELOPMENT OF AN ATOMISTIC UNDERSTANDING OF HIGH-TEMPERATURE HYDROGEN CONDUCTORS

EXECUTIVE SUMMARY

Ion transport membranes composed of proton-conducting materials are a critical component for future fuel processing and energy production systems, as well as ancillary technologies such as fuel cells, sensors, and electrolyzers. Proton conducting membranes are necessary to extract *absolutely* pure hydrogen from mixed gas streams in the processing of fossil fuels and other petroleum and petrochemical processes. The best candidate membrane materials for hydrogen separation at high temperatures are proton-conducting ceramic oxides. However, despite great efforts, a viable ceramic-based proton conductor has not yet been developed. The objective of the proposed thrust is to develop, through the integration of theory, modeling, and experimentation, a scientific understanding of the mid- to high-temperature (<600°C and 700°C) interaction of incorporated hydrogen with the host atoms and structural defects in a new class of oxides and amorphous metallic proton conductors.

Current science and future facilities are well positioned to make these advances. For instance, the more advanced computing systems are providing powerful tools for research through massively parallel implementations of simulation models . High-performance computing is enabling researchers to model materials systems at reduced dimensionality, while at the same time accurate first-principle calculations of materials properties now extend to systems involving thousands of atoms. The advent of powerful pulsed neutron sources is making possible the acquisition of neutron diffraction data on much shorter time scales. These and current neutron facilities will provide the capability to shorten the time scale to tens of seconds for some materials systems as well, which will allow for critical time-resolved in-situ studies of protonic conductors. Specifically, neutron diffraction can be used to locate the coordinates of oxygen and hydrogen (deuterium) ions in bulk polycrystalline solids, which are essential to the conductivity of these materials. This will expand the scientific understanding required to optimize the structure-related properties of crystalline, nanocrystalline, and even amorphous materials for gas separation, hydrogen storage, fuel cell, and other economically important applications.

The advances made by this effort over the next 10 years are critical for the leap-frog development of novel ion conducting oxides and alloys for hydrogen separation membranes. Such a development will allow for the recovery of millions of cubic feet of hydrogen at refineries every day and thus save the petroleum, steel, and petrochemical industries hundreds of millions of dollars annually. It will also facilitate the separation of hydrogen from carbon-dioxide-laden streams, facilitating sequestration.

Summary of Research Direction

A more fundamental understanding is needed of how hydrogen is transported and stored within the atomic lattice, at interfaces in crystalline materials, and within the disordered structure of bulk amorphous metals. Neutron sources offer exciting new opportunities for studying the migration and storage mechanisms for hydrogen in various materials. The ability to also conduct *in-situ* analysis to examine the influence of temperature and environment on transport processes and stability issues will play a major role in developing the next generation of hydrogen conductors. Theoretical studies utilizing such information will be needed to provide a basis for tailoring materials and multicomponent systems. Opportunities also exist for developing new materials by gaining further insights into the behavior of nanocrystalline oxides and bulk amorphous alloys.

New Scientific Opportunities

Proton Conductors. Proton conductors are critical materials for future hydrogen-fueled systems and the related infrastructure required to produce and deliver hydrogen. These can be used as solid electrolytes in fuel cells, ionic membranes and gas sensors. However, the properties of current materials are not sufficient to meet the needs for commercial applications. To date, the available materials are not sufficiently stable in the anticipated service environments and lack the high protonic conductivity and enhanced catalytic properties required. Future research efforts must focus on the fundamental understanding of hydrogen conduction and storage mechanisms and their relation to composition and crystal structure to uncover new protonic conduction materials.

All current proton conductor systems have issues related to insufficient chemical stability and proton diffusivity and/or the dominance of other charge carriers to the total electrical conductivity. For example, hydrate compounds such as $H_3Mo_{12}PO_{40}$:H_2O, $HClO_4$:H_2O, which possess high protonic conductivity, are unstable in dry atmospheres and at temperatures above 100^{o}C. A similar situation is found with the bronze-structured H_2WO_3 or H_xMoO_3 oxides. Despite the fact that these materials have high proton mobility, their electrical conductivity is dominated by the electronic contribution, and protonic conductivity is not major factor in this case. In acceptor-doped perovskites (e.g., $SrCeO_3$, $BaCeO_3$), the electrical conductivity can be enhanced by trivalent dopants that introduce oxygen vacancies and promote the incorporation of protons. Unfortunately, the ratio of hydrogen-to-oxygen transport diminishes at elevated temperatures, and the materials are no longer effective hydrogen conductors.

A major issue is the need to discover materials that are capable of hydrogen storage levels of $10%. Studies of proton storage in oxides indicate that the protons are associated with the oxygen in the lattice and form OH groups in concentrations of only 3-5%, concentrations that are comparable to the oxygen vacancy content. Similarly, the hydroxides such as LiOH can store only ~ 4% hydrogen, while some of the hydrides are reported to store levels approaching 10% but have issues with stability.

***Oxide Conductors*.** In the case of oxide proton conductors a new paradigm is required to overcome past deficiencies. Unique crystal chemical approaches are envisioned to enhance proton conductivity including (1) introduction of vacancies and defects through novel doping schemes; (2) nonlinear enhancement of properties in compositions near phase boundaries; and (3) exploitation of interfacial effects in multiphase compositions in combinations of chemically related but crystallographically dissimilar proton conductors, such as those with layered structures. Another area for research is the development of ion-conducting thin films, which could accelerate the application of proton conductors as ion separation membranes by enhancing hydrogen permeability, even at lower operation temperatures. There is potential for achieving such goals by developing thin film membranes with thickness less than one micron on porous substrates. This could lead to devices with much higher permeation rates than the current devices that utilize one to two millimeter thick bulk membranes.

While this is insufficient, there is an extensive experimental database on perovskite structures, which could serve as the initial basis for developing new oxide systems. The advent of new neutron beam lines will provide a powerful means for establishing the mechanisms of hydrogen storage and transport in these and other oxide lattices. For instance, quasi-elastic neutron scattering could be employed to study the proton-phonon interactions and develop new insights into protonic transport at the atomistic level. This will also require the development of models and analytical tools to be able to interpret such data. Such advances will allow one to examine the real effects of specific dopants on proton transport and provide for critical in-situ studies of the effects of temperature and gas composition. These results would be linked with theoretical studies utilizing first principles and various longer length scale approaches (e.g., molecular dynamics) to describe the role of lattice structure and composition in vacancy formation and the storage and transport of hydrogen within the lattice. With such understanding, it will be possible to develop materials where electrical transport is not limited by lattice diffusion.

In addition, there is a need to search for and take advantage of new mechanisms for protonic transport. There is the potential for novel nanocrystalline oxides as hydrogen conductors. Studies have shown that nanocrystalline perovskites (e.g., Yb-doped $SrCeO_3$) can exhibit over a thousand-fold increase in electrical conductivity, as compared to the conventional micron-grain-sized ceramics. This effect may be related to the more rapid diffusivity expected to occur along grain boundaries in comparison to that through the lattice. In addition at a grain size of 10 nm, the grain boundaries constitute a substantial fraction of the material. This suggests that nanomaterials may have untapped potential for greater hydrogen storage together with more rapid transport.

A new class of hydrogen separation materials may be possible through the synthesis of bulk amorphous alloys and nanocrystalline metals. Metallic alloys in noncrystalline states generally contain significant "free volume" at the atomic scale that may facilitate hydrogen storage and transport in a controlled fashion. Studies in the past of these materials have been limited due to metastability of these alloys. However, stable forms have been demonstrated that enhance their potential for consideration as proton conductors. Thus, bulk amorphous alloys constitute a new and exciting class of metallic materials with unique physical and mechanical properties for functional and structural uses.

Relevance and Potential Impact

For the next several decades, H_2 will be generated from fossil fuels until clean H_2 sources can be developed. Pure H_2 streams will need to be produced via separation from mixed gas streams containing CO, CO_2, H_2O, hydrocarbons and other gases by separation processes. There is a tremendous need for H_2 separation membranes if the H_2 infrastructure is to become a reality. Pure H_2 is needed for fuel cells, to facilitate H_2 storage, to recover H_2 from mixed gas products in the petrochemical industries, and for upgrading of petroleum products to fuels. In the next several decades more H_2 will be consumed converting petroleum into fuel than any other end use. However, at present there are no viable high-temperature separation membranes capable of producing pure H_2 streams. This area of research needs to be rapidly expanded over the next decade if the H_2 economy is to become a reality.

Estimated Time Scale

Improvements in current materials might be accomplished through such studies over the next five years. However, the evolution of new material classes for hydrogen conductors is likely to require another decade of fundamental research.

FUNDAMENTAL COMBUSTION SCIENCE TOWARDS PREDICTIVE MODELING OF COMBUSTION TECHNOLOGIES

EXECUTIVE SUMMARY

The development of predictive computational capabilities for combustion devices is a long-term goal of the DOE that has yet to be realized due to the magnitude of the scientific and computational challenges presented by turbulent, chemically reacting systems. Continuing advances in high-performance computing and laser diagnostics provide an unparalleled opportunity to advance combustion science, leading to science-based engineering design methods that will revolutionize the performance of combustion systems. An integrated program of basic theoretical, computational, and experimental research is needed bring the fundamental understanding of combustion science up to the level needed to provide a basis for predictive computational models for complex combustion systems. This program should involve closely coupled research by scientists at universities and national laboratories using terascale computers, state-of-the-art laser diagnostic capabilities, and web-based tools for data sharing and collaboration. Emphasis should be placed on the chemical kinetics associated with ignition, combustion, and pollution formation in realistic fuels and on the physics of the coupling of turbulent fluid dynamics with chemistry. An integrated approach is required to connect the various aspects of fundamental science needed to address complex combustion systems.

Combustion of fossil fuel is central to the U.S. economy, accounting for $334 billion in fuel costs in 1996 and 85% of annual energy consumption. Combustion of fossil fuels is also responsible for nearly all of the anthropogenic emissions of nitrogen oxides (NO_x), carbon monoxide (CO), soot, aerosols, and other chemical species that are harmful or are suspected to be harmful to human health and the environment. At the global level, fossil fuels will continue to be the primary source of energy required for economic growth. Issues of energy security, global economic competitiveness, public health, and environmental integrity will have a profound impact on the design and operation of the combustion systems of the future. For example, radically new engine designs are the only hope for meeting the near-zero NO_x and particulate emissions commitments proposed for implementation by 2012.

The traditional evolutionary approach to combustion system development, which relies heavily on cut-and-try engineering to test incremental design changes, is inadequate to meet these challenges. A major barrier to rapid development of radically new combustion technologies with reduced emissions and improved efficiency is the absence of truly predictive computational tools for combustion systems. The phenomena that influence combustion span wide ranges of scales in both time and space. Consequently, no foreseeable computational hardware will be capable of running a fully resolved and coupled simulation of combustion in a practical combustion device, which includes detailed chemistry and all scales of turbulent fluid motion, with turnaround times fast enough for design calculations. Physically accurate and computationally efficient models are needed that are based on fundamental combustion science and validated rigorously against detailed experiments. However, there are significant gaps or uncertainties in our knowledge of the relevant chemical kinetics and in our fundamental understanding of the complex dynamic coupling of turbulent flow, molecular transport, and chemical reactions. Today's most advanced turbulent combustion models can only predict simple flames with reliable accuracy. Accurate prediction of phenomena such as soot formation, auto-ignition of turbulent mixtures, local flame extinction and re-ignition in complex flow geometries, flame propagation in heterogeneous mixtures, and stabilization of detached flames will require greater scientific understanding and further development of combustion models.

Science-based predictive capability for complex combustion systems will revolutionize the development of future combustion technologies by moving much of the innovation, design, and optimization process onto the computer. It will facilitate the exploration and development of radically new concepts for high-efficiency, low-emission devices for conversion of fossil energy. It will also greatly reduce the time required for industry to bring new technologies to market or adapt designs to accommodate specific operational requirements, such as fuel flexibility.

Summary of Research Direction

The phenomena that influence combustion span a wide range of scales in space and time. The spatial scales extend from the dimensions of molecules, where chemical reactions occur, up to the scale of the combustion device itself. Temporal scales extend from those associated with the fasted chemical reactions to the residence time of fluid in the combustor. No foreseeable computational capability will be able to encompass phenomena over this range of length and time scale within a single simulation.

A promising strategy to advance fundamental combustion science is to develop a highly integrated effort that combines detailed scientific simulations with state-of-the-art experimentation. Experiments and computations that illuminate the phenomena at each scale are needed to develop computationally efficient models of the dominant behaviors at each scale. These models can then serve as the building blocks of simulations and experiments at successively larger scales.

Processes at disparate scales are not as easily partitioned as this picture suggests, raising critical fundamental scientific issues. The ultimate product of such research would be a set of mathematical models representing key combustion phenomena and their interactions. These models can serve as the basis of a new engineering design paradigm that would shift the focus of technology development from slow, costly prototype construction and testing to efficient, accurate computational design iteration and testing of proposed hardware designs.

Ultimately, reaching the goal of a predictive capability for comprehensive, device-scale combustion simulations will require coordinated research covering the entire range of combustion length and time scales. Specific needs include: (1) Theoretical methods to predict the pressure and temperature-dependent rates of multistep complex reactions, as well as detailed measurements of key individual reactions in order to verify and validate these computational tools; (2) efficient tools to generate complete combustion chemical mechanisms and tools for producing appropriate reduced mechanisms required for modeling macroscopic combustion systems; (3) experimental combustion diagnostics for nonintrusive, spatially and temporally resolved measurements of the concentrations and concentration-gradients of multiple species, temperature, radiation flux, and fluid velocities, typically required for benchmarking and validation of combustion simulations; and (4) high-fidelity numerical simulations of building-block flows that reveal fundamental turbulence-chemistry interactions in combustion. These physical and numerical experiments must be carried out at multiple levels of complexity. In particular, carefully executed benchmarks that are designed to expose or emphasize the role of particular physical subprocesses are required to assure that our scientific understanding is complete. Also, quantitative computational data and experimental measurements in device environments are required to validate the capabilities of device-scale simulations to predict the complex interplay among the many important physical processes over a parameter space that enables the design of future combustion technologies. Figure 1-2 shows the necessary range of computations and experiments required to understand combustion.

The rich nature of the scientific challenge and its connections to combustion technology are illustrated by three example problems:

- soot formation in combustion systems and its coupling to other phenomena;
- the coupling of autoignition kinetics with turbulent mixing, enabling novel control techniques for homogeneous charge compression ignition (HCCI) combustion; and
- extensions of lean-limit combustion via hydrogen fuel blending.

Understanding the inception, growth, transport, and oxidation of soot is vital to controlling particulate emissions from diesel automobile engines, and soot radiative properties are central to heat transfer in boilers and furnaces. The gas-phase chemistry leading to soot formation involves hundreds of species and thousands of chemical reactions. New theoretical and experimental tools and techniques will be needed to elucidate the complex soot-formation chemistry. New theoretical methods are needed to rapidly and accurately predict the pressure and temperature dependent rate constants required to describe the early, rate-limiting steps of soot formation. The thermally-driven ordering of the initially disordered solid particle involves too many atoms for fully detailed simulation, so a reduced description of atom-atom interactions will be needed in simulations of this process. The clumping of soot particles to form wispy aggregates

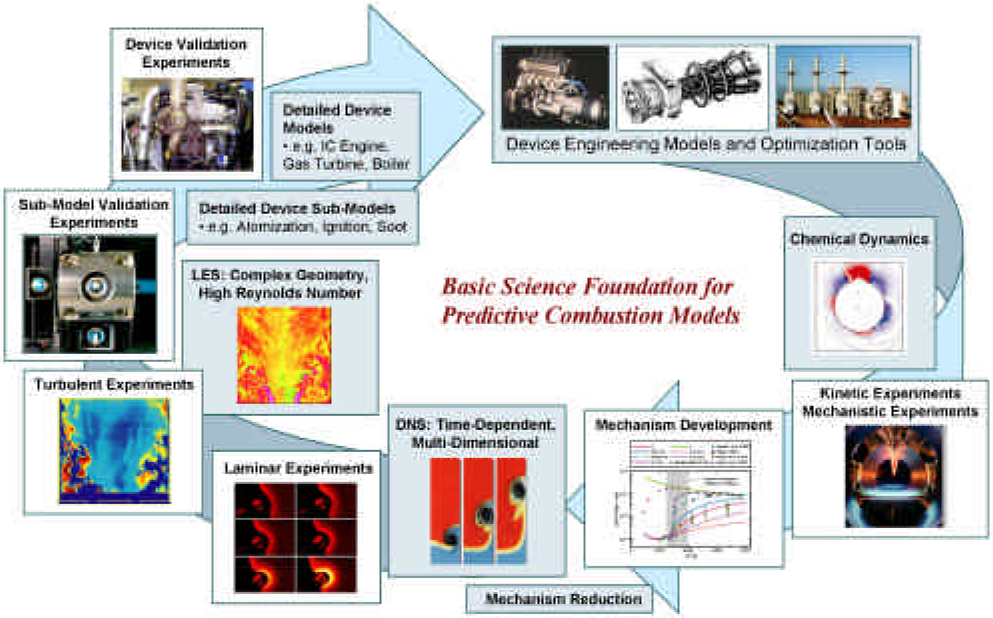

Figure 1-2. Applications of simulation tools and experimental capabilities designed to address combustion science.

cannot affordably incorporate atomic-scale processes, but the knowledge gained from finer-scale simulations will provide adequate surrogate representations. Heterogeneous chemistry experiments will be required to guide and validate model development. New experimental methods will be needed to quantify soot and soot precursors concentrations and morphology in combustion environments. The key role of soot as an absorber and emitter of radiation will be addressed computationally in a simulation that keeps track of the number and mass density of soot aggregates as they are transported through a combustor by turbulent fluid motions. Individual aggregates will not be resolved at this level of simulation. Other soot-related phenomena that will be studied computationally include autoignition and flame stabilization in a turbulent jet to determine the initial distribution of soot precursors, heat exchange between soot and nearby flames, turbulent mixing of soot-bearing gas with surrounding air, and oxidative destruction of the soot.

Homogeneous charge compression ignition (HCCI) combustion is an alternative engine combustion process that can provide high diesel-like efficiencies, while producing ultra-low NO_x and particulate emissions. Unlike a conventional spark-ignited engine, combustion occurs volumetrically throughout the cylinder as the charge is compressed, rather than in a flame front. This permits HCCI combustion to occur at relatively low temperatures, and therefore, dramatically reduce NO_x emissions. There are several outstanding technical barriers that must be overcome before HCCI can be widely applied to transportation engines. Fundamental research is required to control ignition timing and to limit the rate of combustion heat release to allow high-load operation. Overcoming these challenges requires an improved understanding of the close coupling between turbulent mixing and local chemical-kinetic reaction rates related to autoignition of large hydrocarbon fuels. This chemistry is the same as the chemistry associated with knock in spark-ignited engines. Turbulent mixing is thought to play a major role in mixture preparation and modulation of ignition kinetics. The inclusion of detailed chemistry in turbulent models is often impractical and methods for producing high-fidelity reduced mechanisms must be developed. Within practical engines, complete charge homogeneity is unattainable. An important research question is how mixing strategies lead to varying inhomogeneities in the charge, and how these inhomogeneities can be used ultimately to control the heat release rate, emissions and ignition timing.

Ultra-lean premixed hydrocarbon combustion (LPC) is currently one of the most promising concepts for substantial reduction of emissions while maintaining high efficiency. This mode of combustion is operated with excess air to reduce the flame temperature to levels that virtually eliminate NO_x production. Operating at the lean flammability limit poses significant challenges with flame stability, noise, and system dynamic responses. Minor fluctuations in the fuel/air ratio, for example, can lead to flame blowout, combustion instabilities, autoignition and flashback. Moreover, the intrinsic problems described above are compounded at high pressures. Understanding and controlling these phenomena is extremely important for the design of LPC stationary gas turbines and burners. Recently, hydrogen-enriched hydrocarbon fuels are being considered to improve flame stability characteristics during lean combustion. Hydrogen-enriched fuels modify both the flame structure and propagation aspects. Fundamental research is needed to characterize the behavior of combustion of enriched fuels. In addition to potential operational advantages, the development of hydrogen and hydrogen-blended hydrocarbon fuels for gas turbine applications will boost the use of alternative fuels. In the long term, these “designer “ fuels will serve in the transition to a carbon-free fuel economy.

Such challenges will require multidisciplinary teams of computational and experimental physicists and chemists with access to terascale computer systems, state-of-the-art numerical algorithms, the latest advances in computational science, and advanced optical diagnostics in modern experimental facilities. Significant new efforts are needed to describe heterogeneous processes, such as soot growth, and the effects of high pressure, for example in HCCI and LPC devices.

New Scientific Opportunities

Terascale computer systems and advanced experimental capabilities for combustion science offer unprecedented opportunities of synergistic, high-fidelity investigation of combustion phenomena. Direct Numerical Simulation (DNS) and high-fidelity Large Eddy Simulation (LES) methods are on the verge of becoming tools for fundamental investigation of the fully coupled dynamic behavior of reacting flows with detailed chemistry and realistic levels of turbulence. Information from such simulations, combined with detailed laser-based experiments on well-defined benchmark flames, present new opportunities to understand the central physics of flow/flame interaction and develop accurate, physics-based models for turbulent combustion.

Relevance and Potential Impact

Combustion of fossil fuels is the dominant mode of energy conversion, both nationally and globally, and it will remain dominant for decades. The truly predictive computational tools needed to effectively develop new combustion technologies with higher efficiency and lower emissions do not exist today. A focused BES effort dedicated to solving relevant combustion science problems will enable, for the first time, high-fidelity, fully predictive simulation of the next generation of combustion devices. Predictive capability will revolutionize the development process for advanced combustion technologies for transportation, power generation, and industrial processes, and it will greatly accelerate the global implementation of high-efficiency, low-emission systems. Fundamental advances in the science and modeling of chemically reacting flows will also have significant impact in chemical process engineering and atmospheric science.

Estimated Time Scale

The development of predictive simulation capability, which is applicable to a broad range of combustion problems, is a long-term goal. Substantial progress in the development of predictive models for the coupling of turbulence and chemistry in complex combustion systems can be expected within the next 5-10 years under the proposed program. Extension to prediction of complex phenomena, such as autoignition in turbulent heterogeneous mixtures or soot formation in combustion systems, is likely to require sustained effort over a 10-20 year period.

Nuclear Fission Energy

Materials Degradation

Advanced Actinide and Fission Product Separations and Extraction

Fuels Research

Fundamental Research in Heat Transfer and Fluid Flow

MATERIALS DEGRADATION

EXECUTIVE SUMMARY

Future nuclear energy systems will need to provide (1) manageable nuclear waste, effective fuel utilization, and increased environmental benefits, (2) competitive economics, (3) recognized safety performance, and (4) secure nuclear energy systems and nuclear materials. Steady-state coolant temperatures in proposed next-generation reactor concepts range from 370°C to 1000°C, with projected accident transients that could reach temperatures to 1800°C for a short duration. These concepts involve exotic coolants such as lead-bismuth, lead, molten salt, or supercritical water. They must also perform satisfactorily while being subject to neutron damage levels greater than those experienced in any material developed for nuclear systems use to date. These expectations are unprecedented in nuclear energy or any other application and will require the development of a significant fundamental level of knowledge to successfully guide system development. In addition, information on materials performance in harsh nuclear environments is required to enable predictive modeling of material behavior in nuclear waste packages and other nuclear energy systems, such as accelerator-driven nuclear fission and transmutation. Opportunities for radical advances in fundamental understanding of the multiscale mechanisms and processes governing materials degradation are becoming possible through new and emerging advanced scientific facilities and high-performance parallel computing platforms. Integration of novel in situ experiments with theoretical/computational efforts provide the possibility to develop fundamental understanding of degradation mechanisms and kinetics over multiple scales, from atomistic to micron and nanosecond to minutes.

There is insufficient fundamental understanding of radiation effects on materials in nuclear reactor components to reliably predict component properties and thus mitigate service failures. The degradation of core components, including component welds and joints, and cladding in current and future nuclear reactor designs can lead to failures at high levels of neutron irradiation in the reactor coolant environment. The coolant chemistries (e.g., water, supercritical water, liquid metals) can become more aggressive in crevice situations, where component failures are often observed. Since cracking susceptibility requires a combination of radiation, stress and a corrosive environment, the failure mechanism has been termed irradiation-assisted stress-corrosion cracking (IASCC) for water coolants, but similar processes may occur in other coolant environments. Because testing of irradiated materials is difficult and expensive, it is highly unlikely that a purely empirical approach will provide an adequate understanding of corrosion processes. Much of this issue is tied to the co-evolution of equilibrium and non-equilibrium nanostructures and nanochemistries.

Research related to improved storage of spent nuclear fuels is another area of opportunity because there have been very few scientific studies on the behavior of nuclear waste packages. Qualification of new materials for nuclear waste packages needs to be scientifically based. This is critical in the absence of sufficient testing capabilities. Opportunities exist for major advances in this area through new and emerging in-situ experimental and diagnostic capabilities and parallel computational platforms. The properties of the spent nuclear fuel, other solid nuclear waste forms, the storage canister, and the drip shield may degrade in the presence of water, oxidizing environment, and radiation-induced chemistry changes (e.g., radiolysis, radioactive decay products). The fuel or waste forms are also subject to self-radiation-induced degradation from the decay of the radionuclides. This corrosion and radiation damage must be understood well enough that extrapolations of waste package behavior can be made confidently over periods of at least ten thousand years.

Summary of Research Direction

Advancing the fundamental mechanistic understanding of radiation-induced materials degradation to enable the predictive modeling of materials performance in the hostile environments (extremes of radiation field, temperature, stress, thermal/mechanical cycling, corrosive coolants, and oxidizing environments) associated with nuclear waste packages, nuclear reactors, and other nuclear energy systems.

New Scientific Opportunities

The DOE's Office of Nuclear Energy, Science, and Technology (NE), in conjunction with the ten countries that compose the Generation-IV International Forum (GIF), has been investigating nuclear reactor concepts that will be safer, more environmentally benign, longer operating, better performing and economically superior to current designs. The evaluation has included radioactive waste containment systems with the goal of generally optimizing the entire nuclear fuel cycle. This group has recently selected six nuclear reactor concepts for further R&D. The concepts are the Supercritical Water-Cooled Reactor (SCWR), the Very High Temperature (gas-cooled) Reactor (VHTR), the Gas-cooled Fast Reactor (GFR), the Lead-cooled Fast Reactor (LFR), the Sodium-cooled Fast Reactor (SFR), and the Molten Salt Reactor (MSR). The GIF expects the development of these concepts to occur over a 20-30 year time frame. A key to the success of all six concepts is improved structural materials to optimize economic performance and minimize the environmental impact of discharged waste.

There have been continued, but limited, studies of degradation of metal alloys for nuclear reactor components. The major scientific challenge in this area is the co-evolution of all microstructure components and their role in macroscopic material response such as swelling, anisotropic growth, irradiation creep, and radiation-induced phase transformations. Under irradiation the evolution of the microstructure is determined by the dynamic and kinetic response of a complex materials system when driven far from thermodynamic equilibrium. The detailed kinetic processes are both deterministic and stochastic, are coupled, and may evolve into new kinetic processes as the microstructure and phase transformation of the system evolves. The framework for this new era of radiation effects research should be the science of complex systems. While this emerging field is still in its definition phase, the needed understanding for radiation effects in solids provides a well-defined problem. It may, in fact, serve as a prime example or model of a complex system evolving in response to the continuous flow of energy that maintains the system in various states of non-equilibrium.

There is insufficient fundamental understanding of radiation effects on the chemical behavior of nuclear reactor components to reliably predict component properties and thus mitigate service failures. The degradation of core components, including component welds and joints, and cladding in current and future nuclear reactor designs can lead to failures at high levels of neutron irradiation in the reactor coolant environment. The coolant chemistries can become more aggressive in crevice situations, where component failures are often observed. Since cracking susceptibility requires a combination of radiation, stress and a corrosive environment, the failure mechanism has been termed IASCC. Because testing of irradiated materials is difficult and expensive, it is highly unlikely that a purely empirical approach will provide an adequate understanding of IASCC behavior. Much of this issue is tied to the co-evolution of equilibrium and non-equilibrium nanostructures and nanochemistries. Fundamental understanding of IASCC requires mechanistic research and novel approaches to examine reaction thermodynamics and kinetics at surfaces and crack tips. New results show crack-tip openings on the order of nanometers and corrosion/oxidation fronts progressing with solution access through nanometer-size pores. Solution migration, electrochemistry and reaction phase stabilities need to be understood in the constrained dimensions and related to mechanisms controlling the propagation of environmental degradation. Mechanistic understanding of grain-boundary characteristics that control susceptibility of alloys to IASCC remain elusive. Degradation of welds and joints in nuclear components can lead to catastrophic failures, yet there is a critical lack of mechanistic understanding regarding weld microstructures and microchemistries. While there has been some progress in understanding these phenomena for water coolants, the behavior in supercritical water or other coolants is largely unknown. Much less is known regarding environmental degradation in high-temperature reactor systems, where refractory materials, including composites and ceramics, may be employed with gas coolants.

Ceramics are often more robust in durability and corrosion resistance, which is why they have often been proposed for the immobilization of actinides and other partition radionuclides. While ceramic nuclear fuels are currently used in nuclear reactors, future reactors could employ more ceramic composite components, such as in cladding and coatings for nuclear fuel. Advanced computational methods are required to understand, simulate and model the fundamental mechanisms that control the dynamics of radiation effects, diffusion and microstructure evolution in oxide ceramics, as well as at ceramic-ceramic interfaces, in radiation environments over broad ranges of temperatures. In oxide materials, both electronic excitation and elastic collision processes must be rigorously considered, unlike metals and semiconductors where electronic excitations play a lesser role. The critical problem is that the methodologies to perform accurate and reliable computations of radiation-damage processes in oxide ceramics over atomic to macroscopic scales are not currently available within the U.S. or elsewhere. The goal should be to establish a suite of computational methods that can perform modeling of oxide ceramics from the atomic to macroscopic scales on a level equivalent to or exceeding that performed today on metals and semiconductors. This goal is complicated by the mixed bonding character (ionic and covalent) and long-lived electronic excitations that are present in oxide ceramics. Achieving this goal requires development of novel simulation methods, potentials for complex systems, methods to handle complex potentials in parallel computing environments, and integration of electronic coordinates into potential models to implement charge-transfer and electronic excitations within large-scale ionic molecular dynamics (MD) simulations.

The nuclear waste packages for permanent disposition in the oxidizing environment of Yucca Mountain repository in Nevada are currently envisioned as consisting of spent nuclear fuel assemblies (or other solid nuclear waste forms proposed for future fuel cycles) that are contained in metal canisters that may be capped with a drip shield when finally emplaced in the repository. The properties of the spent nuclear fuel, other solid nuclear waste forms, the canister, and the drip shield may degrade in the presence of water, oxidizing environment, and radiation-induced chemistry changes (e.g., radiolysis, radioactive decay products). The spent nuclear fuel or solid nuclear waste forms are also subject to self-radiation-induced degradation from alpha and beta decay of the radionuclides. The environmental degradation due to corrosion and radiation damage must be understood well enough that extrapolations of waste package behavior can be made confidently over periods of at least 10,000 years. Public acceptance of nuclear power as an important energy source depends on developing acceptable solutions to the back end of the nuclear fuel cycle. Scientifically based and carefully engineered solutions are more likely to gain public acceptance.

Many previous models of nuclear fuels and component behavior in current reactors have been semi-empirical in nature and based on large and often incomplete databases. Predicting the performance of new materials for advanced reactor environments and nuclear waste packages in repositories is beyond the capability of current models and databases. Opportunities exist for coupling experimental efforts and multiscale computational approaches to develop new materials and predictive performance models. Realizing this vision requires a large number of fundamental studies, including investigations of

- the thermal and radiation stability of nanometer oxide dispersion strengthened alloys;
- the dislocation interactions and strengthening mechanisms of radiation generated obstacles (voids, stacking fault tetrahedra, dislocation loops, etc.) and oxide precipitates that control plasticity;
- the controlling mechanisms of thermal and irradiation creep, creep cavitation and failure;
- the limited uniform ductility and flow localization at intermediate to low temperatures;
- the ability of nuclear waste packages to achieve long term (centuries) stability; and
- other dimensional effects such as swelling, phase transformations, and amorphization.

Other needs include:

- development of multiscale computational approaches;
- development of new radiation-tolerant materials (e.g., functionally graded, multilayer structures, composites, tailored nanostructures);
- development of a fundamental understanding of intergranular cracking in irradiated components; and
- multiscale modeling of the complex microstructural development of alloys and the relationship of these highly non-equilibrium changes to mechanical, dimensional stability, and corrosion properties.

Relevance and Potential Impact

Although radiation-induced materials degradation is not a new topic, opportunities for revolutionary advances in fundamental understanding of the mechanisms governing materials degradation over multiple length and temporal scales are becoming possible through new and emerging advanced scientific facilities and high-performance parallel-computing platforms. Novel in-situ experiments in realistic environments can be closely integrated with theoretical/computational efforts to develop a fundamental understanding of degradation mechanisms and kinetics over multiple scales from atomistic to micron and nanosecond to minutes. Such advances in this area will provide the underpinning science that will enable licensing nuclear waste packages for emplacement in the Yucca Mountain repository and the development and qualification of new materials for use within Generation-IV nuclear reactors and other nuclear energy systems, such as accelerator-driven nuclear fission and transmutation. In addition, the tools and methods developed in this effort will have a significant impact in the broader field of materials science.

Estimated Time Scale

Anticipated research program duration is 10-20 years.

ADVANCED ACTINIDE AND FISSION PRODUCT SEPARATIONS AND EXTRACTION

EXECUTIVE SUMMARY

Splitting atoms supplies energy to the nation from a uranium isotope that is less than 1% abundant in natural uranium. Ensuring an adequate long-term supply of fissile material is essential to maintaining or increasing electric energy generation using nuclear power reactors. At present world consumption rates, known uranium resources should last for about 65 years without recycling of spent reactor fuel. It is estimated that as yet undiscovered, but recoverable, uranium resources are at least four times larger than known uranium resources. Vastly larger amounts of uranium are present in seawater, although is not currently economically practical to recover such uranium. Energy production using nuclear fission has used two concepts for the final end point: (1) the “once-through” fuel cycle, in which spent nuclear fuel is planned to go directly to a repository, and (2) the “closed fuel cycle,” in which the spent nuclear fuel is reprocessed, with the separated uranium and plutonium going back for use in further fuel and the fission products planned to go to a repository.

Generation-IV reactor concepts are being designed to include reprocessing in order to extract a greater fraction of the energy content of natural uranium and thorium than is achieved currently. Thorium is more abundant in nature than is uranium and, like natural uranium, upon neutron bombardment is converted into fissile material that fissions to a degree as it builds up. By absorbing neutrons, the resulting fission products reduce the efficiency with which new fissile material is created. For this reason, actinide and fission product separation processing with recycling of the fissile isotopes to reactor fuel is being examined for full utilization of the energy content of present actinide resources as well as to minimize the volume of produced waste products. The present roadmap for advanced nuclear fuel cycles suggests that molten salt media may play an important role in the future. Improving separations efficiency is a viability issue for such media and should be addressed in basic research on the fundamental chemistry of thorium, uranium, selected transuranic elements, and salt-forming fission products in molten salt media. Studies under unusual or extreme oxidation and reduction conditions are needed also because little information is presently available under these conditions that may be encountered during a process upset or an accident scenario.

Achieving “green chemistry” is a goal worth establishing in separation processing of actinides and fission products. The term “green chemistry” is defined by the U.S. Environmental Protection Agency, in part, as the promotion of innovative chemical technologies that minimize the use of hazardous substances in the manufacture of chemical products. One step toward that goal is the replacement of presently used organic solvents with less hazardous liquids such as room-temperature ionic liquids (RTIL’s). The timeframe for maximum impact of fundamental studies on RTIL’s and molten salt media to be used is 10-20 years, when the results of such investigations must be factored into plant design decisions.

Innovative methods for recovery of uranium from seawater should be investigated if significant improvement over existing recovery techniques seems achievable. Deliberately designed ligands, perhaps analogues of the very specific ion channels of biological membranes or carbon nanotubes of appropriate radius whose specificity has been enhanced by modification of their interior surface or appropriate decoration of their entrances and exits with specific ion attracting functionalities, provide promising avenues to achieve the required breakthroughs. Economic recovery of uranium from seawater is likely to be an issue in about 50 years.

Proposed Research Direction

Create the fundamental research basis for advanced actinide and fission product separation and novel extraction processes that are essential to ensure sufficient fissile material stocks, reduce costs, achieve proliferation resistance, and minimize environmental impacts and waste repository requirements in the nuclear fuel cycle.

New Scientific Opportunities

Ensuring an adequate long-term supply of fissile material for the nuclear fuel cycle is essential to maintaining or increasing the energy supplied to the nation by nuclear fission. About 0.7% of natural uranium is the fissile isotope U-235. Uranium is about as abundant on earth as are zinc or tin and is found at trace levels in most rocks and soils. Uranium is present in seawater to about 3 parts per billion. At present world consumption rates, the International Symposium on the Uranium Production Cycle and the Environment, held October 2-6, 2000 at the International Atomic Energy Agency (IAEA) in Vienna, concluded that the known uranium resources of 4 million tons (Mt) should last for about 65 years without recycling of spent nuclear reactor fuel. In addition, there are estimates of as yet undiscovered uranium resources of about 16 Mt in ore bodies, although recovery of that uranium is likely to be difficult. By some estimates, recovery of uranium from seawater using present technology would become economical if the price of uranium rose ten-fold.

Generation-IV reactor concepts provide opportunities both for reducing the radiotoxicity of non-fissile isotopes in presently stored spent reactor fuel and for creating new fissile isotopes. Recycling fissile isotopes provides a means of extracting a greater fraction of the energy content of natural uranium and thorium than is achieved in the current “once through” nuclear fuel cycle. Natural thorium is considered to be a “fertile feedstock,” meaning that its neutron irradiation results in the formation of fissile isotope U-233. Thorium is even more abundant in nature than is uranium, and generally thorium is less soluble in ground water or seawater due to its preference for the tetravalent state. If fissile isotopes are produced by neutron bombardment of natural or depleted uranium or natural thorium targets in nuclear reactors or in accelerator-based subcritical assemblies, utilization of nearly the full energy content of present uranium or thorium resources can be achieved. Irradiating such targets creates fissile isotopes that, as they build up, also fission to a degree. Such fission releases useful energy but also creates fission products, some of which strongly absorb neutrons. To achieve optimum neutron economy, actinide and fission product separation processing with recycling of the actinides to targets or reactor fuel is essential to maximize utilization of the energy content of present fissile and fertile actinide resources.

Some existing actinide processing is carried out in molten salt media, such the LiCl-KCl eutectic. The present roadmap of advanced fuel-cycle concepts suggests that molten salt media may play a significantly more important role in future actinide and fission product separation techniques due to the radiation resistance of such media. The fundamental chemistry of thorium, uranium, selected transuranic elements, and salt-forming fission products should be investigated in molten salt media because improving separations efficiency is a viability issue for such media. Investigations under unusual or extreme chemical oxidation and reduction conditions are necessary because little information is presently available on molten salt separations processes under these conditions. Examples of such conditions include molten salt that contains high concentrations of elemental lithium or a transuranic element in metallic form, molten salt that is being sparged with chlorine gas, and molten salt exposed to nitrogen, oxygen, water vapor, or carbon dioxide (i.e., the potentially reactive constituents of atmospheric air), as might occur in an accident scenario. The timeframe for maximum impact of fundamental studies on molten salt separations processing is 10-20 years when the results of such investigations must be factored into plant design decisions.

Green chemistry is defined by the U.S. Environmental Protection Agency (EPA) as the promotion of innovative chemical technologies that reduce or eliminate the use or generation of hazardous substances in the design, manufacture, and use of chemical products. One highly promising approach to achieving “green chemistry” in separation processing of actinides and fission products is the replacement of organic solvents with less hazardous liquids. Certain mixtures of organic cations, such as methyl imidazolium derivatives, and charge-balancing inorganic anions of low complexing ability, such as triflates or hexafluorophosphate, form liquid phases at ambient temperature that are termed room temperature ionic liquids (RTIL’s) (e.g., see Figure 2-1). Only a minuscule fraction of compounds with potential to form such liquid phases have been investigated for their ability to form RTIL’s with useful properties.

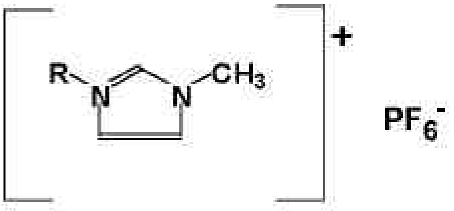

Figure 2-1. Generic structure of the room temperature ionic liquid alkylmethylimidazolium hexafluorophosphate, where **R** is an alkyl group.

Because the constituents of these RTIL’s are ions, no volatile organic carbon (VOC) is released during their use. The plutonium uranium extraction (PUREX) process used in most present aqueous-based separations processing of spent nuclear fuel relies on solvent extraction processing. In PUREX, some metal ions are extracted from an aqueous solution of nitric acid into an organic phase that is a mixture of alkane hydrocarbons (kerosene) and tributyl phosphate. The PUREX process emits both VOC’s and nitrogen oxides. A simplified version of PUREX, termed the UREX process, is the reference head end aqueous separations process for some Generation-IV nuclear reactor cycles. UREX also will emit VOC’s and nitrogen oxides. Although direct substitution of an RTIL for kerosene in PUREX or UREX processing is unlikely to be productive, novel extractant molecules, especially designed for use in an RTIL, hold significant promise for achieving superior performance. Some known RTIL’s have liquid ranges that exceed 300°C. Some are miscible with water or supercritical fluid (SCF) carbon dioxide; others are water- or SCF carbon dioxide-immiscible. A few RTIL’s have exceptionally large electrochemical potential windows, with one having been shown recently to allow electrodeposition of uranium metal. For this reason, selected RTIL’s should be investigated as potential replacements for high-temperature molten salts that are the basis for present pyrochemical and electrometallurgical processing of actinides. The radiolytic stability of RTIL’s is an area that clearly merits early investigation. The timeframe for maximum impact of fundamental studies on RTIL’s is 10-20 years, when the results of such investigations must be factored into plant design decisions.

Given the amount of uranium in seawater, the development of innovative methods for its isolation presents a major challenge. Deliberate design of ligands, using approaches that combine molecular mechanics modeling with experimental verification, is a promising avenue for identifying extraction agents capable of achieving the required breakthroughs. For this purpose, one can envision such molecules attached to solid supports to facilitate extraction and ease of separation from solution by filtration to provide the desired elements, such as uranium, in essentially pure form, when starting from highly dilute solutions. Utilization of synthetic analogues of the very specific ion channels of biological membranes (sodium versus potassium, for example), in which the analogues are embedded in artificial membranes, is a further promising area of investigation. The resulting channels might be stacked complexes of host molecules or be carbon nanotubes so constructed as to have a radius appropriate to the specific translocation across the membrane of particular hydrated ions. Such specificity might be enhanced by modification of the interior lining of the carbon nanotubes or by appropriate decoration of their entrances and exits to facilitate specific translocations.

In a device using biological membranes, a very dilute solution containing a mixture of metal ions, such as seawater, would pass through a network of these membranes with one type of pore in each region of the apparatus; that region would then specifically collect a particular ionic species. Such an apparatus could be used to selectively collect uranium, for example. The economic viability of this approach could be enhanced by concurrent ability to isolate other valuable elements and produce desalinated water. At the other end of the nuclear fuel cycle, such a device could be employed to separate most components of dissolved spent reactor fuel (e.g., a mixture of actinides and fission products) thereby recycling unspent fuel and concentrating the most noxious by-products. These proposals have significant precedence in the natural world (ion channels in neurons or the loops of Henle of the human kidney, for example). Economic recovery of uranium from seawater is likely to be an issue in about 50 years.

Relevance and Potential Impact

The separations and extraction concepts outlined above provide challenging areas for creative fundamental research to generate the scientific knowledge base for creating applications that have immense significance to the production of energy by nuclear fission and the efficient, environmentally-friendly, handling and minimization of resultant waste products. Improving the closed fuel cycle requires efficient and effective recycle of actinides, such as uranium, and significant reduction of waste destined for geologic repositories. Novel separations and extraction methods are essential to meet the possible future needs of the closed nuclear fuel cycle, but they must overcome the current formidable obstacle of not being economical. The complex nature of mixtures of actinides and fission products and resulting radiolysis render profoundly challenging the development of such separation and extraction methods for the nuclear fuel cycle.

Estimated Time Scale

Two timescales are relevant to this research effort: 10-20 years for separation-related studies (to impact plant design decisions) and 50 years for extraction processes that achieve economic recovery of uranium from seawater.

FUELS RESEARCH

EXECUTIVE SUMMARY

In order to play their essential role in meeting future energy needs, advanced nuclear energy systems will need to provide: (1) manageable levels of nuclear waste, effective fuel utilization, and increased environmental benefits, (2) competitive economics, (3) recognized safety performance, and (4) proliferation-resistant nuclear energy systems and nuclear materials. The DOE's NE represents the U.S. and has a lead role in the Generation-IV International Forum (GIF), a group of ten countries working together to develop nuclear energy systems that make improvements in each of these four areas. The Generation-IV program is designed to develop reactors that meet these criteria and could be deployed by 2030. The GIF has recently selected six concepts for further R&D. The concepts are the Supercritical Water-Cooled Reactor (SCWR), the Very High Temperature (gas-cooled) Reactor (VHTR), the Gas-cooled Fast Reactor (GFR), the Lead-cooled Fast Reactor (LFR), the Sodium-cooled Fast Reactor (SFR), and the Molten Salt Reactor (MSR).

The GIF has completed an R&D Roadmap that describes the key viability and performance issues for the development of the six reactor concepts. Advances in fuel performance, including fuels that recycle actinides, have been identified as critical to the success of each. These fuels must achieve long lifetime while operating at high temperature. Additionally, as part of another NE program, the Advanced Fuel Cycle Initiative (AFCI), the DOE is investigating accelerator-based options for transmuting long-lived nuclear waste. These accelerator-based systems will investigate "inert matrix" fuels that do not use uranium and therefore maximize the overall burn rate of long-lived actinides. Because the success of novel fuel types is key to the success of these systems, developing a mechanistic understanding of their properties is critical.

The advanced nuclear energy system initiatives require the development of non-traditional fuel types (including nitride, metallic, dispersion, and inert matrix), the incorporation of large quantities of plutonium and higher actinides, and the inclusion of embedded isotopically-tailored neutron absorbers (burnable poisons). Additionally, each of these fuel cycle advances must be accomplished in a way that maintains an inherent proliferation resistance within the complete nuclear fuel cycle. These requirements motivate the need for fundamental understanding of the chemistry of elements in nuclear fuels; the thermodynamic stability in oxidizing and reducing environments; the physical properties (e.g., density, microstructure and thermal conductivity); the processing techniques for the fabrication of fuels containing actinides, plutonium and burnable poisons; and the response to radiation.

Proposed Research Direction

Provide a fundamental understanding of the chemistry, physical properties, and processing in proposed novel fuel forms and compositions, including nitride, metallic, dispersion, and inert matrix (non-fertile) fuels.

New Scientific Opportunities

The majority of fuels used in current nuclear energy systems were developed during the 1950s through the 1970s. Since then many significant advances in the tools for analyzing material properties have been developed. In studying the fuels for these advanced systems, critical Basic Energy Science analytical tools such as synchrotron light sources, advanced electron microscopes, advanced neutron scattering centers, and facilities for conducting advanced computation need to be applied to ensure the best scientific tools are used to identify fundamental mechanisms of degradation.

In general, a long-term program to develop fuels for deployment entails at least the following four activities:

- fabrication process development,
- property measurement and assessment,
- irradiation testing and safety demonstration, and
- modeling and predictive code development.

Each of these activities must be conducted while remembering the requirement that any new fuels developed must be compatible with the associated recycle process. Current reactor fuels are primarily oxides, while for the Generation-IV systems, novel fuel types such as nitride, metal and dispersion fuels have been proposed. For accelerator-based transmutation systems and some reactor systems, inert matrix (non-fertile) fuels have been proposed. For all of these fuels, much fundamental understanding is lacking. A key fundamental scientific objective is to establish the basis for understanding and predicting fuel behavior (i.e., changes in density, melting point, thermal conductivity, tensile strength, corrosion resistance) under the temperatures, stresses, and radiation fields in the reactor.

Potential research topics include:

- behavior of novel fuel forms exposed to harsh environments (high temperature, high levels of radiation, and stress). These fuels include nitride fuels, metallic fuels, dispersion fuel, and non-fertile (inert matrix) fuels;

- for fuels made from reprocessed materials, the influence of recycled products on fuel behavior, including radiation response; and

- multiscale modeling of fuel thermomechanical behavior.

Generation-IV goals and the transmutation objectives for the AFCI program will present challenging performance requirements for new fuel types. Therefore, improving and optimizing performance potential will require a sound understanding of the mechanisms that impact fuel behavior and, ultimately, fuel lifetime. Such understanding is typically attained through development of mechanistic models for key phenomena and demonstrated through incorporation of those models into validated fuel performance codes. However, establishing mechanistic models requires knowledge of fundamental thermophysical, physical, and mechanical properties. These properties will influence important phenomena such as fission gas retention and release, fuel swelling, irradiation growth, fuel cladding chemical and mechanical interactions, and transient response. In the past, many fuel development programs were limited to empirical approaches that did not have the benefit of knowledge of those properties (although such information was often obtained with continued research on the well-established fuel designs). However, the challenges for the current programs require a coordinated effort to determine key properties for the fuel types (i.e., forms and compositions) as an important contribution to the fuel development process.

Inert matrix fuels do not contain fertile materials (materials that breed additional fissile constituents), such as uranium-238 or thorium-232, which allow a maximum burn rate of higher actinides. Inert matrix fuels are typically proposed as multiphase materials consisting of yttria-stabilized zirconia (YSZ) or magnesium spinel ($MgAl_2O_4$), which are chemically and thermodynamically stable and insoluble in nitric acids. Inert matrix fuels may require the inclusion of burnable poisons to improve the reactivity coefficient profile during its lifetime. Fundamental understanding of the thermodynamic stability, fuel performance (response to irradiation), and fission gas release are needed.

Modeling of fuel performance is critical to predicting operational lifetimes. On a fundamental level, this includes obtaining critical material parameters from first principles calculations. These parameters can then be used in higher-level models such as molecular dynamics, Monte Carlo, and rate theory to describe events that have both short and long time scales and small and large distance scales. The development of these multi-scale computational methods will be critical to obtaining the predictive capability that is needed to extrapolate beyond the available experimental data.

The overall impact of advanced, alternate fuels on a repository program is not clear, and the economics of transmutation and recycling are current obstacles to their use. However, actinide recycle incorporating a fast-spectrum reactor has been identified as a means to manage the disposition of transuranic isotopes, which have long half-lives and dominate the calculated long-term dose associated with releases from repositories such as Yucca Mountain in the U.S. The fast-spectrum Generation-IV concepts are to be designed to accommodate minor actinides in fuel or in special targets. An understanding of minor actinide-bearing fuel materials is not well established. Therefore, key properties, such as thermal conductivity, enthalpy, and melting temperatures must be determined and understood. Other intrinsic characteristics, such as interdiffusion of fuel constituents under temperature gradients and interdiffusion with cladding constituents, must also be understood. The addition of the minor actinides adds a new level of complexity to fuel performance beyond that of “fresh” fuels.

Relevance and Potential Impact

The program of research outlined would produce a broad spectrum of results directly relevant to the DOE NE Generation-IV and AFCI programs. Development of computational tools and methods would be of benefit to the larger materials science community.

Estimated Time Scale

This program is expected to require 10-20 years of research.

FUNDAMENTAL RESEARCH IN HEAT TRANSFER AND FLUID FLOW

EXECUTIVE SUMMARY

The transfer of heat and the flow of fluids are fundamental to understanding and predicting the design of all types of advanced devices ranging from heavy-vehicle engines to computer chips and nuclear reactors. All forms of energy conversion systems, both present and future, require higher temperatures to achieve greater efficiencies. A better fundamental understanding of the processes involved is a critical requirement for the achievement of higher performance and assured licensing. A complete comprehension of the mechanistic phenomena related to multiphase fluid flow and heat transfer is lacking and to date relies on empirically derived correlations to predict the nature of these phenomena. New heat-transfer materials involving nanostructures provide exciting opportunities to extend the properties and applications of these materials. While efforts are on-going in these areas, considerable impact can be obtained over the next 15 years as measurement techniques and computational capabilities both rapidly expand.

Summary of Research Direction

Continued progress on a fundamental understanding of the physics of heat-transfer and fluid-flow issues is of great importance to many different future energy conversion and delivery technologies including transportation, electricity production, and many others. This crosscutting fundamental research direction is of critical importance because a better understanding of the basic features on a molecular level may allow future systems designers to greatly extend new materials and processes to optimize their performance. It is of particular importance to nuclear energy technologies, especially with the development of Generation-IV concepts during the next two decades, that a fundamental understanding of heat transfer under varying conditions be developed in order to reduce the uncertainties associated with the performance and safety of these advanced reactor concepts. Both design performance and licensing issues are driven and determined by the accuracy and uncertainties associated with the analysis of heat transfer and fluid flows in nuclear systems.

Generation-IV reactor concepts include numerous heat-transfer and fluid-flow challenges due to the selection of coolant materials for these systems. Coolants chosen for Generation-IV technologies include liquid metals (lead, sodium, and lead-bismuth eutectics), gases (helium and carbon dioxide) and supercritical water. An advanced understanding of heat transfer and fluid flow that includes a fundamental understanding, even to the point of eliminating the use of correlations for heat transfer and fluid flow analysis, would be very beneficial.

Traditionally, fluid flow and heat transfer in engineering systems are modeled using empirically derived correlations that are often only reliably applied for prescribed conditions and materials. This expedient method allows accurate and currently acceptable results, but as the next generation reactor designs move forward these analyses would be significantly improved by a better fundamental understanding of the basic physics and science at a molecular and atomistic level. Recent and expected future accelerations in computing capabilities can be utilized to probe the fundamental mechanisms related to molecular interactions between fluids and solid materials. Better instrumentation and measurement techniques can be designed to collect more detailed information with respect to heat-transfer and fluid-flow properties to provide better data for these expanded computer codes.

New Scientific Opportunities

To eliminate use of engineering correlations, it is necessary to develop a first principles understanding of multiphase heat-transfer and fluid-flow mechanisms, including the behavior of fluids such as supercritical water, lead and lead-alloys, and molten salts. In addition, there is the need to develop an understanding of fluids with dispersed particles (i.e., nanofluid suspensions).

There are a number of recent advances in multiphase fluid flow and heat transfer. Two-phase fluids using various combinations, including liquid/vapor, liquid/solid, and vapor/solid, offer enhanced heat transfer and fluid flow properties that can be utilized in energy conversion systems designs. Boiling and condensation heat transfer have been utilized for many years without a complete fundamental understanding at the microscopic and molecular scales to enhance heat transfer and system capabilities. Recent developments in microscale probes and non-destructive measurement techniques coupled with advanced computing technology give rise to considerable optimism that better fundamental understanding can be developed in the near future in two-phase flows and boiling and condensation heat transfer.

The recent development of nanofluid suspensions appears to yield novel heat-transfer and fluid-flow properties that provide another exciting possibility for enhanced system performance through the use of new materials and properties. This new class of heat transfer fluids is manufactured by dispersing nanometer-size solid particles in traditional heat transfer fluids to increase thermal conductivity and heat transfer performance. Experiments conducted to date have found that the improvement in heat-transfer properties of several nanofluids is significantly better than that predicted by existing theory. This represents a fundamental discovery in basic heat transfer and considerably more work is required to fully understand the principals of operation and the fundamental physics that give these materials enhanced capabilities. Original efforts by Argonne National Laboratory are being extended through work with Valvoline, Inc.; Nanopowder Enterprises of Piscataway, N.J.; and through collaborations with Purdue University and Rensselaer Polytechnic Institute to investigate the heat-transfer mechanisms in nanofluids. Applications in heavy transportation vehicles, supercomputer circuits, high-power microwave tubes, and advanced nuclear reactors are possible.

Relevance and Potential Impact

A truly fundamental understanding of heat transfer and fluid flow is advantageous to all forms of energy conversion systems, both present and future. Research leading to a comprehensive understanding of multiphase flow and heat transfer at the mechanistic level would yield significant design benefits for all types of advanced devices ranging from heavy-vehicle engines to computer chips and nuclear reactors.

Estimated Time Scale

The necessary research effort is estimated to require15-20 years.

Renewable and Solar Energy

To Displace Imported Petroleum by Increasing the Cost-Competitive Production of Fuels and Chemicals from Renewable Biomass by a Hundred Fold

Develop Methods for Solar Energy Conversion that Result in a Ten-to-Fifty Fold Decrease in the Cost-to-Efficiency Ratio for the Production of Fuels and Electricity

Develop the Knowledge Base to Enable Widespread Creation of Geothermal Reservoirs

Conversion of Solar, Wind, or Geothermal Energy into Stored Chemical Fuels

Advanced Materials for Renewable Energy Applications

TO DISPLACE IMPORTED PETROLEUM BY INCREASING THE COST-COMPETITIVE PRODUCTION OF FUELS AND CHEMICALS FROM RENEWABLE BIOMASS BY A HUNDRED FOLD*

EXECUTIVE SUMMARY

Emerging knowledge in functional genomics and molecular technologies provides new opportunities for the genetic tailoring of plants and microorganisms to produce novel materials, fuels, and chemicals. During the past century, plants have been extensively modified to vastly improve the production of food, feed, and fiber. An understanding of fundamental mechanisms that govern the physical limitations of plant efficiency will allow the design and control of many useful plant properties. These include the control and characterization of plant architecture and composition (lignin, cellulose, hemicellulose, starch, and oils), improvements in the energy efficiency of plant production (reduced nutrients, water, and land requirements), and an expansion in the range of environments that can be used for cultivation (salt tolerance and stress resistance). Further advances in the fractionation of biomass into individual components using physical and chemical treatments offer a major opportunity for cost savings. Metabolic engineering of new microbial biocatalysts offers the potential to produce novel biomaterials and chemicals that will serve as renewable alternatives to current petrochemicals. These improved microbial biocatalysts are required to expand the range of useful conditions for industrial fermentations and reduce costs through process simplification. Substantial cost savings can also be realized by the development of biocatalysts that produce enzymes (i.e., cellulase, xylanase, etc.) for carbohydrate depolymerization as coproducts during fermentation, eliminating the need for separate enzyme production facilities. Application of biochemical and genetic principles provide mechanisms for the rational design of improved enzymes concerned with the depolymerization of plant constituents. Recent expansion in genomic sequences from microbes and plants provides a vast toolkit of genes and enzymes that can now be recombined and used to provide clean and sustainable solutions to our current dependence on imported petroleum.

Summary of Research Direction

The modern industrial revolution has been powered by the use of solar energy from ancient plants and microalgae that formed vast deposits of petroleum, coal, and natural gas. The ancient photosynthetic processes that produced these reservoirs of fossil energy also shaped our climate and the composition of our atmosphere. Storage of carbon in relatively inert fossil forms reduced atmospheric carbon dioxide and other compounds associated with planetary heating and produced our oxygen-rich atmosphere. The vast scale of biological conversion processes offers the opportunity to replace part of our dependence on fossil residues for energy with contemporary sources of renewable biomass. Biological transformations of renewable biomass materials also offer the opportunity to displace current petroleum-based chemicals and plastics using environmentally friendly processes. Co-production of these higher value chemicals from renewable biomass is essential to reduce the cost of liquid fuels such as ethanol or biodiesel from biomass.

Approximately 0.2% of the current U.S. energy needs are supplied by renewable biomass, principally through direct combustion (heating or electricity) or ethanol as a fuel extender and oxygenate (providing 2

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*This document served as the basis for a subsequent Proposed Research Direction from the Energy Biosciences Team entitled “Energy Biotechnology: Metabolic Engineering of Plants and Microbes for Renewable Production of Fuels and Chemicals.”

billion gal/yr or 1.3% of total automotive fuel). Both the areas of liquid fuels (i.e., ethanol and biodiesel) and combustion offer tremendous opportunities for expansion through the development of improved methods for the solubilization of plant constituents and the application of our emerging knowledge of plant and microbial genomics.

Near term expansion of research should focus on the development of improved bioconversion processes to produce chemicals (e.g., ethanol, longer chain alcohols, fatty esters, etc.) that can be blended with currently used automotive fuels (i.e., gasoline and diesel) and on the development of microbial processes for higher value coproducts (i.e., commodity chemicals and bio-based plastics) that displace imported petroleum and increase revenues. Underutilized residues from current agriculture and forestry with little or no current value should be used as feedstocks for this near-term expansion. Approximately 30 million tons (Mt) of corn is currently converted to fuel ethanol in the U.S. by a mature industry using very efficient processes that take advantage of the highly digestible nature of starch by microbial enzymes. While this can continue to expand and make an important contribution to the energy security of our nation, the energy-intensive nature of corn farming and competing uses of corn as food and feed will prevent the substantial replacement of automotive fuel by ethanol from corn alone. In contrast, the use of undervalued lignocellulosic residues as feedstocks should have minimal impact on consumer costs for the primary products from agriculture (food, feed and fiber). This new use represents an expanded benefit with minimal investment of additional energy. Additional fuels from lignocellulosics can be blended with gasoline to reduce petroleum imports while maintaining the benefits of corn-based ethanol production.

The high capital cost and increased risk associated with process complexity have thus far blocked the industrial implementation of many promising new technologies. Much of this process complexity can be reduced through the genetic engineering of improved microbial biocatalysts, the genetic tailoring of the plants for specific applications, and by improvements in plant fractionation technologies that increase efficiency and reduce costs. Even with process simplifications, the barrier of risk associated with the first implementation of a novel technology should not be underestimated.

New Scientific Opportunities

Many aspects of process complexity can be improved by the application of knowledge from microbial and plant genomics. Genomic sequences provide a catalogue of genes that can be used to alter cellular structure, composition, and function. These sequences provide a starting point for our understanding of integrated processes that limit the efficiency of water and nutrient use, the partitioning of photosynthate among cellular constituents, tolerances to extreme environments, and bioconversion processes by microorganism. A logical next step is to expand these genetic catalogues by adding fundamental knowledge concerning the integration of gene functions and physiological activities.

Cellulose depolymerization by enzymes is arguably the single most expensive step associated with the bioconversion of lignocellulose to fuels and chemicals. Increased understanding of the molecular mechanism of glycohydrolases may lead to creation of more efficient enzymes that resist product inhibition. Additional approaches include the coproduction of glycohydrolases by the microbial biocatalysts during fermentation and the coproduction of glycohydrolases in the tissues of plants prior to harvesting for bioconversion. Significant reductions in added cellulase will also be achieved by improved understanding of the fundamental chemical and physical processes involved in the fractionation and solubilization of biomass.

Our increasing facility and knowledge of plants should also support a more radical approach to biomass feedstocks, the genetic tailoring of plant composition for specific bioconversion processes. Continuing investigations of fundamental mechanisms that regulate the partitioning of photosynthate between carbohydrate polymers (i.e., cellulose, hemicellulose, and starch), protein, lipid, and lignin should now allow rapid improvements in plant composition for fuels and chemicals equivalent to those that have been realized in food crops. For instance, increasing the lignin content with reduction in carbohydrate content would increase the energy density of plant residues intended for use in combustion. Alternatively, increasing the production of carbohydrate polymers that can be readily degraded by enzymes (i.e., starch and hemicellulose) and reducing the content of cellulose and lignin could eliminate the need for cellulase enzymes in bioconversion processes. Relatively small lignin and cellulose residues that remain after enzyme treatments of such materials could be burned to provide steam and power.

Broad implementation of biomass as a primary energy source in the U.S. and in the world will depend upon the genetic modification of plants to expand the range of soil environments for productive cultivation, to minimize nutrient requirements, and to increase crop productivity (tons/acre per year). These improved plants will become the feedstocks of the future. Areas of particular interest include salt tolerance, metal tolerance, and improved efficiencies for the use of water and nutrients. This is a longer term goal where sustained investment in fundamental research is essential. Again, the field of genomics provides a wealth of information by cataloguing the genes. However, continuing fundamental studies are essential to understand the mechanisms that have evolved to control these macro functions in plants and microorganisms. Results from these investigations will serve as a guide for the rational design of future improvements using both traditional and molecular approaches.

Relevance and Potential Impact

The efficiency with which we have converted fossil biological energy sources into fuels and chemicals has allowed a tremendous expansion in population and improvement in the quality of life throughout the industrialized world. As we look toward a future that must rely upon alternative energy sources, the same fundamental biological processes that created fossil deposits and our oxygen-rich atmosphere can be harnessed to provide a renewable source of energy and chemicals. Traditional plant breeding coupled with chemical and microbial conversion processes has allowed hundred- to thousand-fold increases in the production of food and food products over the past the century with small recent contributions from genomics and molecular methods.

Estimated Time Scale

These new methods, together with new advances in materials science and chemistry, offer the opportunity for even greater improvements in bio-based products over the next 50 years and provide the basis for the conservative estimate of a hundred-fold increase in contribution of renewable biomass (meeting 20% of the nation’s energy needs) to our national security.

DEVELOP METHODS FOR SOLAR ENERGY CONVERSION THAT RESULT IN A TEN-TO-FIFTY FOLD DECREASE IN THE COST-TO-EFFICIENCY RATIO FOR THE PRODUCTION OF FUELS AND ELECTRICITY

EXECUTIVE SUMMARY

The grand challenge for solar energy utilization is to develop conversion systems that are stable and robust for a 20-30 year period and that result in a ten-to-fifty-fold decrease in the cost-to-efficiency ratio for the production of electricity and fuels. To reduce the cost of installed photovoltaic systems to $0.20 per peak watt of solar radiation, a cost level that translates into $0.01-$0.02/kWh, or to reduce the cost of solar fuels to $1.00/GJ, costs that would make solar photoconversion very attractive economically in today's energy market, will require truly disruptive technologies that do not exist at the present time.

To achieve low solar cost- to- power (electrical or chemical) ratios, at least three approaches are possible. In a first approach, chemical methods are needed to enable inexpensive photoconversion materials (like polycrystalline, nanocrystalline, and organic materials) to perform as if they were expensive single crystals. A second approach is to produce so-called interpenetrating networks. Such an approach relaxes the usual constraint in which the photogenerated carriers must exist for long enough times to traverse the entire distance of the cell and be efficiently separated and collected. Instead, the materials consist of a network of interpenetrating regions that facilitate effective charge separation and collection over very short distances. A third approach involves developing novel methods to obtain extremely high conversion efficiencies at modest cost. Present photon conversion devices based on a single threshold absorber and full thermal relaxation of the photogenerated carriers, including semiconductor photovoltaics, have a theoretical thermodynamic conversion efficiency of 32% in unconcentrated sunlight, but the conversion efficiency can be increased, in principle, to 45-65% if carrier thermalization can be prevented. Multiple bandgap absorbers in a cascaded junction configuration can offer high efficiencies, particularly when highly concentrated sunlight can be used, but the materials are expensive. Approaches to achieving high efficiencies at moderate materials cost might utilize semiconductor quantum dots, quantum wells, organic dyes, and related nanostructures. In either of the above approaches, the interfaces necessary to separate and collect the charge carriers can be formed using solids, liquids, or polymers, but the resulting photoconversion structures must be inexpensive and manufacturable on a large scale.

Summary of Research Direction

The efficiency of photovoltaic devices has been increasing steadily. Nevertheless, current technologies all lie on a relatively common cost/watt (W) scale. The underlying reason for this roughly equal cost/W trade-off is that the photovoltaic materials now available suffer from the same fundamental physical limitations. Large-grain pure materials, with a long lifetime capable of making efficient solar cells, are costly to produce. Alternatively, cheaper materials with smaller grain sizes have grain boundaries that act as recombination sites, resulting in inefficient solar cells. A similar trade-off is found for organic ("plastic") photovoltaics. If pure inorganic single-crystal materials, like silicon and GaAs, are replaced with much cheaper organic materials, the materials are inherently disordered and therefore are cheaper but more inefficient. The net result is that one can ride anywhere on this cost/W trade-off scale, but nevertheless end up at the same cost/W ratio to within a factor of 20%. To reduce the cost of photoconversion systems for the production of solar electricity to $0.20/peak W of solar radiation and solar fuels to $1.00/GJ cost levels that would make solar photoconversion very attractive economically in today's energy market, will require scientific breakthroughs and associated truly disruptive technologies that do not exist at the present time.

One important strategy to attain these goals is to identify approaches that produce ultrahigh conversion efficiency at modest cost. Present photon conversion devices based on a single threshold absorber, including solid-state semiconductor photovoltaics, all operate within a regime wherein the ultimate thermodynamic conversion efficiency is limited to about 32% with unconcentrated sunlight. In this regime, the photogenerated electrons and holes are in thermal equilibrium with the phonons (quantized lattice vibrations) of the light-absorbing material. This means that the energy of photogenerated electrons and holes in excess of the threshold energy (i.e., the bandgap) is not utilized for useful work, but rather is converted into heat. Furthermore, in this regime, photons less energetic than the threshold energy are not absorbed. Recent research has shown that the equilibration of electrons and phonons (also referred to as hot electron cooling) can be slowed by one to two orders of magnitude in semiconductor quantum dots, quantum wells, and related nanostructures. Thus, useful electrical or chemical work may possibly be extracted before thermalization occurs, resulting in higher conversion efficiencies. Other researchers have shown that conversion efficiencies above the 32% limit may also be achieved by: (1) the formation of resonant impurity bands in photoelectrodes produced from quantum dot solid arrays that can absorb two sub-bandgap photons to create one electron-hole pair; (2) photon up-conversion, whereby a higher energy photon is produced from two lower energy photons; and (3) photon down-conversion, whereby two smaller energy photons are produced from one energetic photon. Another approach to achieving high conversion efficiency, also yielding a theoretical thermodynamic maximum of about 65%, is to use multiple bandgap absorbers in a cascaded tandem configuration. In the limit of threshold absorbers matched to the solar spectrum the limit is 65%, but two tandem bandgaps are estimated to yield about 40% conversion and three tandem bandgaps to yield about 50% conversion.

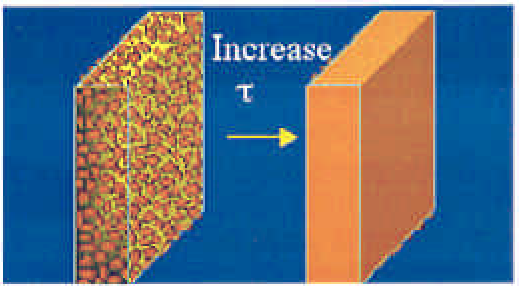


Figure 3-1. Solar paint passivates grain boundaries in inexpensive photovoltaics, causing them to perform like expensive single crystal materials.

Another approach to meet these cost/W goals is to find chemical methods to fool the inexpensive photoconversion materials (like polycrystalline, nanocrystalline, and organic materials) into performing as if they were expensive single crystals, without actually incurring the costs to grow the expensive crystals themselves. This approach involves chemically treating these inexpensive materials so as to fool their grain boundaries or interfaces into thinking they are part of the periodic crystal that this material is trying to emulate (e.g., see Figure 3-1). A related strategy is to produce so-called interpenetrating networks. Use of such networks relaxes the usual constraint in which the carriers that are excited must exist long enough in their excited states to traverse the entire distance of the cell. Instead, the materials consist of a network of interpenetrating regions. There are two examples of these approaches that are just emerging. Neither of them are economically or technologically viable today, but they seem like good approaches in the long run to achieve the difficult cost goals of #$0.01-$0.02/ kWh.

New Scientific Opportunities

In either of the above approaches, the interfaces necessary to separate and collect the charge carriers can be formed using solids, liquids, or polymers. In any successful system, the resulting photo conversion structures must be inexpensive and manufacturable on a large scale. Photoelectrochemical cells, polymer/ inorganic semiconductor junctions, thin-film photovoltaic materials deposited by chemical methods, and organic conductors and semiconductors are all possible materials that should be explored for this purpose.

An interesting feature of photoelectrochemical cells is that they are inherently more tolerant of grain boundary effects than solid-state systems and additionally such cells can be configured to store the photogenerated electricity by using part of the photogenerated power to charge a third electrode in the cell, which can discharge in the dark. Such a cell becomes a photochargable battery that can deliver power day and night. In the end, regardless of which materials system is implemented in the conversion device, the fabrication and assembly of the conversion device will have to be as cheap as painting your house and will need to be mass produced as inexpensively as printing the daily newspaper or making photographic film.

Relevance and Potential Impact

Recent detailed analyses indicate that from 10-30 TW-yr of annual carbon-free energy will be required by the year 2050 to accommodate the world's expected population combined with a modest annual global economic growth rate of about 2%. The range of required carbon-free energy depends upon the level of atmospheric CO_2 that can be tolerated. About 10 TW-yr of carbon-free energy annually will be required to stabilize CO_2 at 750 ppm, while about 30 TW-yr annually will be required for stabilization at 400 ppm. The current atmospheric CO_2 level is 275 ppm, compared to 175 ppm before the industrial revolution. Today, the total annual consumption rate of energy is about 12 TW-yr. Thus intense energy research and development is required to enable the introduction of such large amounts of carbon-free energy into the world's energy infrastructure on this timescale.

The solar constant is 1.76×10^5 TW, which is much larger than the 12 TW mean global energy consumption rate from all sources at the present time. Hence, there is ample solar energy potential to provide all of our energy needs from a renewable, carbon-free power supply. From the 1.2×10^5 TW of solar energy that strikes the earth's surface, a practical siting-constrained terrestrial solar power potential value is about 600 TW. The numbers range from very conservative estimates of 50 TW to optimistic estimates of 1500 TW, depending on the land fraction devoted to power generation. A good number to use for onshore electricity generation potential is probably 600 TW. Thus, for a 10% efficient solar farm, at least 60 TW of power could be supplied from terrestrial solar energy resources. For calibration, photosynthesis currently supplies 90 TW globally to make the biosphere run, so the amount of power available from the sun is very large.

The land area that is required to produce 20 TW of carbon-free power from solar energy is 0.16% of the earth's surface, or 5×10^{11} m^2. Producing 3 TW (the current U.S. energy consumption rate from all sources) with 10% efficiency would require covering 1.7% of the land in the U.S., an area comparable to the land devoted to the nation's interstate highways.

Estimated Time Scale

10 Years

DEVELOP THE KNOWLEDGE BASE TO ENABLE WIDESPREAD CREATION OF GEOTHERMAL RESERVOIRS

EXECUTIVE SUMMARY

There is a critical need to significantly increase the power generating capacity globally over the next 50 years, while minimizing the environmental impact. The natural thermal gradient of the earth's crust represents an extensive global geothermal resource, limited only by our inability to tap the gradient by creating productive and sustainable geothermal reservoirs. For example, exploitation of the geothermal gradient in the western U.S. alone could add as much as 0.1 TW of base load electrical power. The extent to which this vast potential resource can contribute to increasing demand will depend on conceptual and technical advances related to the creation and sustainability of productive reservoirs, where natural permeability and/or fluid content are limited. To meet this goal, basic research on all aspects of fractures and fracture networks in competent crystalline rock will be required. Specific critical research areas include: (1) the need for reliable high-resolution techniques for remote fracture mapping, (2) coupling mechanical properties and the local state of stress of reservoir rocks to stimulated fracture geometry, (3) mechanical and chemical techniques for sustaining stimulated fracture permeability, (4) new techniques for quantitative assessment of the coupled thermal and chemical interaction of injected fluids with the stimulated reservoir fractures and reservoir matrix, (5) new materials and coatings to enable drilling and heat harvesting at temperatures above 300°C, (6) new sensor technologies that will work at these temperatures, and (7) the same technologies at temperatures from 500-1000°C.

Summary of Research Direction

Geothermal energy is derived from the inherent heat content of the earth's crust. Circulating groundwater mines the heat from hot crustal rocks and energy is extracted from the heated groundwater. With research support from the U.S. DOE, significant progress in defining U. S. geothermal resources has been made. Resources with obvious geothermal manifestations, such as geysers, hot springs, fumaroles, mud volcanoes, etc., have been developed or tested, and currently provide ~2800 MW_e of geothermally derived electricity. It is conceivable that improvements in exploration and production technologies could increase the output from natural systems by as much as a factor of ~2-10. However, given the predicted need for 10-30 TW of clean power by the mid-21st century, extensive technological advancements will be required if the vast geothermal energy potential of the earth is to be exploited and added to the global energy mix. To meet future demands, geothermal research should be directed at tapping the inherent heat of the earth's crust by creating engineered geothermal systems.

Past research efforts have demonstrated the technical feasibility of creating an engineered geothermal resource. However, no commercial systems have been constructed and there is no conclusive proof that productive sustainable reservoirs can be developed. Never-the-less, the vast energy potential represented by the earth's natural thermal gradient should be a resource target. Ideally, a successfully engineered system will be one in which the inlet and outlet conditions of fluid pressure, temperature, flow rate, and water chemistry can be constructed, manipulated and controlled. Engineered systems, like their natural counterparts, will likely be hosted in competent crystalline rocks, where fluid flow and heat exchange is fracture controlled.

New Scientific Opportunities

To meet this scientific challenge will require extensive basic research into the nature and all aspects of fractures, fractured rocks, and the interaction between the water circulating through the fractures and the heat contained in the matrix rock hosting the fractures. Specific critical research areas include: (1) the need for reliable high-resolution techniques for remote fracture mapping, (2) the ability to couple mechanical properties and the local state of stress of reservoir rocks to the stimulated fracture geometry, (3) the development of mechanical and chemical techniques for sustaining stimulated fracture permeability, (4) new techniques for quantitative assessment of the coupled thermal and chemical interaction of injected fluids with the stimulated reservoir fractures and reservoir matrix, and (5) extending drilling technologies to higher temperatures than presently accessible.

High resolution remote fracture mapping. Fundamental research in the area of subsurface imaging, with a focus on geophysical methods, will enable the development of technologies for remote fracture mapping. Seismic methods are obvious candidates, since it is known that fractures scatter seismic energy, cause mode conversions, and trap and guide seismic waves. Further work is needed to establish a more quantitative relationship between fracture properties of interest, such as length, connectivity, and permeability, and of changes in the wavefield. Further work is also required to establish quantitative attributes of the seismic signature typically measured in the field. Seismic amplitudes can be used if the relative contribution of scattering and intrinsic attenuation can be better understood, particularly under the multiphase chemically reactive environment of a geothermal reservoir.

Field application of seismic methods will involve deployment of surface and subsurface sources and receivers. In this regard, the huge amount of experience in the petroleum industry is not easily transferred to geothermal. There are few geothermal reservoirs located in sedimentary environments for which conventional acquisition strategies have been developed. Passive source concepts should be further explored, since it is known that geothermal production activities yield many microseismic events.

The difference in the geologic environments of petroleum and geothermal resources also means that data processing techniques from the petroleum industry are not easily adapted to geothermal applications. Fundamental research is needed to derive new algorithms for processing of the seismic wavefield generated in very heterogeneous strongly scattering media.

Other geophysical methods, such as electrical and electromagnetic, gravity, and surface deformation, are of lower resolution than seismic but potentially provide information to compliment seismic measurements. Further fundamental research on the effect of fractures on potential field measurements is needed.

Rock mechanical properties, local stress, and stimulated fracture geometry. The fundamentals of rock fracture have been studied extensively for 40 years. Nonetheless, the technology for fracture stimulation of geothermal reservoirs is not well defined, despite several field-scale attempts. Further fundamental research needs to be focused on understanding fracture initiation and propagation in rock in which there is a network of pre-existing fractures containing fluids of multiple phases subjected to large thermal and hydrologic pulses. The relative contribution of brittle and ductile processes needs to be studied for the hydrothermal conditions and rock types present in geothermal reservoirs. Though it is known that microseismic activity accompanies such stimulation processes, further research is needed to quantitatively interpret these events in terms of changes in hydraulic properties of the rock.

Sustaining stimulated fracture permeability. Experience in reservoir stimulation using such techniques as fluid acidification, injected propellants, hydro-fracturing, sand injection, etc. has demonstrated the feasibility of enhancing near-well bore permeability. Engineered geothermal systems introduce a new level of complexity, because permeability must be enhanced and sustained over the distance between an injector and production well and over long periods of time. Long-term success of an engineered system will require future research in physical and chemical methods for maintaining open fluid pathways.

Coupled thermal and chemical interaction between injected fluid and reservoir rock. The thermal power performance of an engineered reservoir will depend on the coupled efficiency of fluid circulation and heat extraction. Surface seismic methods can define a seismic reservoir volume. Conservative fluid tracers can map fracture connectivity between an injection and production well. However, there is no direct measurement that couples the seismic volume and fracture connectivity to the effective heat-transfer volume. The latter is a necessary parameter for understanding, modeling and predicting thermal power performance.

A major objective of future research should be to develop reliable techniques for determining the effective heat-transfer efficiency over an integrated fluid-flow path. Fundamental research is needed to develop the chemical, isotopic, and advanced microscopic techniques for geochemical characterization of fluid-rock systems from the microscopic, to the molecular, to the field scale. For instance, presently it is not well understood why fluid-rock reaction rates determined in laboratory-scale experiments are up to several orders of magnitude faster than similar reaction rates measured on a field scale. Of fundamental importance is the ability to model fluid transport, fluid-rock interaction, the rate and distance scales over which these processes occur, and an effective surface area of fluid-rock exchange.

High-temperature drilling technologies. In order to extend the geothermal resource potential to greater depths and higher temperatures, high-temperature drilling technologies will need to be advanced. Future research should focus on developing new materials and coatings to enable drilling and heat harvesting at temperatures above 300^{o}C, new sensor technologies that will work at these temperatures, and the same technologies at temperatures from 500-1000^{o}C.

Relevance and Potential Impact

The natural thermal gradient of the earth's crust is ~30-100^{o}C/km and represents an extensive global geothermal resource of high potential. For instance, exploitation of the thermal gradient in the western U.S. alone could add as much as 0.1 TW of baseload electric power. Access to this resource is limited only by our present inability to tap the natural thermal gradient and create geothermal systems. To create a productive and sustainable geothermal power resource from the natural thermal gradient, the biggest scientific challenge will be engineering the appropriate mix of permeability, fluid pressure, water flux, and heat exchange. In most regions, adequate heat is accessible with present drilling technologies. Access to deeper and hotter systems, thus extending the geothermal resource, would require future advances in high-temperature drilling technology.

Estimated Time Scale

Initial goal is 0.02 TW of baseload electric energy from engineered systems by the year 2020. Secondary goal is 0.1 TW by the year 2040. Final goal is technological development for exploiting deeper hotter systems in regions of normal and higher than normal thermal gradients.

CONVERSION OF SOLAR, WIND, OR GEOTHERMAL ENERGY INTO STORED CHEMICAL FUELS

EXECUTIVE SUMMARY

In one approach, electricity would be produced by the conversion devices and then converted separately into storable fuels. For this approach to be cost-effective and energy efficient, new catalysts are needed to facilitate multi-electron transformations, such as evolving hydrogen and oxygen from water or reducing CO_2 to methanol, ethanol, or other carbon-based fuels. In a second approach, the fuel is made directly or in an integrated system with the energy conversion device. Direct solar photoconversion is the process whereby the energy of solar photons is converted directly into fuel starting from simple and renewable substrates, such as water, CO_2, and N_2. These processes require photoactive organic, inorganic, or biological molecules or materials that can absorb a large fraction of the solar irradiance and drive the chemical reactions that produce the fuels of interest.

Summary of Research Direction

Direct solar photoconversion is the process whereby the energy of solar photons is converted directly into fuels starting from simple and renewable substrates, such as water, CO_2, and N_2. These processes require photoactive organic, inorganic, or biological molecules that can absorb a large fraction of the solar irradiance and drive the chemical reactions that produce the fuels of interest. Direct formation of fuels will require development of inexpensive, robust, and efficient thermal and/or photochemical catalysts for the formation of such fuels from abundant, inexpensive, recyclable chemicals. Important targets include the direct photochemical splitting of water into H_2 and O_2; catalysts that could be used, either in an integrated fashion with photoelectrochemical devices or in a modular fashion with photovoltaic systems, and that individually reduce water to hydrogen and oxidize water to oxygen; and catalysts that effect the reduction of CO_2 to organic fuels (such as methanol or methane) or that utilize H_2 and CO_2 to form hydrocarbon fuels.

Three branches of science and technology can be defined for direct solar photoconversion: photoelectrochemistry, photochemistry, and photobiology. They all depend upon photo-induced charge generation (i.e., electrons and positive holes) followed by efficient positive and negative charge separation at various types of interfaces that ultimately produce oxidation-reduction (redox) chemistry. Photoelectrochemistry involves semiconductor-molecule interfaces, photochemistry involves molecule-molecule interfaces, and photobiology involves biological interfaces with other biological and non-biological molecules.

Fuels produced by solar photoconversion are derived from endoergic reactions wherein the photon energy is stored as chemical free energy in the reaction products. Extremely important examples of this process are hydrogen from photolytic water splitting and formation of methane, methanol, or ethanol by the reduction of CO_2 in water. The latter can be termed "artificial photosynthesis," since biological photosynthesis uses the same reactants of CO_2 and H_2O to form biomass and O_2. However, the term "artificial photosynthesis" is also applied more generally to all fuels and chemical products produced via solar photochemistry. The photoactive molecules and materials used to create and separate electrons and holes and to drive the appropriate redox chemistry are semiconductors (inorganic or organic) in photoelectrochemistry, molecular structures in photochemistry, and biological structures (e.g., *in vivo* water-splitting blue-green algae or *in vitro* reaction centers) in photobiology.

The best reported conversion efficiency (rate of H_2 free energy output divided by the input solar power) for the photolytic splitting of water by semiconductor structures is about 12%. This efficiency was achieved using a monolithic tandem cell structure that consisted of two series-connected p-n junctions of GaAs and $GaInP_2$ with noble metal catalysts deposited on the anodic (oxygen evolving) and cathodic (hydrogen evolving) sides of the layered structure. However, the cost of this cell is very high, and the use of such high-efficiency tandem cells is usually reserved for space applications. Photobiological production of hydrogen by photosynthetic blue-green algae has recently been achieved without the usual poisoning of the algae by the evolved oxygen. However the conversion efficiency is very low (< 1%). Systems in between these limits, in terms of both cost and efficiency, have also been developed and include the photoelectrolylsis of aqueous HBr using Si microspheres and the photoelectrolysis of aqueous HI using pure semiconductor crystals. Combination approaches are also possible in which non-biological chromophores are used to drive photosynthetic processes in cells and, conversely, in which photosynthetic reaction centers are modified to produce different fuels than are normally produced by the natural biological system.

Underlying all of these approaches are inexpensive photoconversion systems and effective, robust fuel-forming catalysts. The reactions of interest are multi-electron transfer processes that are difficult to perform near their thermodynamic potential using known inexpensive catalysts. Important targets include the direct photochemical splitting of water into H_2 and O_2, catalysts that individually reduce water to hydrogen and oxidize water to oxygen and that could be used either in an integrated fashion with photoelectrochemical devices or in a modular fashion with PV systems, and catalysts that effect the reduction of CO_2 to organic fuels (e.g., methanol or methane) or that utilize H_2 with CO_2 to form hydrocarbon fuels.

New Scientific Opportunities

Biological systems offer proof of concept that such catalysis is possible, because enzymes such as hydrogenase, nitrogenase, and the oxygen-evolving components of photosystem II drive these fuel-forming reactions with extremely high energy efficiency. At present there is little understanding of how to remove such catalysts from the biological system and maintain their function or how to design biological catalysts for such reactions that are inexpensive and robust under expected operating timescales and environmental conditions. There is a critical need to develop catalysts, likely transition-metal based, that can enable this fuel-forming function, whether in direct solar conversion systems or as a module in conjunction with solar-to-electric systems, and that as a system enable the production of fuel from the solar energy resource.

Relevance and Potential Impact

The same considerations for inexpensive conversion of solar energy apply to systems that would enable inexpensive storage and fuel production from solar energy. All the possible strategies for high-efficiency, low-cost, high-stability and long-lifetime solar photoconversion systems must be examined and compared to find the optimum system(s) to achieve the important goals described above for producing stored chemical free energy in fuels or electricity from renewable resources. This is particularly vital since photoconversion is a direct solar conversion process that utilizes the largest available renewable energy resource and has the potential to operate with ultrahigh conversion efficiencies and with very low-cost materials in an integrated system that provides the solar energy conversion and storage functions while producing useful fuel from a renewable energy resource.

Estimated Time Scale

10-20 Years

ADVANCED MATERIALS FOR RENEWABLE ENERGY APPLICATIONS

EXECUTIVE SUMMARY

Photovoltaic conversion is one of the leading contenders for renewable energy sources. The basic physical principles of photoconversion are now well understood, leaving system design and materials development as the primary challenges for widespread implementation. Solar cells made from polycrystalline (including amorphous silicon, a-Si) semiconductors on low-cost substrates are a promising direction requiring significant materials advances. Hybrid solar cells combining a porous wide bandgap semiconductor with a light-sensitive dye offer high potential for low-cost unconventional photovoltaic conversion. Opportunities and prospects associated with hybrid conversion materials are very promising and create many attractive materials research directions. In the longer term, nanostructured materials offer qualitatively new opportunities and challenges for solar conversion, exploiting quantum dots, carbon nanotubes and nanofibers, and organic semiconductors. Early successes demonstrate significant impact of nanoscale materials on photoconversion and promise dramatic advances in material design and performance.

Summary of Research Direction

The most likely scenario for renewable energy utilization generally envisions a mix of technologies, with photovoltaics (PV) being the leading contributor. The factors that are most detrimental to widespread PV applications are cost and effective storage of the electrical energy produced. The storage problem is such a severe limitation that any discussion of materials for PV conversion for the future should include consideration of materials problems relating to the storage device (e.g., batteries) itself. Revolutionary progress in photovoltaic conversion of energy depends on developing materials that will work effectively, reliably, and are inexpensive to implement.

Single crystal conventional cells. Consider first high efficiency single-crystal silicon cells. Efficiencies have progressed to a remarkable point in the last 10-15 years, but at an enormous increase in the cost and complexity of the cells. The materials problems associated with Si itself have largely been overcome because of its widespread use in the semiconductor industry. Recent gains in efficiency have been made by improved fabrication techniques for antireflection coatings, texturization of the surface for light trapping, buried contacts to increase the active area, etc. If one considers other semiconductors such as GaAs, the materials situation is less well developed, but still the research has been at a respectable level. Multi-junction cells, even for concentrator applications, are very complex and the materials issues even more demanding. Again, these avenues have been thoroughly explored and it seems that a breakthrough of the magnitude needed is not to be found in this area. The driver is not efficiency, but cost.

Thin-film cells on low-cost substrates. The driving force for the development of this approach to PV is again cost. The high-efficiency cells mentioned above all utilize the material itself to support the active part of the cell. Even in Si with its indirect bandgap, very little of the material is utilized for the actual PV conversion. Consequently, thin films deposited on low-cost substrates would seem to offer a path to drastic reductions in cost. Let us consider three such paths that have been extensively explored.

At one time, a-Si solar cells were considered the hope of the photovoltaic industry for large-area applications, but their potential has not been realized and now almost universal pessimism about them prevails. For one thing, degradation due to Stabler-Wronski effect has not been satisfactorily overcome. Efficiencies remain comparatively low. To increase the efficiencies, research on multi-junction a-Si cells has been pursued, but the fabrication of such cells is costly and the efficiency/cost equation was never that favorable for them. Also, there is the question of the substrates, usually glass or very thin stainless steel, which can become prohibitively expensive in the quantities and quality needed. Materials research for a-Si has been both intensive and extensive and it is difficult to identify new areas that might lead to a breakthrough.

Another somewhat similar approach uses polycrystalline Si on low-cost substrates. The problems here arise primarily from grain boundary effects in the semiconductors and interdiffusion from the highly impure inexpensive substrates. To minimize grain-boundary effects, the grains must be fairly large, which puts severe restrictions on deposition processes. High temperatures (near the melting point of Si) are required for the film deposition itself or else a subsequent recrystallization step must be introduced. In either case, the demands on the low-cost substrate materials at these high temperatures are extremely severe. Although progress with this approach has been slow to date, it is possible that a concerted effort in the materials area could yield truly worthwhile gains.

Yet another approach in this category that has been extensively studied utilizes thin films of small-grained, direct bandgap materials such as CdTe and $CuInSe_2$ on low-cost substrates. Here, the deposition temperature may be quite reasonable and not a problem, although the deposition process itself requires close control. It remains an area where further research could be fruitful. The grain-boundary effects in these materials, often quite subtle, are still not well understood nor readily controlled. Consequently, reproducible fabrication is a problem.

Dye-sensitized mesoporous solar cells. A recent, very encouraging development is the success some groups have had with the so-called Grätzel cell. In this approach, a porous, fairly wide band gap semiconductor such as TiO_2 is impregnated with a light-sensitive dye (usually a transition metal complex whose molecular structure is specifically designed to have the required properties). The dye absorbs the photons and the excited electrons are injected into the conduction band of the TiO_2. Electron-hole separation occurs so rapidly at the TiO_2/dye interface that recombination is practically eliminated. Because the internal surface of the film is much higher than its projected geometric surface, there is a large interfacial area between the dye and the semiconductor. Due to the small size of the particles/pores, the film does not scatter visible light. Also, visible light is not absorbed by the oxide if the bandgap is large enough.

Solar cells from nanophase materials. Since the pores in the porous materials of the Grätzel-type cell may be very small, the conceptual progression to nanophase materials is a natural one. While it is too early to predict what the impact of nanoscience engineering and technology on PV conversion may have, it is difficult to believe that it will be of no consequence. The capability to tailor both optical and electrical properties of arrays of quantum dots has already been demonstrated. The outstanding electrical, thermal, and mechanical properties of carbon nanotubes and nanofibers are widely appreciated, even though severe obstacles to their applications in large-scale systems remain formidable. The flexible thin-film features of both nanophase and organic semiconductors are important for applications, leading perhaps to photovoltaic "cloth" and "plastic wrap". The already well-established self-organizing capabilities of some systems, such as block copolymers and nanoporous oxide templates, could be important for Grätzel cell type applications.

New Scientific Opportunities

Thin-film cells on low-cost substrates. In the area of low-cost substrates, concerted efforts in materials areas could yield truly worthwhile gains. Efforts should be aimed at understanding and controlling grain boundaries better and the development of substrates that retain their low cost while remaining practically inert to the thin-film deposition process itself. In particular, reproducible fabrication techniques are desperately needed. Intensive materials research in this area of grain-boundary effects might lead to steady progress, if not to a breakthrough.

Dye-sensitized mesoporous solar cells. While the efficiencies that have been obtained so far are relatively modest (~10%), the approach is quite different from the conventional ones described above and warrants much further study. Unlike conventional cells, the light absorption process and the electron-hole charge separation are differentiated. A multitude of crucial questions about the most effective materials and materials combinations (semiconductors and dyes) remain to be explored. Since the dyes are frequently organic materials, the oft-discussed marriage of organic and inorganic materials, primarily semiconductors, is a fundamental aspect of the approach. It perhaps should also be pointed out that porous materials of a somewhat similar type are expected to have important applications for catalysis and a variety of other technologies. Thus, a wider spectrum of scientific expertise might be brought to bear on the problems. This is an exciting area for fundamental materials research with practical applications.

Solar cells from nanophase materials. The possibilities for nanophase materials are too numerous to be discussed here, but their potential importance is undeniable.

Relevance and Potential Impact

Within DOE, successful research on new materials for renewable energy is particularly relevant to the Energy Efficiency and Renewable Energy Program on Solar Energy Technology. Since nanomaterials will potentially play a prominent role in new approaches to photovoltaic materials, the research is directly related to the National Nanoscale Science, Engineering, and Technology initiative that crosses many federal agencies.

Estimated Time Scale

Materials research on conventional single-crystal solar cells is well developed and evolutionary progress is expected to continue. The materials issues governing the performance and cost of polycrystalline, thin-film solar cells and a-Si are much less well understood and are likely to see significant breakthroughs enabling discontinuous progress in the next five years or more. Progress on dye-sensitized mesoporous cells requires path-breaking research on photoconversion and charge collection in hybrid materials, a promising and fertile opportunity for creating qualitatively new materials with tailored properties over the next ten or more years. Nanophase materials for photovoltaics offer the broadest horizon and the highest potential for spectacular progress. Understanding and controlling the behavior of single- and multiphase photoconversion materials at the nanoscale can make revolutionary progress in the cost and performance of solar cells. This area is now in its infancy and will be fruitful over the next two decades or more.

Fusion Energy

Multiscale Modeling of Microstructural Stability of Irradiated Materials

Deformation and Fracture Modeling

Plasma-Surface Interactions

Thermofluids and “Smart Liquids”

Plasma Aerodynamics

MULTISCALE MODELING OF MICROSTRUCTURAL STABILITY OF IRRADIATED MATERIALS

EXECUTIVE SUMMARY

Fundamental research is needed to identify the key physical processes that will enable materials to maintain microstructural stability during prolonged fusion neutron irradiation. By utilizing physically rigorous bridging of the gaps between different spatial and temporal modeling regimes (nanoscale to continuum), a comprehensive predictive capability for modeling the stability of prospective advanced nanoscale materials can be attained. Several longstanding, unresolved materials science issues could be answered by this research program (e.g., "one-interstitial" versus "two-interstitial" model for point defect migration). The successful development of fusion energy will require materials that are capable of withstanding exposure to intense radiation fields over a broad range of temperatures. A sound physics-based understanding of the stability of materials in the anticipated fusion environment is key for establishing the viability of fusion as a future energy source. This fundamental information is also of importance for advanced Generation-IV fission reactor materials.

Summary of Research Direction

Materials are key to achieving attractive fusion energy. Opportunities in the area of multiscale materials modeling for a comprehensive predictive capability of the response of fusion materials are extensive. They range from basic theoretical developments of fundamental processes at the atomic, mesoscopic and continuum scales to highly complex simulations of surface and bulk phenomena. Surface processes include sputtering and other erosion mechanisms, implantation, re-deposition and co-deposition of tritium, near surface damage and microstructure evolution, enhanced atomic transport (diffusion, trapping/detrapping and desorption), and surface roughening and restructuring. Bulk processes include crystal lattice displacement damage, creation of atomic and clustered defects, microstructure evolution (e.g., voids, bubbles, dislocations and new phases), dimensional instabilities (e.g., swelling and creep), shear bands and localized plasticity, and a host of embrittlement phenomena at both low and high temperatures. The recommended approach is to utilize multiscale materials modeling, covering atomistic simulations (e.g., ab initio quantum methods, molecular dynamics, and Monte Carlo), mesoscopic simulations (e.g., dislocation dynamics and statistical mechanics), and continuum simulations (e.g., rate theory and the Finite Element methods). A critically important aspect of the multiscale materials modeling is to use physically rigorous bridging of the gaps between the various spatial and temporal modeling regimes. Specific recommended thrust areas associated with this multiscale modeling paradigm include the following:

- Development of improved interatomic potentials, including directionality effects, magnetic effects (very important for ferritic steels), alloying effects. Since interatomic potentials are the fundamental building blocks used for many higher-scale materials models, it is crucial that these descriptions of atomic interactions be physically meaningful. It is well known that many of the state-of-the-art interatomic potentials currently available do not accurately describe many fundamental material properties, and therefore further work using atomistic and quantum chemical techniques is needed to achieve improved, more realistic descriptions of the interatomic interactions.

- Numerous recent molecular dynamics (MD) simulations (using interatomic potentials of dubious quantitative accuracy) have predicted the possibility of long-range one-dimensional transport of matter via self-interstitial crowdion bundles. This mechanism has enormous potential consequences on the interpretation of existing experimental data (due to the different reaction kinetics for 1-D versus 3-D transport), and reopens the highly controversial condensed-matter physics debate (dating back to the 1960s and never fully resolved) regarding the “one-interstitial” versus “two-interstitial” model for point defect transport. The prospect of 1-D migration of defect clusters would also have an impact on non-nuclear fields, for example, semiconductor processing by ion beam implantation methods (providing either an obstacle or an opportunity for creating unique nanoscale structures via ion implantation).

- Development of physically rigorous multiscale microstructural evolution models based on molecular dynamics, kinetic Monte Carlo and kinetic rate theory techniques. The predictions from these multiscale materials models would be experimentally validated by comparison with specific well-controlled experiments performed on model metallic and ceramic material systems. An overarching question associated with this activity is whether nanoscale structures can be designed with extremely high resistance to radiation damage and transmutant helium degradation.

- Phase stability under irradiation, with particular emphasis on the following three aspects: (1) development of improved physics-based models of radiation-induced or -enhanced solute segregation to interfaces (grain boundaries, etc.) due to inverse Kirkendall, solute drag, and other mechanisms; (2) evaluation of the effect of solute segregation on corrosion resistance; and (3) displacement cascade dissolution of second-phase particles (most of the available models date from the 1970s and do not correctly predict the experimentally observed behavior). Improved models are needed to describe both solute segregation processes and precipitate/solute cluster ballistic dissolution processes. Specific materials systems of interest for fusion applications include the stability of (Y, Ti, O) clusters in nanocomposited ferritic steels and Ti(C,O,N) precipitates in V alloys.

- Transport and clustering of helium. Helium produced by nuclear transmutation events may ultimately determine the operating lifetime and maximum use temperature of materials in fusion systems. Grain-boundary embrittlement due to accumulation of helium bubbles is a well-known phenomenon that limits the maximum operating temperature of helium-containing materials, but recent experimental research suggests that special types of grain boundaries may exhibit significantly different response to helium accumulation. A fundamental understanding of the role of different types of grain boundaries on helium transport within the grain boundary is lacking. If this effect could be properly understood, it might eventually lead to developing materials with specifically designed grain boundaries in order to attain significantly higher resistance to helium grain boundary embrittlement.

New Scientific Opportunities

By utilizing physically rigorous bridging of the gaps between different spatial and temporal modeling regimes (nanoscale to continuum), a comprehensive predictive capability for modeling the stability of prospective advanced nanoscale materials can be attained. This research could answer several longstanding unresolved materials science issues (e.g., “one-interstitial” versus “two-interstitial” model for point defect migration).

Relevance and Potential Impact

The successful development of fusion energy will require materials that are capable of withstanding exposure to intense radiation fields over a broad range of temperatures. A sound physics-based understanding of the stability of materials in the anticipated fusion environment is key for establishing the viability of fusion as a future energy source. This fundamental information is also of importance for advanced Generation-IV fission reactor materials.

Estimated Time Scale

~10 years: development of improved interatomic potentials (including directionality effects, magnetic effects, alloying effects)

~10 years: multiscale microstructural evolution and nanoscale solute segregation models of irradiated materials based on Molecular Dynamics and kinetic Monte Carlo techniques

~10 years: development of improved physics-based models of radiation-induced or –enhanced solute segregation to interfaces (grain boundaries, etc.) and their resultant effect on corrosion resistance

DEFORMATION AND FRACTURE MODELING

EXECUTIVE SUMMARY

A fusion energy system requires a high level of material performance to function safely and economically. In a fusion energy system, structural materials must perform at damage levels and with gaseous and solid transmutants well beyond those of other nuclear systems. Multiscale modeling of material deformation and fracture is of tremendous need for fusion energy systems, because this can accelerate the design and development of materials to meet these demands while comprehensive models could also aid in the design process as well. New opportunities exist to understand and predict the effects of radiation on deformation and fracture. Multiscale modeling involving atomistic simulations (e.g., ab initio quantum methods, molecular dynamics, and Monte Carlo), mesoscopic simulations (e.g., dislocation dynamics and statistical mechanics), and continuum simulations (e.g., rate theory and the finite element methods), coupled with greatly expanded computational capabilities, allow us to understand phenomena and predict behavior beyond that which has been possible with experimental approaches.

Summary of Research Direction

New multi-scale modeling opportunities that cover the atomistic to continuum scales exist today and can provide new fundamental understanding of some complex problems that have been studied for a number of years. This includes understanding of radiation effects problems that have been studied for a number of years along with application to understanding and predicting the behavior of new materials. The introduction of new materials, such as nanoscale reinforced materials and radiation resistant composite materials, into fusion energy systems can occur in a shorter time frame with the fundamental understanding that is possible with new modeling. Also, a better understanding of radiation phenomena will also allow tailoring of conventional materials to gain improved performance. Some examples covering both new materials and a description of some well-known problems are given below.

- Newly developed ceramic matrix composites present new opportunities for radiation environments and challenges to model their deformation and fracture behavior. Multiscale modeling must incorporate details from the atomistics of the fiber/matrix interface (e.g., effect of gaseous transmutants, thermal transport, and interfacial fracture strength) to a model for the bulk deformation based on localized microcracking.

- This topic was highlighted at a recent NE/BES workshop on Higher Temperature Reactor Materials (ANL-02/12, June 2002). It is critically important for Generation-III+ and -IV fission reactors and future fusion systems to develop materials that do not suffer unacceptable degradation in ductility and fracture toughness during low-temperature neutron irradiation. The international fusion materials community is actively investigating many of the underlying mechanisms responsible for the mechanical property degradation. Teaming with BES researchers would lead to acceleration in the understanding of the mechanisms. Key issues include: (1) dislocation interactions with SFTs, (2) conditions for or limiting cross-slip of irradiated materials, and (3) physics of channel development and effects on fracture

- Radiation embrittlement can now be understood at the atomistic level and in fact semi-empirical modeling has been successful in predicting shifts in the fracture transition from ductile to brittle behavior. However, improved interatomic potentials and multi-scale models incorporating dislocation dynamics have the capability to reveal new insights into our understanding of radiation embrittlement. This knowledge at the atomistic level could provide the opportunity to design new radiation resistant materials.

- Radiation embrittlement and fracture deal with the initiation of flaws that are critical in size in terms of conventional fracture mechanics. Subcritical sized cracks initiate and grow with time to become critical sized flaws that induce fracture. The initiation and propagation of subcritical sized flaws often involve interactions between external and internal nano- and microchemistry, nano- and microstructure and loading conditions at the tip of a crack. There are opportunities to use ab initio modeling of local chemistry, molecular dynamics modeling of crack-tip deformation, mesoscale modeling of plastic zone scale processes and continuum modeling of far-field effects to provide new insight and understanding to this field. A key challenge involves merging chemistry, physics and mechanics modeling tools.

- High-temperature deformation mechanisms, such as irradiation creep, have been the subject of numerous fundamental research projects over the past 40 years or so, but one of the important new twists is the possibility that new nanoscale materials may behave differently from conventional materials (recent experimental results on nanoscale oxide-dispersion-strengthened ferritic steel suggests this may be the case). If nanoscale structures can be tailored to provide superior creep strength, this could usher in a whole new class of high-performance materials for a broad range of applications. Another new twist is the high-temperature deformation, creep and irradiation creep of ceramic composites. These materials deform by local microcracking and link-up to produce macroscopic strain. Comprehensive models describing irradiation effects on high-temperature deformation and fracture are needed.

New Scientific Opportunities

The current understanding of radiation effects on deformation and fracture of new materials is inadequate. New multi-scale modeling capability has the potential to make breakthroughs in understanding and designing these new materials.

Relevance and Potential Impact

A fusion energy system requires a high level of material performance to function safely and economically. In a fusion energy system, structural materials must perform at damage levels and with gaseous and solid transmutants well beyond those of other nuclear systems. Multiscale modeling of material deformation and fracture is of tremendous need for fusion energy systems because this can accelerate the design and development of materials to meet these demands. Comprehensive models could also aid in the design process as well.

Estimated Time Scale

Considerable phenomenological understanding of radiation effects on deformation and fracture has been obtained over an extended period. Modeling developments have also been occurring over a shorter time period than the experimental work but still over a relatively long period of time. These time periods were needed because of the complexity of the problem. Opportunities for utilizing multi-scale modeling to understand and predict these complex problems exist today but will also require an extended period because: (1) models must address complex systems and (2) experimental verification of the models will require an extended period of time. Given the current schedule to produce a fusion demonstration plant and the time frame for bringing new materials to commercial production, these results are needed in the next 10 years.

PLASMA-SURFACE INTERACTIONS

EXECUTIVE SUMMARY

One of the most important issues concerning the basic feasibility of fusion as an energy source, and a major issue for present-day high-temperature plasma confinement experiments, is the interaction of intense heat and particle fluxes with plasma-facing components. These interactions need to be understood in terms of the basic phenomena so that they can be controlled. Potential impacts include contamination of the plasma and short lifetimes of the components.

Another related issue is developing high-power targets for future accelerators and particle colliders for nuclear and high-energy physics as well as for space applications. Understanding basic mechanisms of material destruction and lifetime enables the design and development of materials that meet these harsh environments. This effort will increase the basic understanding of critical issues related to plasma-surface interactions including photon radiation transport, “potential” sputtering, and material erosion under intense power loadings. Developing multi-scale and integrated models of these issues using powerful computational capabilities will significantly increase our basic knowledge to best optimize and enhance plasma and material performance.

Summary of Research Direction

One important area that determines many of the plasma-surface interaction effects is photon radiation and transport in both optically thin and optically thick plasmas with intense line populations. Developing 3D direct photon transport computer models (Monte Carlo, ray tracing, etc.) in a highly charged, hot and dense plasma is quite important in various basic research areas. This is an extremely important effect, since it will define/control plasma time evolution and the degree/intensity of plasma-material interactions of nearby components.

Another important topic is a recently discovered physical phenomenon that is not well understood called “potential sputtering”. This occurs during the interactions of highly charged ions with target materials. The sputtering coefficient is several orders of magnitude higher than the values for well-known physical sputtering (100-1000 times). An important related area is basic understanding of details of interatomic potentials. Developing phenomenological models and 3D molecular dynamics methods to understand this effect is, therefore, highly desired. This has many potential benefits, such as preventing “explosive” erosion of materials or the use of these methods for highly effective etching of materials.

Understanding fundamental models of material erosion and destruction under intense power applications is another vital topic. Material destruction and lifetime issues take many forms including fragmentation, splashing, brittle destruction, spallation, etc. Most of these issues require detailed understanding of the microstructure evolution dynamics during the intense-power deposition phase. Up to now there is no comprehensive understanding of all of these effects. These issues are of significant concern in many basic research science [e.g., beam/plasma-on-target effects for high-energy physics (muon collider, neutrino project)], nuclear physics [high-power accelerator, Spallation Neutron Source (target concerns)], medical applications (high-power electric arc effects and injuries), and plasma interactions with electrodes in plasma guns, Z-pinch, dense plasma focus, and others.

New Scientific Opportunities

Development of a deeper understanding and models for key plasma-surface interactions involving intense particle and heat loads.

Relevance and Potential Impact

One of the most important issues concerning the basic feasibility of fusion as an energy source, and a major issue for present-day high-temperature plasma confinement experiments, is the interaction of intense heat and particle fluxes with plasma-facing components. These interactions need to be understood in terms of the basic phenomena so they can be controlled. Potential impacts include contamination of the plasma and short lifetimes of the components.

Another related issue is developing high-power targets for future accelerators and particle colliders for nuclear and high-energy physics as well as for space applications. Understanding basic mechanisms of material destruction and lifetime enables the design and development of materials that meet these harsh environments.

Estimated Time Scale

The research activities described here have typically a 10-year period.

THERMOFLUIDS AND “SMART LIQUIDS”

EXECUTIVE SUMMARY

The proposed research is to develop a fundamental understanding of, and capability to control, flowing electrically-conducting fluids in complex environments that include electromagnetic fields. Magnetohydrodynamic (MHD) forces can affect liquid motion from the largest, integral scales down to the finest scales of turbulence. These fundamental changes in the liquid motion have an impact on practical considerations, like how much energy it takes to force fluids to flow through pipes or what happens to hot interfaces when subjected to intense heating conditions.

MHD phenomena also provide one means of controlling the liquid flow to mitigate undesired consequences and even improve the capability of a fluid flow to perform some function. Clever ideas that modify local magnetic field or supply externally injected electric currents may be utilized to accelerate liquids in desired directions. This electromagnetic control may be necessary for the use of liquids as virtual first walls of magnetic and inertial confinement fusion reactors, where they would act as continuously self-healing surfaces in contact with the burning plasma, one which would be immune to radiation damage effects. Other ideas to modify the fluid properties themselves through chemical systems engineering and micro and nano technologies could potentially work hand-in-hand with electromagnetic effects to maximize potential for a given engineering application. Ultimately, fluid properties can be tailored so that such “smart liquids” can be shaped and steered, as well as mixed and separated in such novel fashions only now being conceived.

Summary of Research Direction

From the fusion perspective, the establishment of liquid walls or liquid surface divertors (for MFE and IFE) that allow high-heat-flux handling, high reliability, long lifetime and high efficiency heat extraction would be extremely significant. The behavior of such unrestrained flows in complex, temporally and spatially varying magnetic and electric fields poses a significant challenge in terms of numerical and experimental simulation. Magnetohydrodynamic forces can affect the liquid motion from the largest integral scales all the way down to the finest scales of turbulence. The particle- and heat-removal capabilities of such flows will depend heavily on the flow conditions, so that accurate simulations are necessary for the determination of feasibility and performance. Even for more conventional closed-channel cooling systems, similar motivation for better understanding of interactive, multi-scale flow processes and heat transfer exist. The ultimate idea is something like the creation of “smart liquids” via a number of engineering science disciplines. Specific suggestions that might be of interest to BES include the following:

- Numerical simulation of the effect of magnetohydrodynamic forces on turbulence in incompressible and stiffly compressible liquid conductor flows and their related transport of heat and mass, especially near solid and free interfaces. Studies can include: (1) evolution of 3D turbulence entering strong magnetic fields regions to 2D-like turbulence to complete turbulence suppression, (2) turbulence generated from shear flows completely “grown” inside a strong magnetic field, (3) instability and collapse of boundary layers and shear layers, and (4) compressible effects coming from rapid heating and incident surface shocks.

- Control of liquid-metal flow motion and velocity profiles via applied magnetic and electric fields and currents. The ability to control the flow of free-surface liquid-metal walls is a similar challenge to the magnetic control of fusion plasma itself. Simulation of the motion of the liquid wall, including interaction with complex geometry, electrically conducing structures, and electromagnetic coupling to the plasma will be an important part of establishing the feasibility of the liquid wall idea.

- Modification and control of fluid properties and behavior via complex chemical doping and micro-additives. Taking advantage of the revolution in MEMS and nano-technology and new simulation capabilities for chemical/material systems, concepts and basic proof-of-principle simulations and experiments should be developed to apply these ideas to the control of the micro-processes in the liquid flows to give benefits like reduced-surface evaporation; improved surface gettering of hydrogen, helium and impurities; reduced wall corrosion; and many others.

New Scientific Opportunities

Several avenues for improvement in computation methods for complex physical problems are mandated by this work.

- 3-D direct numerical simulation (DNS) and large eddy simulation (LES) and other methods of incompressible, turbulent, free-surface fluid flow in strong electromagnetic fields and complex geometries. Improvement of free-surface tracking techniques like Level-Sets and Front Tracking will be required, as well as complex unstructured finite-volume and finite-element grids.

- Stiffly compressible liquid modeling, with intense sources of heat and particles that allow for phase change, cavitation and fracture of initially condensed liquid flows. Free-surface tracking techniques like Phase Field and accurate equations of state will be required.

- Near-surface molecular dynamics and similar techniques to simulate changes in surface properties from dopants and nano-additives as well as kinetic interaction with energetic particles.

Application and expansion of these numerical modeling techniques to gain better efficiency and fidelity in simulating these complex multi-scale physical systems, as well as data-visualization techniques required to interpret the voluminous data.

Relevance and Potential Impact

Fusion energy seeks to contain star-like conditions within physical barriers. The environment includes elevated temperatures, radiation and kinetic debris. To solve the resulting materials problems, increasing attention is being given to liquid walls in both magnetic and inertial fusion. Liquids can be pumped through the harsh reactor environment and out to a benign area where liquid refurbishment can be performed. “Smart liquids” may enable unique solutions to direct flow, especially free-surface flow in complex, fusion reactor geometries, and control heat-transfer and particle-pumping effects that depend heavily on the small-scale near-surface turbulent motion.

The impact of smart liquid development would hardly be confined to the fusion reactor application only. The control of free-surface flows by electromagnetic and other means has a myriad of potential applications in industry including fuel injectors and other combustion processes, water jet cutting, ink jet printers, continuous casting, flood/jet soldering, hull design, ocean/river hydraulic engineering, crystal growth and many others.

Estimated Time Scale

The feasibility of employing liquid wall concepts in fusion power systems should be established in the next 10-20 years. The in-depth, scientific understanding of the thermofluid science involved in such concepts should be established in the next 10 years.

PLASMA AERODYNAMICS

EXECUTIVE SUMMARY

Efficient access to space, hypersonic transport, and the development of high-performance re-entry vehicles are areas of national importance. Vehicles that operate in these regimes suffer from extremely high heat loading and must contend with very complex flow physics, including laminar-to-turbulent transition, shock wave boundary layer interactions, nonequilibrium gas dynamics, and supersonic combustion. For air-breathing hypersonic vehicles, the inlet geometry must be mechanically modified for each flight Mach number to avoid unacceptable performance and catastrophic engine stall. It has recently become apparent that the use of weakly ionized plasmas may revolutionize the capabilities of these vehicles. Weakly ionized plasmas can be used to locally deposit energy into the air to control shock location, produce virtual vehicle geometries, control transition to turbulence, reduce drag, avert engine stall, and accomplish other objectives not currently possible with mechanical devices. In addition, weakly ionized plasmas are electrically conducting, and, therefore, provide the opportunity of incorporating magnetohydrodynamics into the vehicle design for control, power extraction, thrust augmentation, and vehicle steering. The potential application of these concepts involves a detailed understanding of plasma formation properties, including nonequilibrium molecular phenomena, plasma contraction and filamentation, electron beam interactions, microwave coupling; and other approaches to achieve both high-efficiency energy deposition and high-efficiency generation of conductivity. Modeling of aerodynamic processes must include full electromagnetically coupled, dynamic three-dimensional flow-field calculations, including nonequilibrium and turbulence.

Summary of Research Direction

The area of plasma aerodynamics is just beginning to be explored. There are numerous fundamental issues that need to be understood.

- Because the plasmas are so expensive in power to establish and sustain, one of the critical areas to understand is the time scale of the phenomena. Moving from continuous to pulsed plasmas may reduce the overall power requirement and improve the performance of the process. It is important to know how long various effects last after the plasma is turned off and whether pulsing is preferable to continuous operation. It may also be possible to achieve the desired plasma effects by using nonuniform plasmas that consist of streamers or multiple simultaneous or sequentially formed localized plasmas. This may further reduce the power requirement.

- In many of the plasma aerodynamic applications, the presence of instabilities may become a serious limitation. Filamentation will cause a glow discharge to collapse and generally happens when the pressure rises and where large electric field gradients are present. This may limit the operation of MHD power extraction or low observability plasmas. On the other hand, filamentation permits the delivery of large amounts of heat to localized regions, so it may be preferable in some circumstances. The high velocity of the flow, high magnetic field strength, and the coupling of the plasma to the flow may lead to unexpected instabilities.

- Mechanisms for the efficient creation of air plasmas also need to be understood. These may be very different depending on whether the plasma is needed for conductivity or for heat addition.

- Perhaps the most difficult issue is the establishment of scalability relations. Almost no experiments can be done on full-scale vehicles, so the community will be relying on sub-scale experiments. The very different nature of plasmas as a function of air pressure, temperature, electric and magnetic field strength, fluid motion, and molecular species make sub-scale experiments very difficult to extrapolate. Numerical simulations may help guide development of flight tests to generate scalability data.

New Scientific Opportunities

A plasma aerodynamics program will establish models for treating the interaction of plasma and electromagnetic forces with three-dimensional flow fields and aerodynamic shapes. Since, in general, aerodynamic plasmas are expensive to create, it is important to understand the impacts that they may have on vehicle control, heat-load mitigation, and performance enhancement. For example, the ability to control the inlet shock structure may remove the need for hydraulically-driven inlet flaps and deformable duct walls. Since a large fraction of the aircraft weight is associated with these mechanical devices, the cost penalty of the plasma formation mechanisms may be small by comparison. Plasmas and MHD processes provide the capability of achieving new methods for controlling air flow and may enhance the capabilities of the vehicle well beyond those that can be achieved with mechanical systems. For example, modeling suggests that off-body plasmas can be used to suppress far-field shock coalescence and, therefore, minimize sonic boom. If this is true, it may open up supersonic flight to commercial air transport. New plasma technologies combined with new multifunctional lightweight materials may provide highly capable re-entry vehicle geometries with low-heat loading or wide cross-path landing capability for emergency return of astronauts. The scientific opportunities focus on understanding the effects that plasmas can have on aerodynamic interactions with vehicles for control, power extraction, heat-load mitigation, and performance enhancement.

Relevance and Potential Impact

Weakly ionized air plasmas have a high potential for impact on advanced aerodynamics. Specifically, plasmas and MHD processes may be capable of mitigating peak thermal loads, extracting high levels of power, reducing drag, reducing observability, reducing sonic boom, and suppressing noise. Plasmas may be employed to facilitate stability and control by optimizing inlet shock position, controlling turbulence by initiating or suppressing transition, and steering the vehicle with localized heat addition. Internal aerodynamics may be affected by virtual shaping of the internal ducting through plasma heating, elimination of shock reflections by localized surface plasmas, enhanced mixing, and control of ignition and enhancement of combustion rates.

Estimated Time Scale

Research activities have a 5-10 year period.

Distributed Energy, Fuel Cells, and Hydrogen

Advanced Hydrogen Synthesis

High-Capacity Hydrogen Storage for Distributed Energy of the Future

Novel Membrane Assemblies

Designed Interfaces

ADVANCED HYDROGEN SYNTHESIS

EXECUTIVE SUMMARY

Hydrogen has the potential to offer solutions to two major challenges in future growing energy use, the security of the energy supply and the preservation of the environmental quality. To realize this potential, our understanding of the principles of hydrogen useage, and their development and incorporation into novel technologies for massive hydrogen synthesis systems, needs to be accelerated.

Currently, about 9 million tons of hydrogen are produced per year in the U.S. alone, primarily from steam reforming of fossil fuels such as natural gas. While natural gas can continue to supply hydrogen for the near term, in the mid-to-long term (>20 years), other production technologies using sustainable feedstocks must be brought on line. Mid-to-long-term processes that hold promise to produce hydrogen domestically, without net CO_2, emissions include gasification of biomass or organic wastes, electrolysis of water using electricity from renewable resources (i.e., photovoltaic, wind, solar-thermal-electric, and geothermal) or nuclear power.

Fundamental advances in catalysis, membranes, and gas separation could enable more efficient, lower cost fossil hydrogen processes. Understanding the feasibility of carbon capture and sequestration is key for long-term use of fossil hydrogen with near-zero emissions (i.e., geoscience and flows in porous media). Leap-frog technologies for the longer-term include solar photolytic methods and thermochemical water-splitting driven by nuclear or solar heat.

The direct and effective coupling of light harvesting to catalytic processes that produce hydrogen is a grand challenge. This builds on the BES research programs in photochemistry and catalysis. However, fundamental studies of catalysis need to be expanded to include electrocatalysis. Corrosion and materials selection are significant issues for semiconductor photolytic processes and in high-temperature thermochemical water-splitting systems.

Thermochemical water-splitting uses high-temperature heat (typically ~500 to 900^0C) to drive chemical reactions to separate water into hydrogen and oxygen. One key to discovering, evaluating, and developing feasible and economic thermochemical water-splitting cycles is having a firm scientific basis for the chemical thermodynamic data, as well as for the models of the chemical reaction systems. The current thermal chemical cycles that are being considered for coupling to nuclear energy suffer from the need for materials that can withstand extreme corrosive environments at these elevated temperatures. Alternative cycles based on novel redox systems may be devised that operate at lower temperatures, thus reducing the daunting corrosion problems. For solar-driven systems, cycles that lend themselves to hot/cold (day/night) cycles can offer considerable potential if coupled with such reduced-temperature redox cycles.

Summary of Research Direction

Fossil Hydrogen Production. Today most commercially produced hydrogen is made at large scale from fossil fuels via steam reforming of natural gas or partial oxidation of heavier hydrocarbon feedstocks, such as residual oil or coal. Hydrogen is then used in chemical applications, including ammonia and methanol production and oil refining. Large-scale hydrogen production from fossil fuels for the hydrogen economy is under consideration by oil companies such as Shell and British Petroleum (BP). A variety of small-scale fossil-based hydrogen production systems are under development for application to distributed hydrogen production (e.g., for use in fuel cells).

Light-Harvesting Systems Directly Coupled to Catalytic Processes to Generate Hydrogen. A photolytic process utilizes the fact that the entire visible spectrum of light has sufficient energy to split water into hydrogen and oxygen. Water is transparent and does not absorb this energy. The key then is to find an efficient light-harvesting system that can collect the solar energy and directly transmit towards a catalytic water-splitting reaction. Both photobiological and photochemical processes have shown the capability of using light energy to produce hydrogen and oxygen from water and sunlight. We propose fundamental studies of photoelectrochemical light-harvesting systems directly coupled to catalytic processes for hydrogen production.

Photoelectrochemical water-splitting, also known as photoelectrolysis, represents an advanced alternative to a photovoltaic (PV)/electrolysis system. The incident light, absorbed in a semiconductor electrode immersed in an aqueous solution, splits water directly. This is equivalent to combining a solar cell and an electrolyzer into a single monolithic device. In operation the semiconductor collects the light energy, and directs the energy to a catalyst on the surface of the semiconductor. Hydrogen is produced at the surface of an illuminated p-type semiconductor. Oxygen is produced at the surface of an illuminated n-type semiconductor. This occurs due to injection of electrons into the solution (for p-type) or because holes (e.g., electron vacancies) appear at the semiconductor/electrolyte interface (for n-type). The other component of the water-splitting reaction (oxygen or hydrogen, respectively) is generated in a separate compartment.

A one-step monolithic system of this configuration eliminates the need to generate electricity externally and subsequently feed it to an electrolyzer. This combination then reduces semiconductor processing, since surface contacts, interconnects and wiring are no longer necessary. Only the piping necessary for the transport of hydrogen to an external storage system or gas pipeline is required. An additional advantage of photoelectrochemical water-splitting is that H_2 and O_2 can be generated separately, and separation steps are not necessary. Another major advantage of a direct-conversion system is that the area used for electrolysis approximates that of the solar cell. Depending on the solar intensity and the type of semiconductor material, this translates to a current density of 10-30 mA/cm^2. At these current densities, the voltage required for electrolysis is much lower than standard electrolysis [in the range of 1.35 V (at 25^{o}C)], and therefore the corresponding electrolysis efficiency is much higher [close to 90% (LHV)], resulting in an efficiency increase of up to 30% over a separated PV/electrolysis system, without the added cost of the electrolyzer. Finally, semiconductors can be very efficient light absorbers, resulting in a very high (>25%) theoretical solar-to-hydrogen conversion efficiency.

Thermochemical water-splitting cycles. Thermochemical water-splitting uses a set of thermally driven chemical reactions to separate water into hydrogen and oxygen. The process takes in only water and high-temperature heat and releases only hydrogen, oxygen and low-temperature heat. While high temperatures are needed (typically ~700 to 900^{o}C), the heat can be provided by any source, including solar and nuclear energy. Advanced solar processes to produce hydrogen have significant potential, although basic research remains to be done.

New Scientific Opportunities

Fossil Hydrogen Production. Fossil hydrogen production methods, such as steam methane reforming, are well-established commercial processes, capable of providing hydrogen in large quantities. However, further research can optimize existing fossil hydrogen production approaches for use in future hydrogen energy systems. Fundamental advances in catalysis, membranes, and gas separation could enable more efficient, lower cost fossil hydrogen technologies. Processes that combine hydrogen generation and separation in a single reactor (for example, membrane reactors for methane steam reforming) could improve conversion efficiency and reduce emissions. Very pure (99.999%) hydrogen is needed for some applications, in particular proton exchange membrane fuel cells (PEMFCs), so that hydrogen purification technologies need further development.

Existing fossil-based hydrogen production processes release significant amounts of carbon dioxide. Near-zero emissions of greenhouse gases and air pollutants must then be a characteristic of future hydrogen production. Capture and sequestration of carbon during hydrogen production from fossil fuels are key technologies to enable long-term use of fossil-derived hydrogen. (This is particularly necessary for coal-derived hydrogen). Understanding the feasibility of carbon capture and sequestration is vital for long-term use of fossil hydrogen with near-zero emissions. This includes basic understanding of the geological processes that may be involved in carbon dioxide storage.

Light Harvesting Systems Directly Coupled to Catalytic Processes to Generate Hydrogen. The main issue with this approach is that the usual semiconducting materials that are stable in water and can do the water-splitting reaction do not absorb enough sunlight to be efficient, and the materials that absorb sunlight efficiently either corrode in aqueous solution or do not have the proper energetics to effect the water-splitting reaction. Research is needed that is directed at: (1) discovery of possible semiconductor materials that have appropriate light-absorption characteristics and are stable in aqueous solutions; (2) development of techniques for the preparation of catalytic coatings and their application to semiconductor surfaces; and (3) identification of environmental factors (e.g., pH, ionic strength, solution composition, etc.) that affect the energetics of the semiconductor, the properties of the catalysts, and the stability of the semiconductor.

An area of interest that is cross-fertilized with the solar industry is the study of photovoltaic multi-junction cell technology as applied to photoelectrochemical water splitting. Multi-junction cell technology connects photovoltaic layers (p-n junctions) with different semiconductor bandgaps in series, one behind the other in a single-cascade device. This arrangement provides the highest theoretical conversion efficiency of any photoconversion system (maximum of 66%). This approach may allow a material that would otherwise corrode in aqueous solution to be protected by another semiconducting material that is stable. The combination then provides a higher efficiency than each would offer alone.

Thermochemical water-splitting cycles. One key to discovering, evaluating and developing attractive thermochemical water-splitting cycles is having a firm scientific basis for the chemical thermodynamic data and models for the chemical reaction systems. Also critical is the need for materials that can withstand the corrosive environments and elevated temperatures projected for the current thermal chemical cycles that are being considered for coupling to nuclear energy. For example, in the S-I cycle, I_2 and SO_2 are added to water, creating H_2SO_4 and HI. These are separated and then decomposed by heating to release H_2 and O_2 and recycle the I_2 and SO_2. The system must be able to withstand SO_2 and H_2SO_4 corrosion in the

700°C range, and HI and I_2 corrosion in the 450°C range. This is a very demanding materials problem. Development of new membranes to separate O_2, H_2O, and SO_2 could result in lowering the reaction temperature, reducing the demands on other materials in the system.

In the area of solar-driven thermochemical water-splitting systems, cycles that lend themselves to hot/cold (light/dark) cycle are key. A conceptual example here could be a metal (Me)/metal oxide (MeO) cycle or, in general, a metal oxide redox cycle:

(1) $MeO_x + H_2O \longrightarrow H_2 + MeO_{x+1}$ (dark/cold)

(2) $MeO_{x+1} + \text{heat} \longrightarrow MeO_x + 1/2\ O_2$ (sunlight)

The elaboration of such cycles, which would involve less demanding materials properties, can be effective ways to produce hydrogen in combination with solar concentrators.

Relevance and Potential Impact

The DOE Hydrogen, Fuel Cells and Infrastructure programs in the Energy Efficiency and Renewable Energy and the Fossil Energy Programs have active development and demonstration programs for advanced hydrogen production technologies, in addition to enabling technologies such as membranes for gas separations and carbon sequestration. The proposed research supports these efforts by concentrating on the understanding of the fundamental mechanisms involved in advanced hydrogen production systems. The proposed research could lead to development of more efficient, lower cost methods for hydrogen production, with near-zero emissions.

Expected Impact and Time Scale

The proposed research direction looks toward basic research with practical implementation, perhaps 20 years in the future, as it is likely that low-cost fossil hydrogen production methods will dominate commercial production in the U.S. over the next few decades.

HIGH-CAPACITY HYDROGEN STORAGE FOR DISTRIBUTED ENERGY OF THE FUTURE

EXECUTIVE SUMMARY

Hydrogen has been proposed as the future low-polluting energy carrier. Nearly every energy-related application of hydrogen requires a safe and efficient hydrogen storage technology, especially in transportation, where there are serious weight and volume constraints. In fact, stagnation of the hydrogen storage technology near its present stage would require profound changes in attitudes toward transportation and significantly obstruct the prospects of a hydrogen economy. A new paradigm is required for the development of hydrogen storage materials to facilitate a hydrogen economy.

Hydrogen may be stored as a compressed gas, a cryogenic liquid, or as a hydrogen-rich solid. The first two approaches require substantial energy expenditures. Therefore, improved energy efficiency of hydrogen compression and liquefaction is desired.

Over the past three decades, solid-state hydrogen storage has involved nearly exclusively metals and metallic alloys, where the metal matrix is expanded and filled with hydrogen atoms located in interstitials. Capacities of two hydrogen atoms per metal atom have been demonstrated. However, the metal matrices consist of relatively heavy elements, such as Ti, La, Ni, etc., and storage capacities usually do no exceed 2 wt% hydrogen. Few, if any, options to modify the properties of conventional hydrogen storage alloys remain unexplored. A material approaching the required volumetric and gravimetric capacity, at reasonable temperatures and pressures, has not been discovered.

Lightweight metals, such as Li, Be, and Mg, can form high-capacity binary hydrides. However, they release hydrogen at 300-600°C, or are toxic. Carbon-based hydrogen storage has not achieved its initial promise. Experimental results are controversial and irreproducible, and significant storage is only realized at cryogenic temperatures in combination with high pressure. Such conditions are not practical for general transportation.

The ultimate hydrogen storage compound is methane, where four hydrogen atoms surround a single carbon atom. However, methane is gaseous, and the nature of the hydrogen-carbon bond does not allow easy dehydrogenation and is nearly impossible for direct rehydrogenation.

Novel materials [e.g., alanates (aluminohydrides) and borohydrides], where a metal or a metalloid atom is surrounded by four to six hydrogen atoms forming a complex negatively charged anion, mimic methane and may provide a much needed breakthrough in solid-state storage of hydrogen. Their hydrogen capacities are high (from ~10-18% by weight), but multiple basic issues related to their hydrogen storage properties must be addressed. To date, even the atomic structures of many complex hydrides are either unknown or have been determined with insufficient accuracy. On the other hand, the nature of complex hydride solids (i.e., the ionic bonding of hydrogen-rich anions with various cations) opens a way for precise chemical substitutions in the cation sublattice, thus bridging the gap between hydrogen-poor intermetallic hydrides and hydrogen-rich LiH, BeH_2, and MgH_2. It is in this area that a significant research program is proposed.

Summary of Research Direction

Compressed storage of hydrogen is presently certified for use with 5,000 psi tanks. Research and development continues, which may result in future certification of 10,000 psi tanks. It is not certain whether higher pressures could be achieved practically and safely. This technology results in 7-10% energy lost during the compression.

Liquefied hydrogen production is an existing technology. However, energy requirements are presently too high (approximately 30% energy is lost during the liquefaction). Furthermore, cryogenic tanks are inconvenient and costly, and cryogenic storage of hydrogen has intrinsic hydrogen boil-off losses.

Over 40 years of research in conventional metal hydrides, such as $LaNi_5$, $ZrNi_2$, TiFe, and related alloys did not produce a material capable of reversibly storing more than 2 wt% of hydrogen. Regardless of virtually limitless possibilities to modify alloy chemistry and microstructure, no further improvements are in sight.

Binary hydrides of several light metals, such as MgH_2 (7.7 wt%), LiH (~12 wt%), and BeH_2 (~18 wt%), could provide sufficient hydrogen storage. However, hydrogen can be released only at high temperature (300-600°C), or the material is highly toxic (BeH_2). Chemical and structural modifications without capacity loss are severely limited and only minimal improvements can be envisioned.

Complex hydrides offering high-hydrogen capacities include: $Al(AlH_4)_3$ (10 wt%), $LiAlH_4$ (~10.5 wt%), $NaBH_4$ (10.6 wt%), Li_3AlH_6 (11.1 wt%), $LiBH_4$ (18.3 wt%), and others. To date, 7.6 wt% hydrogen release has been demonstrated for $LiAlH_4$ (5.1 wt% at room temperature plus 2.5 wt% below 150°C). The entire hydrogen content of $Al(AlH_4)_3$ is available below 100°C. The actual structures of a number of ternary and majority of multicomponent complex hydrides and their hydrogen storage behavior remain unknown and unexploited. Basic research effort to explore hydrogen storage properties of complex hydrides is virtually nonexistent, except for some recent work on the relatively low capacity $NaAlH_4$, which contains 7.4 wt% hydrogen total.

New Scientific Opportunities

While design of a solid with 25 wt% hydrogen or more appears unfeasible (the four-coordinated carbon stores 25% hydrogen in methane), light metal-based complex hydrides with 10-18 wt% hydrogen exist. Hydrides where four to six hydrogen atoms coordinate a single metal or metalloid atom, thus forming complex $[MeH_n]^{p-}$ anions, are especially promising. Novel hydrogen-containing solids based on light elements should be engineered, synthesized, and fully characterized. This effort may include partial or complete substituting on the cation sites or exploring the feasibility of creating a variety of different kinds of anions (both in chemical composition and structure) stabilized by lightweight counterions. Thus, studies of the phase diagrams, structures, and chemical and physical properties of new hydrides are especially important. New materials chemistries could be designed, which should facilitate high hydrogen storage capacities coupled with acceptable dehydrogenation and hydrogenation pathways. Major emphasis should be placed on solids with total hydrogen content 10% by weight or more.

Bonding states of hydrogen in novel solids are different from conventional metallic hydrogen absorbers, and understanding of hydrogenation-dehydrogenation transformations at length scales from 10^{-1} to 10^3 nm has emerged as a complex fundamental problem. Especially intriguing is self-assembly of $[MeH_n]^{p-}$ anions, which occurs in the solid state. The in-depth understanding of the mechanisms of the solid-state transformations occurring during the dehydrogenation and rehydrogenation of complex hydride solids is critical if satisfactory reversibility of hydrogen in this broad class of materials is ever to be achieved. State-of-the-art characterization of crystalline, nanocrystalline, and amorphous solids is essential because it is the only reliable way to establish the structure and intrinsic properties of hydrogen-containing solids and correlate them with their hydrogenation-dehydrogenation behavior. Although thermodynamics favor hydrogenation of complex hydrides, this has been achieved in the past via solvent processes and at high hydrogen pressures.

An issue in hydrogen storage employing complex hydrides, which requires considerable basic research, is overcoming high hydrogenation pressures. Often, hydrogenation and dehydrogenation kinetics are limiting steps. Conventional wisdom to overcome kinetic limitations calls for increased temperature, but this requires a further increase of hydrogenation pressure. Other forms of energy (e.g., mechanical, electromagnetic, sound, etc.) should be explored to improve kinetics.

Apart from gravimetric and volumetric capacity, the critical issue for novel materials to be considered for hydrogen storage and distribution is the reversibility of hydrogen release and uptake. Since in many cases it is easier to develop a method for hydrogen extraction than it is to recombine the resulting residue with hydrogen, various experimental approaches to direct solid-state synthesis of complex hydrides from elements should be studied in detail. Kinetics of solid-state transformations leading to breakdown and formation of complex $[MeH_n]^{p-}$ anions should be explored and understood before hydrogen delivery and recharging could be controlled with the required precision. Intimate combination of the first principles theory with the state-of-the art experiment is likely the most feasible way to design ultra high capacity hydrogen-containing solids. Prior extensive studies of the conventional intermetallic hydrides fully support the notion that the processes of the absorption and recovery of hydrogen are controlled by the thermodynamic properties of materials, complex hydrides included. Recent significant improvements of the computational methods for *ab initio* calculations of the thermodynamic and electronic properties of intermetallic compounds should be extended and applied to complex hydride materials.

Relevance and Potential Impact

The DOE Hydrogen, Fuel Cells and Infrastructure programs in Energy Efficiency and Renewable Energy and the Fossil Energy Programs have active development in fuel cells intended to be served by hydrogen in the hydrogen economy. Without a practical storage method, however, the hydrogen economy is unlikely to become a reality.

Estimated Time Scale

The proposed research could lead to development of effective hydrogen storage methods. The proposed research direction will require concerted efforts extending well over 10 years.

NOVEL MEMBRANE ASSEMBLIES

EXECUTIVE SUMMARY

Membranes that conduct hydrogen ions and oxygen ions, either alone, in combination, or together with electrons, are essential components of a broad range of energy conversion devices and fuel-conditioning systems, and play a role in nearly every energy storage scenario. The required combination of properties for these membranes, including a useful temperature range of operation, high conductivity, extreme stability, and economy, is rarely if ever achieved. Practical operating conditions may impose undesirable materials selections for the complementary system components, such as platinum catalysts below 200°C or expensive ceramics above 600°C. It is precisely in this 200-600°C temperature range that functionally useful membranes are yet to be discovered. The essential difficulty is that fundamental theories to date are inadequate for the prediction of the physical and chemical properties of single-phase, composite, and, particularly, nanocomposite membranes, their adjoining electrode materials, and their interfaces. While a complex and very challenging task, the development of such predictive theories, together with experimental exploration and verification, could dramatically accelerate the rate at which practical discoveries can be expected that have a beneficial impact on energy technology.

The benefits of novel membranes and membrane/electrode assemblies (MEAs) may be appreciated by considering the following examples. The operating temperature, efficiency, and catalytic activities of a PEMFC is limited by the dependence of the hydrated proton [i.e., $H(H_2O)_n^+$] on the water content of the membrane polymer. Polymer and polymer/inorganic composite membranes of exclusive, high proton conductivity, but independent of humidity in the temperature range of 100-200°C, may enable variants to the PEMFCs with higher tolerance of anode catalyst to carbon monoxide poisoning. Thermal management would be significantly simplified, and parasitic losses associated with air pressurization could be reduced or avoided altogether.

For solid oxide fuel cells (SOFCs), reducing the temperature to 300-600°C with the accompanying development of effective oxygen and fuel electrodes would allow dramatic cost reductions for electrical interconnects and for the balance-of-plant (BOP). It would extend the domain of use of SOFCs to smaller residential or even mobile units, where bottoming turbine cycles are not indicated, operating directly on natural gas, fossil fuels, alcohols, or hydrogen.

Novel membrane assemblies must be sought to reduce the polarization resistances at membrane-electrode interfaces that limit the overall electrolytic device performance. In particular, novel membranes assemblies must facilitate: (1) the reduction of oxygen in fuel cells cathodes, (2) the oxidation of hydrogen or direct oxidation of carbon-containing fuels in fuel cell anodes, and (3) the synthesis of pure hydrogen or the reforming of carbon-containing fuels to hydrogen.

In conclusion, novel organic or inorganic membranes and their composites, assembled with high-performance electrodes and targeted for operation in the 200-600°C range, will lead to a new generation of electrochemical devices that are exceptionally effective in the energy conversion and utilization sector. Basic research can accelerate their development by stimulating the relevant theoretical studies in combination with materials experimentation, particularly in the area of nanocomposite membranes.

Summary of Research Direction

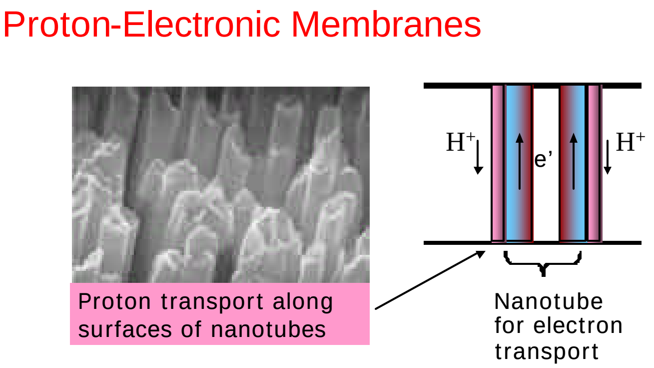
Membranes that conduct hydrogen ions and oxygen ions, either alone, in combination, or together with electrons, are essential components of a broad range of energy conversion devices, fuel-conditioning systems, and play a role in nearly every energy storage scenario. Most prominent among these are the fuel cells, of which the PEMFC and the SOFC are the target of much commercial development. Yet broad deployment of these fuel cells, which would be ideally suited to a hydrogen economy and to its fossil fuel transition phase, is hindered by the present nature of the membrane and its electrodes. The required combination of properties for these membranes, including a useful temperature range of operation, high conductivity, extreme stability, and particularly economy, is rarely if ever achieved. Practical operating conditions impose undesirable materials selections for the complementary system components, such as noble metal catalysts below 200°C and ceramics above 600°C. It is precisely in this 200-600°C temperature range that functionally useful membranes are yet to be discovered. The essential difficulty is that fundamental theories to date are inadequate for the prediction of the physical and chemical properties of single-phase, composite, and particularly nanocomposite membranes, their adjoining electrode materials, and their interfaces.

PEMs rely on a hydronium-based transport mechanism that requires liquid water within the membrane and limits the fuel cell operating temperatures to less than 100°C, unless operated at elevated pressures. The pressurized perfluorosulfonated ionomer PEM and its variants lack the properties to operate much above 140°C. Humidification of the membranes is required to maintain the water content and conductivity of the membranes. Even at operating temperatures as high as 140°C, the PEM fuel cell is quite susceptible to carbon monoxide poisoning and is most effective when operating on pure hydrogen. The low operating temperature reduces the PEMFC's utility for combined heat and power (CHP) applications, but the high power density of the PEM fuel cells make them well suited for automotive applications when operating on pure hydrogen. The high power density is a result of high catalytic activity at both electrodes and the development of highly efficient systems for thermal management combined with product water removal. Hydrogen fuel utilization (as high as 99%) and high efficiency have been achieved in PEM fuel cells operating at atmospheric pressure. Pressurized fuel cells typically sacrifice as much as 20% of the available power pressurizing the air for the cathode.

SOFCs offer promise for a clean and highly efficient system for chemical-to-electrical energy conversion when operating on fossil fuel. At 800-1000°C in a combined cycle, efficiencies of over 80% can be projected. Their fuel flexibility, from carbon-containing fuels to hydrogen, makes them well suited for the transition to a hydrogen economy. The high operating temperature of SOFCs is currently required for sufficiently fast electrode reactions (oxygen reduction and fuel oxidation) near the membrane-electrode interfaces and for fast ionic transport across the electrolyte membranes. However, this high operating temperature is at the same time the source of a range of problems, including necessity of limited and uneconomic component and material choice, complex system designs, slow cold start, and limited deployment. Accordingly, the cost of the current SOFC systems is still prohibitive for broad commercialization. To be economically competitive, both the cost of materials and the cost of fabrication for SOFC systems must be dramatically reduced. To achieve this, the SOFC operating temperature must be significantly reduced. At sufficiently low temperatures, interconnects, heat exchangers, and other structural components can be fabricated from much less expensive materials. Further, as the operating temperature is reduced, many technical difficulties can find easy solutions, system reliability and operational life increase, and the possibility of using SOFCs for a wide variety of applications becomes possible.

The essential grand challenge is to design ionic and mixed-conducting membranes with high conductivity, stability, and selectivity over a broad temperature range, especially temperatures below 600°C. Of particular interest are membranes transporting one or more of the following charged defects: proton, oxygen vacancy, oxygen interstitial, electron, electron hole, and OH$^-$. Such membranes must be combined with anodes and cathodes of high catalytic activity for oxygen redox reactions, for direct oxidation or reforming of hydrocarbon fuels, and for synthesis of cleaner fuels. This can only be achieved if relevant theory development combines effectively with experimental investigation. In particular, considerable potential for innovation, both on the theory and practical side, exists in the study of nanocomposite membranes and transport along their internal interfaces, as for example shown in Figure 5-1.

Similar concepts may be applied to create nanocomposite membranes that exhibit exceptionally high selectivity for molecules rather than ions. Such composite membranes may lead to revolutionary means of fast gas separation that in turn may profoundly impact on hydrogen and other gas separations beneficial to fuel cells and hydrogen production.



- Hydrogen separation/purification
- Electrodes for fuel cells based on proton conductors

Figure 5-1. Conceptual example of a possible nanocomposite membrane.

New Scientific Opportunities

While the quantum effects in optical and electronic processes have been extensively studied, transport of ionic species and catalytic reactions at nanoscale are yet to be examined. A fundamental approach to the ionic and electronic transport in nanoscale composite membranes, such as the one sketched in Fig.1, involves both phenomenological theory development as well as *ab initio* calculations. These are used to obtain insight into mechanisms of ionic and electronic transport along or near interfaces in nanocomposites where the surface of the particulates, such as carbon nanotubes, have been functionalized with organic or inorganic adducts, and where the carbon may transport electrons. A membrane with rapid transport of both electrons and protons may be used for hydrogen separation, purification, and electrosynthesis of cleaner fuels.

For ceramic membranes, predictive theories, such as advanced molecular dynamics treatments, must be developed that clarify the rate limits, temperature dependence and mechanisms of ionic conduction, particularly for oxygen ions and protons. This will facilitate both novel membrane design and electrode formulations.

It is proposed: (1) to explore ionic and mixed transport with both phenomenological theory development as well as *ab initio* calculations; (2) to combine these theory developments effectively with parallel experiments; (3) to characterize transport mechanisms and other emergent phenomena relevant to ionic transport using the advanced facilities, such as high resolution electron microscopy, neutron scattering, and advanced light sources, available at the DOE National Laboratories; (4) to design rationally nano-structured membranes with rate of ionic and electronic transport several orders of magnitude higher than any existing membranes in the 200-600°C range; (5) to fabricate nano-structured membranes exploring templating and self-assembly processes; and (6) to seek effective electrodes that in combination with the novel membranes lead to economic energy conversion and utilization devices in the 200-600°C range.

Relevance and Potential Impact

The novel membrane assemblies that result from the proposed work would have an impact most directly on the applied DOE programs in Fossil Energy, Energy Efficiency, and Renewable Energy. These membrane assemblies include:

- *proton membranes* for PEM fuel cells, hydrogen separation and purification, hydrogen sensors;
- *oxygen ion membranes* for low-temperature SOFCs, electrolyzers, partial oxidation and reforming of hydrocarbon fuels, contaminant removal, and oxygen sensors;
- *mixed-conducting membranes* for hydrogen separation/purification, oxygen separation, reforming/partial oxidation of hydrocarbons (e.g., methanol); and
- *membrane-electrode* assemblies (MEAs) for increased efficiency and reduced cost of fuel cells, batteries, hydrogen separation/purification, oxygen separation, reforming/partial oxidation of hydrocarbon fuels, contaminant removal, gas sensing, and other processes relevant to energy storage and conversion.

Estimated Time Scale

10-20 years for full theory development, with first practical payoff within 5–10 years.

DESIGNED INTERFACES

EXECUTIVE SUMMARY

The utilization of hydrogen- or carbon-containing fuels in electrochemical systems depends critically on the properties of interfaces that need to fulfill specific and often conflicting functions. Among these functions are structural, dimensional and chemical stability; rapid electron, ion, and mass transfer; and catalysis or electrocatalysis; all under a wide range of temperature, temperature changes, and gas partial pressures variations. This multitude of interactive factors vastly complicates the fundamental understanding of interface processes in electrochemical energy conversion devices and hinders the development of practical and economic fuel cells. The direct predictive first-principles computation of the responses of an electrochemical interface to input variables which includes factors such as chemical composition and ionic and electronic conduction, is likely to remain intractable. Yet, progress in this field could be dramatically accelerated if means were created to combine phenomenological and computational interface theory with experimental data. The neural network approach to this complex problem is envisioned to offer the possibility of pointing the way to novel interface concepts, of which the expected properties may be at least qualitatively if not quantitatively predicted.

As improved theories mature, and the reliable experimental database expands, the predictive capability of the neural net can be expected to expand from small excursions from known behavior to more speculative concepts. It is likely that nature of the various network nodes and their transfer functions will have to be modified from current models to be able to deal with the mix of theory and experiment. The construction of a dependable neural net for the expected properties of various interfaces in electrochemical systems can be invaluable in the design of such interfaces at all levels.

Summary of Research Direction

The neural network approach to problem solving evolved from attempts in the 1930's to understand and mimic cognitive processes. A network topology is constructed, inspired by the structure of biological neurons and their interconnections, consisting of input nodes that receive data; the transmission of these input data to hidden nodes via weighted interconnects; the evaluation of the all-weighted input data by a hidden neuron layer using various activation functions, which may be linear, non-linear, binary, or probabilistic; and an output neuron layer which produces the results by applying again some activation function to the weighted sums of the outputs of the hidden nodes. The process is schematically illustrated in Figure 5-2.

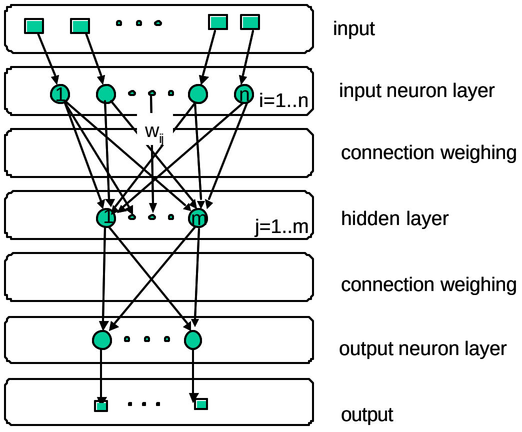


Figure 5-2. Schematic of the basic neural network. All "input neurons" *i* are connected to all "hidden neurons" *j* by an interconnect *ij*, of which the importance *(i.e.* the weight wij) is adjustable.

The "knowledge" resides in the weights of the interconnects. Thus, adjusting the weights w_{ij} to reach a known output from a defined input constitutes learning.

Neural networks in combination with fuzzy logic have been used successfully in optical pattern and in speech recognition. They have been applied to an increasing range of applications as diverse as banking failure prediction, mortgage credit approval, process management and control, hotel room pricing, and medical diagnosis. In materials development, the neural network approach has been successful (e.g., in the design of improved nickel-based superalloys for airplane engines and for power plant turbines).

New Scientific Opportunities

A neural network approach to the design of low-impedance interfaces and electrode surfaces with high electrocatalytic activity has not yet been attempted. The construction of such a neural network would require innovation in the integration of existing and new theory of electrochemical interfaces with extensive reliable data sets obtained from well-characterized interfaces. Initially, problems may be formulated such as the alloying of a nickel surface to reduce its sensitivity to sulfur poisoning, minimally compromising its catalytic activity for hydrocarbon oxidation.

Relevance and Potential Impact

The potential impact of a predictive neural network approach to design electrochemical interfaces would be far-reaching, providing accelerated development of practical fuel cell systems, hydrogen generators, and related devices under active consideration in the DOE programs on Fossil Energy, Energy Efficiency, and Renewable Energy.

Estimated Time Scale

This new enterprise may reach maturity in 10-15 years, with significant practical results generated as it evolves.

Transportation Energy Consumption

Integrated Quantitative Knowledge Base for Joining of Lightweight Structural Materials for Transportation Applications

Vehicular Energy Storage

Fundamental Challenges in Fuel Cell Stack Materials

Integrated Heterogeneous Catalysis

Thermoelectric Materials and Energy Conversion Cycles for Mobile Applications

Complex Systems Science for Sustainable Transportation

INTEGRATED QUANTITATIVE KNOWLEDGE BASE FOR JOINING OF LIGHTWEIGHT STRUCTURAL MATERIALS FOR TRANSPORTATION APPLICATIONS

EXECUTIVE SUMMARY

Although the use of new strong light-weight alloys, composites and other materials in vehicles will reduce consumption of fuel and reduce emissions, the maximum benefit from the use of these materials cannot be achieved without a detailed, quantitative knowledge base of how materials transform and behave under the extreme conditions characteristic of joining processes. Spatial and temporal gradients of temperature, composition and structure are a common result of materials joining. The component physical processes depend strongly upon the materials system and the joining process. While various component physical processes of materials joining have been modeled individually in metallic and, to a far lesser extent, nonmetallic systems, integration of these individual models is needed to predict the results of joining. This is typically a very highly complex process. For example, in metallic systems, the component physical processes in fusion welding include heat transport from a source such as a laser beam, a plasma arc, or an electron beam to the materials being joined; the fluid flow, heat transfer and mass transfer in the liquid region; the absorption and desorption of gases; the vaporization of alloying elements; solidification and phase selection processes; and solid-state transformations. Each of these processes has been modeled with various degrees of quantitative fidelity, but no integrated model exists. In another example, for the joining of certain important ceramics, a process such as diffusion bonding may be used where thermal diffusion and interfacial phase formation are important to joint strength and toughness. Joint interfacial reactions also play an important role in affecting joint integrity in other materials. The ability to incorporate advanced materials into future transportation systems will be greatly enhanced by an integrated predictive capability for joint geometry, microstructure and chemical composition to address such critical issues as strength, reliability, manufacturability and cost of the structure that contains the joint. The broad scope of this quest will require contributions from several scientific disciplines and will require coupled experiments and predictive modeling. During integration of the various component models, new scientific opportunities will arise at the crossroads of basic and applied sciences. Direct benefits of the work will be the easier incorporation of advanced materials into transportation systems with attendant lower costs and improved reliability in mass-produced structures. Alternate repair strategies can also be easily explored.

Summary of Research Direction

Defect free, structurally sound and reliable joints are often fabricated by empirically adjusting variables through trial and error. Although this practical approach often produces an acceptable end result, it ignores the potential competitive technological advantage that is attainable through fundamental understanding of the underlying science. Furthermore, the ranges of variables chosen empirically do not always produce optimum results.

Predicting and controlling joint geometry, composition, structure and properties are difficult because the joining processes are highly complex and the fabricated joint is compositionally and structurally non-homogeneous. For example, in metallic systems, the component physical processes in fusion welding include heat transport from a source such as a laser beam, a plasma arc, or an electron beam to the materials being joined; the fluid flow, heat transfer and mass transfer in the liquid region; the absorption and desorption of gases; the vaporization of alloying elements; solidification and phase selection processes;

and solid-state transformations. In another example, for the joining of certain important ceramics, a process such as diffusion bonding may be used where thermal diffusion and interfacial phase formation are important to joint strength and toughness. Joint interfacial reactions also play an important role in affecting joint integrity in other materials. In addition, the fabricated joints typically contain spatial gradients of composition, structure and properties. These special features of the joints, and the diversity of the simultaneously occurring component physical processes in joining, make the prediction and control of joint properties a highly complex venture.

Recent advances in computational hardware, software and numerical models have made many complex processes tractable. In the field of fusion welding, significant progress has been made in the numerical modeling of several important component physical processes. These include formulation and testing of models of heat transfer, fluid flow and thermal cycles, mostly for simple geometry; numerical simulation of grain growth and phase transformations in some alloys; and calculation of residual stress and deformations. In addition, numerical models to avoid formation of simple defects such as porosity have also been proposed and tested. However, many of these models are fairly complex and computationally intensive. Furthermore, the component physical processes have not been synthesized into a single comprehensive model. The ability to predict joint geometry, microstructure, chemical composition and properties will greatly enhance the quality, reliability and serviceability of structures that contain the joints.

The broad scope of this quest will require contributions from several scientific disciplines and will require coupled experiments and predictive modeling. The constituent sub-models may or may not be phenomenological in nature, depending on the materials system and complexity. For example, a phenomenological approach is often adapted for the representation of heat transfer, while a neural network type model has been more successful for the prediction of mechanical properties of joints. During integration of the various component models, new scientific opportunities will arise at the crossroads of basic and applied sciences. Direct benefits of the work will be the easier incorporation of advanced materials into transportation systems with attendant lower costs and improved reliability in mass-produced structures. Alternate repair strategies can also be easily explored.

New Scientific Opportunity

As a result of significant advances in computational hardware and models, opportunities now exist to integrate numerous important constituent models into a usable knowledge base for predicting the response of new materials systems to a selected joining process. While many component physical processes of materials joining have been modeled individually in metallic and non-metallic systems, integration of these individual models is needed to predict the results of joining, typically a very highly complex process. The interdisciplinary nature of the task will require synthesis of knowledge from various disciplines such as plasma physics, thermodynamics, chemistry, materials science, transport phenomena, and various engineering fields such as mechanical, chemical and electrical engineering.

Relevance and Potential Impact

An important component to achieve energy efficiency in the transportation sector is the replacement of traditional structural materials by lighter and stronger materials, which results in direct reduction in energy use. Although the proposed research direction in joining will benefit the transportation sector, its impact will also be realized in all segments of applied energy programs where joining of structural materials is important. These applied energy programs include fossil, nuclear, energy efficiency, renewable energy and fusion.

Estimated Time Scale

As component models are synthesized into large comprehensive models, there will be progress toward a science-based prediction and control of composition, structure and properties of joints. Achievement of this challenging but realistic goal, an important milestone in the advancement of joining technology, is well within the reach of the research community, provided adequate resources are available. It is expected that the benefits of the work will be fully realized in several decades.

VEHICULAR ENERGY STORAGE

EXECUTIVE SUMMARY

High energy-density storage materials will be needed if strategic energy goals are to be satisfied for the transportation sector. Unlike stationary demands, mobile requirements dictate both high volumetric and gravimetric energy density. At present, the transportation sector is almost totally dependent on petroleum fuels for its energy needs as they satisfy the principal need of high energy density. Attempts to replace petroleum fuels with other sources of readily transportable and abundant energy have met with limited success, due principally to the inability to store on-board a vehicle, sufficient quantities of the alternatives to provide vehicle performance that is competitive with petroleum fuels.

Among the candidate energy carriers, hydrogen and electricity are two that can satisfy the abundance requirement but which are low in energy density.

Hydrogen sorbents and hydrides may offer a means of obviating high pressures and/or low temperatures to attain higher volumetric and gravimetric energy densities. In fact, metal hydrides are presently capable of volumetric densities greater than that of liquid hydrogen, but fall short of the requirements for high gravimetric density. In order to satisfy gravimetric energy density requirements, sorbents based on low atomic number (Z) materials will need to be used. Our present knowledge of known stable hydrides, based on low Z materials that serve as suitable candidates for gravimetric and volumetric hydrogen storage, is limited to systems with thermodynamic and kinetic barriers that are too high to be of use to the transportation sector. Such systems may also suffer from irreversible hydrogen cycling limitations. Systems based on complex hydrides can offer possibilities for high volumetric and gravimetric storage but are poorly understood. For example the $NaAlH_4$ system, which is closest to engineering realization, has multistep hydride/dehydride reactions with differing kinetic and thermodynamic values. These are only realized in the presence of a dopant (catalyst) with a poorly understood role. This circumstance makes the understanding of hydride materials an imperative if new materials are to be developed for attaining the goal of hydrogen-fueled vehicles.

In the near term (5-10 years), it is expected that batteries possessing enhanced energy and power densities as well as lifetimes will be needed to enable hybrid/electric vehicles having performance characteristics comparable to conventional internal combustion (IC) engine/petroleum fueled vehicles. Present state-of-the-art technology using Li batteries offers the highest energy densities [twice that of NiMH batteries that are used in hybrid and electric vehicle (EV) technology] and cycle life, but the components, including cathode, electrolyte and separator, are costly. Provided improvements to energy density over current Li technology can be made, batteries might still be used as the primary power source for a pure electric vehicle. In any event, high energy density systems with high cycle life will still be necessary. Even for hybrid technology, batteries are a vital part of the overall power system for hybrid vehicles that utilize regenerative braking. Candidate systems based on Li battery technology offer the highest known energy densities available, but these systems still fall short of automotive design goals that would make such vehicles competitive with petroleum-based systems. An effort to better understand and design suitable cathodes, anodes and separators for Li batteries would benefit the transportation sector as well as the area of portable electronics.

Summary of Research Direction

A research direction based on the study of the thermodynamics, kinetics and phase stability of energy storage materials is proposed. These basic scientific issues are germane to the two specific areas we highlight below for hydrogen storage materials and batteries.

Hydrogen Carriers. The DOE's technical targets of 6 wt% (7.2 MJ/kg energy density) gravimetric storage and 1100 Wh/L (4 MJ/L energy density) volumetric storage for hydrogen systems for transportation applications illuminate the scientific and technological gap in establishing fuel cell viability for commercial markets. The current state-of-the-art energy storage technology can be categorized broadly into physical and chemical storage. Physical storage would consist of cryogenic systems and high-pressure tanks. Liquid hydrogen and compressed hydrogen systems presently fall short of the minimum performance goals (>6MJ/kg and >6MJ/L) sought after by the transportation sector and fall far short of the ultimate technological gravimetric and volumetric target goals (>12MJ/kg and >12MJ/L). From a refueling standpoint, these systems are extremely inefficient. For example, hydrogen liquifaction consumes an equivalent of 30% of the energy density of liquid hydrogen itself (to get to 20 K). Also, multistage compressors are required to achieve the high pressures (690 bar or 10,000 psi) for the compressed hydrogen systems that are being developed.

Chemical storage systems, which would include hydrogen sorbents or hydrides, may offer a means of obviating these inefficiencies by allowing high gravimetric and volumetric energy densities at non-cryogenic temperatures. For example, MgH_2 has a density of 1.45 g/cc or 0.11 g(H_2)/cc. This material thus has a gravimetric density of 7.66 wt% (9 MJ/kg of MgH_2, materials basis only) and 110 kg/m^3 (13 MJ/L). Unfortunately, Mg dehydrides at too high a temperature to be a practical source of hydrogen for vehicular applications (~600 K). To work with presently available fuel cell proton exchange membranes, the desorption temperature would need to be closer to 350 K. In any event, rehydriding is also problematic for MgH_2. At present, Ti-catalyzed $NaAlH_4$ shows potential as a storage material but again falls short in gravimetric density (5.6 wt% or 6.7 MJ/kg materials basis).

Hydrogen physisorption might also work for storage applications but, to be of use for vehicular applications, will require an adsorption enthalpy of 20 to 40 kJ/mole (~200 to 400 meV), if sorbent dehydriding/hydriding near ambient temperature and moderate pressures is to be achieved. In addition, physisorption will require effectively high surface area materials that have a suitable number of adsorption sites to accommodate molecular hydrogen.

If the criterion of high volumetric density was the only concern, a number of metal hydrides would work. The concomitant requirement of high gravimetric density restricts the possible hydride candidates to a limited portion of the periodic table or alloy/chemical constituent components. To date, though, few systematic efforts have looked into suitable candidate materials. The payoff from systematic efforts can be seen when considering that $NaAlH_4$ was discarded as a candidate material because this material was regarded as too volatile and with too low a melting point before hydrogen was released. Over 20 years later, however, it was discovered that a Ti catalyst added to $NaAlH_4$ could promote the kinetics of dehydriding while the material was still in the solid state, bringing it to the point of engineering viability [B. Bogdanovic and M. J. Schwickardi, J. Alloys Compd. 253, 1 (1997)]. At present however, the role of this catalyst is still unknown.

The choice of candidate sorbents or hydrides can be reduced further on the basis of free energy and heat of formation data (thermodynamics) to systems that can operate over temperatures of engineering interest. Applying information gleaned from the JANAF Thermochemical Tables is helpful but understanding multicomponent systems may also require information not yet available but possibly calculable. For instance, Miedema heats have been used to understand the behavior of AB_5 hydrides, and their utility in other systems should be established in order to limit the phase space of elements and compounds deemed suitable for vehicular applications. Furthermore, the kinetics of dehydriding and rehydriding will also be important in addressing fuel uptake and refueling. Finally, issues related to the cycle life of the sorbent or hydride (phase stability) need to be addressed.

Batteries. Lead-acid battery technology, which was developed nearly 150 years ago, is still being used for vehicular applications. These batteries have a gravimetric density of 0.16MJ/kg and 0.25 MJ/L. Ni-metal-hydride batteries have gravimetric and volumetric energy densities nearly twice that of lead-acid, and Li batteries (0.5MJ/kg and 1MJ/L) have values twice that of NiMH. The United States Advanced Battery Consortium has set a long-term goal of 0.72 MJ/kg energy density. At present, it is difficult to imagine improving on the energy density of Li batteries unless improvements to cathodes (typically $LiCoO_2$) are found. Incremental improvements are on the horizon through partial substitution of Co by Ni yielding ~15% improvement in charge capacity (resulting from the phase stability of $LiNi_{0.8}Co_{0.2}O_2$ to retain a stable phase to discharge levels to $Li_{0.4}$). Longer term goals aimed at improving energy density in Li batteries should consist of studying Li insertion/de-insertion kinetics and phase stability of both cathodes and anodes in non-Co based materials. Also, Li-based systems have specific charge/discharge requirements requiring specialized electronics designed to control limits and rates for each cell of a battery pack. Cathodes and anodes that offer the possibility of higher robustness to high discharge rates and overcharging may allow for the simplification of Li-based systems. For instance, Li_2S-based systems demonstrate such robustness and have shown capacities as high as 0.65MJ/kg. A combination of doubling of the energy density of Li secondary (rechargeable) batteries in conjunction with robust cathode/anode systems would be the enabling factors in implementation for the transportation sector as well as offer huge benefits for other sectors like portable electronics.

New Scientific Opportunities

The issues surrounding all high energy density materials fall within the traditional scope of BES in addressing the thermodynamics (temperature), kinetics (hydriding/dehydriding and charge/discharge rates) and phase stability (cycle life) of materials. A focused basic research effort into materials of specific interest for high energy density would greatly benefit those areas with specific technological goals for vehicular applications.

Relevance and Potential Impact

The *National Hydrogen Roadmap* calls for a coordinated national program to advance hydrogen storage materials as no current technology satisfies the storage criteria of manufacturers and end-users. Current research and development efforts are cited as insufficient as storage is noted as a critical enabling element in the hydrogen cycle. While technical goals are easy to identify, fundamental improvements in hydrogen storage processes remain to be fully understood. Developing this understanding should be the long-term goal and a necessary step before the challenges of addressing technical goals is met.

Estimated Time Scale

A coordinated effort over a period of ~10 years is likely required to meet the challenges outlined here.

FUNDAMENTAL CHALLENGES IN FUEL CELL STACK MATERIALS

EXECUTIVE SUMMARY

Offering enormous potential for high-efficiency, pollution-free propulsion, fuel cells (FCs) are of great interest in the transportation sector. The PEMFC is the leading candidate for the primary power source in FCEVs, with hydrogen as the fuel and water and heat as the only by-products. SOFCs are under consideration as auxiliary mobile power units in heavy-duty trucks. While considerable progress has been made in moving FCs closer to economic viability, many major scientific and technological hurdles remain. A hand-built prototype PEMFC presently costs thousands of dollars per kilowatt. Elimination of the hurdles will allow dramatic cost reductions, which will, in turn, hasten large-scale commercialization of FCEVs.

Among the technical challenges are a variety of materials issues related to the FC stack, the array of individual cells linked in series to form a power unit. For PEM stacks the needs include cost reduction, simplified heat, air and water management; higher efficiency; and improved reliability and durability. These objectives may be achieved through research in high-temperature and low-relative-humidity membranes, modeling and diagnostics, improved cathode kinetics, base-metal CO-tolerant catalysts, and improved bipolar plate materials. For SOFC stacks the critical issues are thermochemical integrity and reliability, interconnect durability and performance, power density enhancement, and direct reformation of hydrocarbon fuels. All of these challenges can be addressed through fundamental materials research focused on new membranes, bipolar plates, electrodes, and electrolytes, coupled with theoretical modeling to accelerate their design and evaluation.

Summary of Research Direction

FCEVs represent a potent option in the portfolio for meeting the future transportation needs of the U.S. Despite significant advances in FC technology over the past few decades, however, many fundamental scientific and technological barriers stand in the way of large-scale commercialization for mobile, as well as fixed station, applications. Associated with the FC stack itself are a variety of basic materials research challenges that can be addressed by a sustained and coordinated effort. For the cost per kilowatt to be reduced sufficiently to enable widespread use of FCs and FCEVs, novel materials having improved properties for FC stacks must be discovered, developed, and understood.

New Scientific Opportunities

PEMFC stacks. In view of its advantages with respect to energy efficiency, emissions, and feedstock diversity, the PEMFC is the leading option as the primary power source in FCEVs. Fueled with hydrogen (having a spectrum of possible production methods), the PEMFC can operate at average efficiencies twice as high as today's internal combustion engines, with water and heat as the only by-products. Large-scale commercialization of FCEVs, however, will require dramatic reduction of the cost of the FC stack, which is a critical issue dependent upon groundbreaking fundamental research on a number of fronts for resolution. These include:

- High-temperature membranes. Fuel and air streams in current systems, operating at ~80ºC, must have relative humidity (RH) at about 100% to maintain high conductivity in the membrane and catalyst layers. Substantially improved system efficiency (stack, and water and heat management) could be achieved with higher operating temperature (~120ºC), but a 120ºC system is not feasible with available membranes because of excessive pressure and water recirculation demands. Membranes capable of sustaining ~0.1 S/cm conductivity at RH ~ 25% and 120ºC are required. Specific research topics in this regard are (1) new proton/anion conductivity mechanisms not dependent on high RH, (2) new membranes/polymers with improved *ex situ* properties (i.e., conductivity, hydrogen/oxygen permeability, mechanical robustness) for high temperature application, (3) improved basic understanding of membrane chemical degradation in a high-temperature FC environment, and (4) studies of polymer interaction with other FC components (e.g., the effect of new ionomers in contact with catalysts on cathode kinetics).

- Stack modeling and diagnostics. Materials and stack design have been done empirically thus far. There is a genuine paucity of predictive models for flow-field and current-density distribution as well as methods to measure key component properties. Computational fluid dynamics (CFD) models have not yet had an impact on design because of excessive computation times and lack of verification. The effects of liquid water are poorly understood, the nature of flooding is unclear, and there is insufficient knowledge of water transport in diffusion media and flow fields. Relevant research topics are (1) liquid water formation and transport in porous media and through FC channels, (2) measurement of membrane electrode assembly properties (proton conductivity, gas permeance, current density, kinetics, interfacial and bulk thermal conductivities as functions of pressure), (3) novel characterization techniques that will enable broader insight, and (4) development of useful CFD models.

- Improved cathode kinetics and improved CO-tolerant catalysts. Major stack efficiency losses, causing heat rejection problems, are associated with poor cathode catalyst kinetics. There is a critical need for low-cost, non-noble metal catalysts and catalyst localization techniques. Also, anode CO tolerance also requires fundamental catalyst development.

- Improved bipolar plate materials. Currently the thickness required for carbon/polymer composite plates to have sufficient physical stability and durability is too large, resulting in volumetric energy density too low for automotive use. These high-carbon-content materials entail expensive processing and are brittle. Available metallic plates (e.g., stainless steels, titanium) are sufficiently thin (~0.1 mm), but noble-metal conductive coatings are needed for low contact resistance. In some cases corrosion of the plate substrate and the coating is an issue. Novel and economically feasible plate materials that overcome these challenges are imperative.

SOFC stacks. Current SOFC prototype stacks operate at 750-1000ºC and have potential as auxiliary power units functioning at high overall efficiency in mobile applications. Major challenges confronting stack performance and operation are (1) thermomechanical integrity and reliability of a complex structure, (2) interconnect durability and performance, (3) intrinsic power density, and (4) direct reformation of available hydrocarbon fuels.

These challenges can be addressed through advancements in new electrodes and electrolytes having substantially higher electrochemical activity and intrinsic power density, thus allowing for reduction in operating temperature and alleviating the challenges associated with mechanical durability and interconnect degradation. Cathode materials have improved only slowly over the past two decades, progress having been achieved through intensive semi-empirical investigations of narrow classes of materials. Rapid further advancements require a fundamental understanding of oxygen adsorption and transport in the cathode and at the cathode/electrolyte interface. The effect of materials composition can be probed with real-time *in situ* interrogation of these surface and bulk phenomena using surface diagnostic tools, augmented by electrochemical characterization. Improved understanding of the effects of surface features and local chemistry in both real and model electrode materials can spur rational design of new cathode compositions. In addition to fundamental studies of oxygen reduction, computational chemistry can be employed to predict the effects of various materials combinations and crystal structure on the electrocatalytic reduction of oxygen. Combinatorial methods for preparing and screening samples having compositions selected with the guidance of model predictions can enable accelerated testing, evaluation, and discovery of radically improved materials. Novel compositions with optimized microstructure could be fabricated by means of emerging synthesis/deposition techniques, and possibly self-assembly of tailored porous microstructures as well, to promote high electrochemical activity. Close coupling of predictive electrochemical modeling tools with formulation and testing of new oxide electrode materials can provide fundamental understanding of the roles played by microstructural features and chemistry and speed the design of materials with better performance.

Similarly, the design of new functional anode systems must be based on an improved understanding of fuel oxidation kinetics in porous ceramic and ceramic-metal composite systems. Improved anode systems could help meet key challenges to anode performance, including the need for direct fuel oxidation or *in situ* fuel reformation and tolerance to fuel impurities. With improved electrodes, there will be an increasing need for electrolytes characterized by high ionic conductivity at lower temperatures. As outlined in the approach to electrode understanding and design, computational chemistry tools and combinatorial synthesis capability can also be harnessed to design new and better electrolyte materials.

Relevance and Potential Impact

Current industry and DOE (FreedomCar, Hydrogen, and Fossil Energy) programs are generally aimed at component and system hardware demonstration, along with core technology development for stacks or balance-of-plant. This proposed research direction on stacks through BES is aimed at addressing the more fundamental materials and surface issues governing electrochemical performance, using both experiment and modeling. The understanding of electrochemical transport through membranes and interfaces, and new materials and mechanisms developed under this program, should directly feed into the applied programs funded by DOE and industry, helping to accelerate the pace of FC penetration in transportation, and stationary applications.

Estimated Time Scale

A sustained effort in fundamental research over a period of ~10 years is likely required to meet the challenges outlined here, and enable the transition to FC powered vehicles over the next two decades.

INTEGRATED HETEROGENEOUS CATALYSIS

EXECUTIVE SUMMARY

Catalysis currently plays a significant role in the economic and strategic needs of the country. More yearly Gross Domestic Product (GDP) is produced from catalysis in the U.S. than the entire GDP of most developed nations. In particular, catalysis has and will continue to play a central role in the transportation sector, a sector that will have a considerable impact in determining our nation's future energy security. The needs for fuels synthesis and storage, for efficient fuels utilization, and for environmental mitigation of the deleterious effects of transportation on our environment are enabled through fundamental catalysis research.

The development of novel catalysts and catalytic processes for energy security applications is hampered by the lack of detailed structure-function relationships that serve to drive the development of a predictive capability for new catalyst process concepts and in catalyst materials design. Such new processes and materials will have an impact on future choices in transportation fuels and for efficient fuel utilization processes. Therefore, it should be a national priority to foster and support an integrated world-leading, vibrant and dynamic research infrastructure in catalysis. Such an infrastructure must necessarily involve highly integrated cross-disciplinary thrusts that take advantage of existing, emerging, and new structural tools; computational modeling and simulation techniques; experimental and theoretical reaction pathway modeling; and data fusion techniques that merge the output from these disparate sources into a coherent, predictive description of heterogeneous catalyst structure and activity. For example, the expected impacts of catalysis research for the transportation sector range from catalysts and processes for the abatement of lean-burn internal combustion engine exhaust in the short-term to the longer term developments directed at the rational design of catalysts that will enable the synthesis and utilization of future fuels for combustion, fuel cells, and other yet-to-be-discovered energy production concepts for vehicular and aircraft propulsion. The need to minimize the environmental impacts of any new energy production technologies also argues for a continued fundamental science research emphasis on catalytic emission control processes. Many of the short-term technological goals of the 5-10 year time frame map onto current 'FreedomCar' initiatives (DOE EE/RE). The longer term scientific goal of an integrated research infrastructure in catalysis to support the transportation sector falls to DOE's Office of Science (OS), and is the primary focus of this brief report.

Summary of Research Direction

The development of novel catalysts and catalytic processes for energy security applications is hampered by the lack of detailed structure-function relationships that serve to drive the development of a predictive capability for new catalytic process concepts and for the design of new catalyst materials. Such a predictive capability will have an impact on future choices in transportation fuels and fuels utilization processes.

A number of recent BES workshops have identified the importance of catalysis to the economic and environmental well being of the U.S., and the reader is directed to the reports that have been issued or will be issued in the near future. Historically, catalysis has been driven by the preeminence of the U.S. chemical and petrochemical industries, where catalysis is a core technology. The linkage between catalysis and transportation is crucial and will continue to be so into the foreseeable future. Catalysis is a central technology to the current atom- and energy-efficient production of today's hydrocarbon fuels from petroleum and emerging low-sulfur diesel fuels from natural gas, the abatement of undesirable emissions resulting from the utilization of these fuels, and the synthesis of lubricants for vehicles. Catalysis also plays a central role in fuel cell technology (both low temperature electrocatalysis in polymer electrolyte fuel cells for mobile applications and catalysis of high-temperature processes in solid oxide fuel cells proposed for auxiliary power applications in heavy vehicles). In this way and in many others, catalysis will be an enabling technology for a possible future 'hydrogen economy'.

For transportation, heterogeneous catalysis is one of the key cross-cutting technologies for which the underpinning fundamental science needs are highly compelling. The focus on heterogeneous rather than homogeneous catalysis was arrived upon by the particular needs of vehicular application or the need for the very large-scale processes needed to provide for fuels of the future.

The short-term needs for catalysts in the transportation sector are at some level being partially addressed by DOE's EE/RE FreedomCar programs. For example, applied research to address the abatement of pollutants, such as NO_x and particulates from lean-burn internal-combustion engines using both catalytic and plasma-based approaches, are currently funded at some level by DOE EE/RE. Importantly, however, as pointed out in several recent National Research Council reports and reports prepared for the Office of FreedomCar and Vehicle Technology related to heavy-duty engines, the current technology options are still inadequate to allow for the introduction of these fuel-efficient engines into the U.S. economy, particularly because the pollutant targets become more aggressive entering the next decade. These reports continue to stress the need for increased investments for fundamental science that enables breakthroughs in emissions abatement to enable reductions in the energy intensity of the transportation sector.

Short- to medium-term applied research sponsored by EE/RE on the optimization of electrocatalysts for PEMFC stacks is also well underway in the U.S. Here again there are many fundamental catalysis science issues that need to be addressed to move these technologies forward. Of perhaps primary importance, however, are longer-term fundamental research needs that must be met for advanced transportation systems that are beyond the time horizons of DOE's technology offices, and fall within the boundary of DOE's OS. It is the latter longer-term catalysis research that the topical team focused on.

Broad areas (both short- and long-term) of catalyst science needs for advanced transportation systems were identified:

- catalysts for the generation of H_2 (either photocatalysts, electrocatalysts, or thermocatalytic systems);
- chemical and biocatalysts for the generation of liquid fuels from natural gas and biomass;
- catalysts for the synthesis of tailored, high-energy-density napthenic fuels for the aviation sector;
- catalysts for reducing emissions from high-efficiency lean-burn combustion engines;
- catalysts to enable rapid H_2 uptake and release in high-energy-density hydrogen storage materials; and
- electrocatalysts, particularly oxygen reduction catalysts having improved O_2 reduction kinetics, for improved fuel cells for transportation.

Because catalysis science is a crosscutting area, it is not surprising that the Fossil Energy and the Distributed Energy, Fuel Cells, and Hydrogen Topical Groups also addressed several of these areas in more detail, and those interested in the role of catalysis in those topical areas should refer to those sections of this workshop report.

Today, it is not uncommon for practitioners of homogeneous catalysis to have considerable knowledge of the orientation of ligands, bound substrates, intermediates, or products to a metal center using a combination of nuclear magnetic resonance, infrared, and other spectroscopies. If this complex is not *the* active catalyst but rather a precatalyst, it is often very closely related compositionally or structurally to the active catalyst. This information allows for a rapid assessment of the influence of the subtle changes in steric and/or electronic structure effects, not only by rational modification of the ligands on catalyst reactivity, but also by more detailed theoretical modeling and simulation of the molecular and electronic structures of the active catalyst. Structural knowledge of enzymes has led to bioinspired synthetic homogeneous model systems that in turn, have helped to guide interpretation of the spectroscopic signatures observed during complex enzyme catalysis. The field of heterogeneous catalysis does not share these luxuries afforded by a detailed knowledge of the local structural details of a heterogeneous catalyst.

The last decade of heterogeneous catalysis research has led to advances in theory and experiment that have moved the field of catalysis incrementally closer to the much sought-after *de novo* design of heterogeneous catalysts. More recently, high throughput experimentation has improved the rate at which catalyst compositions may be varied and tested, driving the data-driven design of catalysts forward. Concepts of homogeneous– and bio–catalysis have inspired new heterogeneous catalyst synthesis efforts. New methods of catalyst characterization have emerged that allow more insights into catalyst reactivity. Theoretical approaches have been able to provide hints and guidance to some problems in catalysis, albeit based upon scant structural evidence. These are all efforts that have been ongoing, and have been providing glimpses of the workings of active catalysts.

New Scientific Opportunities

The continued lack of *detailed* knowledge of catalyst structure under realistic operating conditions has hindered catalysis science from making great strides forward in the development of a predictive understanding of the complex behavior of heterogeneous catalysts. So what has changed that leads us to believe that there are new scientific opportunities in this field? Why now? The key barriers to developing this understanding are the need to develop detailed knowledge of the *local* structure of the catalytically active site [the constituents at the active site(s) and their spatial arrangement at the atomic and molecular levels], the manner in which substrates and products interact with the active site, the temporal nature (activation, deactivation, and poisoning) of these interactions, and a detailed description of the overall reaction pathway(s). Detailed *local* structural information through an integrated approach would provide the necessary input to modeling and simulation tools that even at present can provide a good deal of insight where experiments are as yet unable to yield information directly. The development of new and emerging approaches to local structure determination have profited from the excitement for nanoscience and properties related to nanoscale entities over the last several years. Improvements in a variety of techniques and development of wholly new approaches to the study of materials properties have spawned emerging capabilities in structure determination of highly disordered or differently ordered systems, where the length scales of the important interactions are on the order of nanometers)the same length scale that has always been central to heterogeneous catalysis). Improvements in synchrotron X-ray sources and techniques;

local structure by neutron scattering brought about by brighter sources; new and vastly improved surface science techniques, such as scanning tunneling microscopy (STM); new solid-state NMR approaches to measure interatomic distances or temporal phenomena; and ever-improving computational capabilities that have enabled new simulation and modeling techniques are all poised to yield integrated new capabilities that can be brought to bear on complex, catalyst systems that to date have defied structural definition.

Because catalyst materials and processes are so complex, breakthroughs in catalysis will follow from an integrated approach. These breakthroughs will support development of efficient processes that generate, store, and utilize fuels for our future energy security. No single technique is capable of this task, and multiple particle-, photon-, or neutron-based, and advanced spectroscopic techniques must be brought to bear simultaneously on a catalyst system. Data from these disparate techniques and the observed reaction chemistry must be analyzed in a coherent fashion to yield a self-consistent depiction of the catalyst structure and dynamics. This will require new computational techniques with greater accuracy to allow for the integration with high fidelity of data from the various techniques. Improved and new theoretical approaches must be developed to allow for the interpretation, interpolation, and extrapolation of structure and properties when experimental techniques cannot access the needed data directly.

In the future, it is anticipated that new scientific developments, both experimental and theoretical, that allow for detailed descriptions of catalyst structure and dynamics under reaction conditions will have an impact on all aspects of catalysis research. In the transportation sector, the predictive capability generated by detailed structural information of reacting heterogeneous catalysts will have an impact on future developments in fuels synthesis (hydrogen, biofuels, etc.), energy storage (hydrogen, batteries), and fuels utilization (fuel cells) and will continue to play an important role in the mitigation of the environmental impacts of energy production and fuel utilization. The role of new experimental and theoretical approaches to defining the structure and properties of heterogeneous catalyst systems will have an impact on the fields of electrocatalysis and photocatalysis.

Major science needs for the future include:

- Further development of emerging and discovery of wholly new local structural tools that can probe the length scale of 0.1 to 2 nm.
- Developments that will allow the application of the techniques under realistic (in situ) catalytic reaction conditions, as well as applying multitechnique approaches for studies of active catalysts.
- Catalysis-related infrastructure (sample activation, *in-situ* reactivity studies, etc.) at DOE User Facilities, including catalysis end stations at beam lines and flight paths at X-ray and neutron sources and *in-situ* reactors for state-of-the-art surface science and NMR facilities.
- Computational models of the governing catalytic reactions and approaches to integration of structural and spectroscopic data from the above to yield self-consistent models of catalyst active sites, gas conversion and particulate oxidation.
- New nanoscale synthetic approaches that will allow generation of model active sites identified from knowledge achieved in the above pursuits.

Relevance and Potential Impact

Research will enable a considerably more secure energy future by providing fuel and fuel utilization options through more atom- and energy-efficient new catalysts and catalytic processes. It will have relevance to several applied DOE programs including the FreedomCar and Hydrogen Programs, Alternative Feedstocks for Fuels/Biofuels Programs, and Industrial Technologies Programs under EE/RE: Coal and Natural Gas Conversion Programs, Electric Power and Fuels R&D Programs (FE); and Science and Technology Programs (EM).

Estimated Time Scale

It will take approximately a decade to establish capability to fill the knowledge gaps.

THERMOELECTRIC MATERIALS AND ENERGY CONVERSION CYCLES FOR MOBILE APPLICATIONS

EXECUTIVE SUMMARY

Thermoelectric materials, in which heat can be transformed directly into electrical energy and that can act as solid-state heat pumps, have begun to be used in transportation systems. As such they have the capability to mitigate the energy loss in transportation systems associated with heat loss. At present, theoretical considerations suggest that automotive efficiencies could be increased by 20% simply by capturing the waste heat, an efficiency gain comparable to what would be obtained by converting the U.S. car and light-truck fleet to diesel engines, but without the penalty in NO_x or particulate emissions. In addition, thermoelectric materials will lead to an all solid-state, reversible automotive air conditioning system that does not use greenhouse gases and can be simpler and more efficient to operate. Realizing such gains depends on finding materials which behavior meets theoretical limits. These theoretical limits are rooted in the transport properties of materials, which in turn depend on their nanostructure and composition. For example, quantum wires and dots embedded in a suitable matrix appear to have greater potential for use in thermoelectric devices than alloys or other homogeneous materials. Prototypical systems built to demonstrate the above gains are likely to be realized in practice, again depending on the discovery of appropriate materials and the means for fabricating them. Recent new heat exchange cycles between the thermoelectric elements and the working fluids (i.e., exhaust gas, passenger compartment air, or liquids) have also been proposed that make optimal use of each thermoelectric element in a thermoelectric pile and can potentially lead to a substantial increase in system efficiencies.

Summary of Research Direction

A combination of environmental, economic, and technological drivers has led to a reassessment of the potential for using thermoelectric (TE) devices in several transportation applications. In order for this technology to achieve its ultimate potential, new materials with enhanced thermoelectric properties are required. Also, as each TE element is small, unconventional thinking in the area of new heat exchangers between the TE elements and the working fluids will lead to new TE energy generating and cooling systems. These will lead to further increases in efficiencies.

Thermoelectric materials convert heat into electrical energy with an efficiency that is a function of a material parameter defined as the thermoelectric figure of merit, Z. When used as solid state heat pumps in cooling systems, the coefficient of performance of the system (COP), defined as the ratio of the heat extracted at the cold side to the total energy consumed, is again a function of the same figure of merit Z. It is usual to express Z in dimensionless units by multiplying it with the average operating temperature, T. Commercially available thermoelectric materials have a dimensionless figure of merit, $ZT = \sim 0.9$ near room temperature. For a temperature difference of 40^{o}C, typical of an automotive air conditioning system, the COP is on the order of 0.25.

Recent engineering developments with cross-flow heat exchangers that make optimal use of the thermoelectric elements within the cooling modules more than double the COP that can be obtained with a material of a given ZT, and similarly could double the efficiency of TE generators. Even with this, the efficiencies and COP's that can be reached with commercial TE materials are still insufficient. Recently nanoscale thermoelectric materials have been demonstrated that have ZT=2. With such materials, refrigerator systems can be calculated to reach COPs competitive with vapor compression. Waste-heat recovery systems could theoretically reach 13% efficiency, potentially improving the mileage of vehicles by over 20%.

The above improvements in ZT are a direct result of recent progress in the understanding of electronic and thermal transport properties in two areas of solid-state physics: (1) semiconductor quantum wells, wires and dots, and (2) crystalline solids with low thermal conductivities. These transport theories may need further development, but they point to the possibility of further increasing ZT to 4 or even 6, resulting in COPs close to double that of vapor compression air-conditioning and waste heat recovery. This could result potentially in a theoretical increase in fuel economy perhaps larger than could be expected from increasing the use of diesel fuel systems in the U.S. fleet.

New Scientific Opportunities

Scientific research on new material systems which properties approach the theoretically predicted improvements should include nanocomposites and crystals with glass-like thermal conductivity. New concepts to synthesize the new materials in industrial quantities must be explored. New concepts for the optimal use of these materials in complete TE systems, in which segmentation of the thermocouples, the efficiency of the heat exchange with the working fluids, and the problems of making low-resistance contacts to the TE materials are paramount, will greatly improve the efficiency and the economics of heat recovery systems and air conditioners.

Relevance and Potential Impact

Heat recovery systems. In a gasoline engine, roughly two-thirds of the chemical energy of the fuel is wasted as heat, half in the engine coolant and half in the exhaust gas stream. An additional ~5% of the energy is wasted in friction losses and 2-10% goes to the alternator, leaving 15-35% of the fuel energy for propulsion. TE systems can directly and simply convert waste heat into electricity. There are two potential uses for this. In a conventional vehicle (see Figure 6-1), the TE generator can potentially unload the alternator, which (depending on the operating regime) utilizes 2-10% of the energy in the fuel. Assuming a reasonable system efficiency (i.e., 6-9%), a TE generator could supplant the alternator, producing a fuel economy improvement of 2% of the fuel energy or ~5-10 % in the vehicle's mileage.

In future vehicles with hybrid or electric propulsion (see Figure 6-2), the electrical energy saved can be used for propulsion. The efficiency of the TE generator now comes into play directly. With an ~10% conversion of waste heat to electricity, roughly 5% of the chemical energy of the fuel can be recovered. Assuming that, on average, only about 25% goes to propulsion overall, this represents a potential 5%/25% or ~20% improvement in fuel economy. Such benefits are comparable to those obtained by using diesel engines rather than gasoline engines, but without the environmental issues (i.e., NO_x and particulate emissions) associated with diesel technology.

Transportation R&D is a major component of the DOE's EE/RE program.

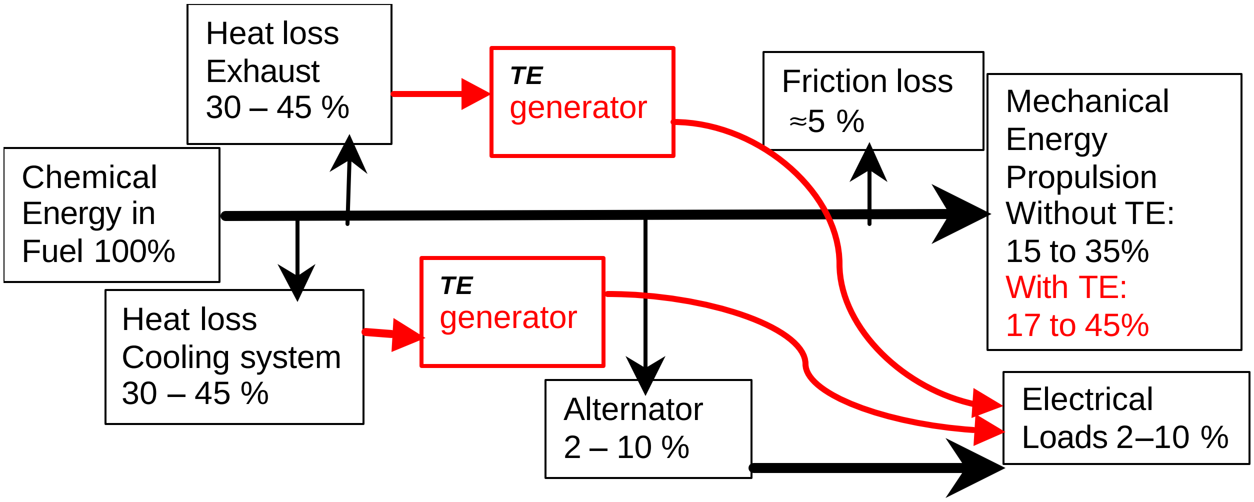


Figure 6-1. Energy use in a conventional vehicle (black lines). A thermoelectric generator (red line) can unload the alternator, leading to a fuel economy improvement of 4-10%.

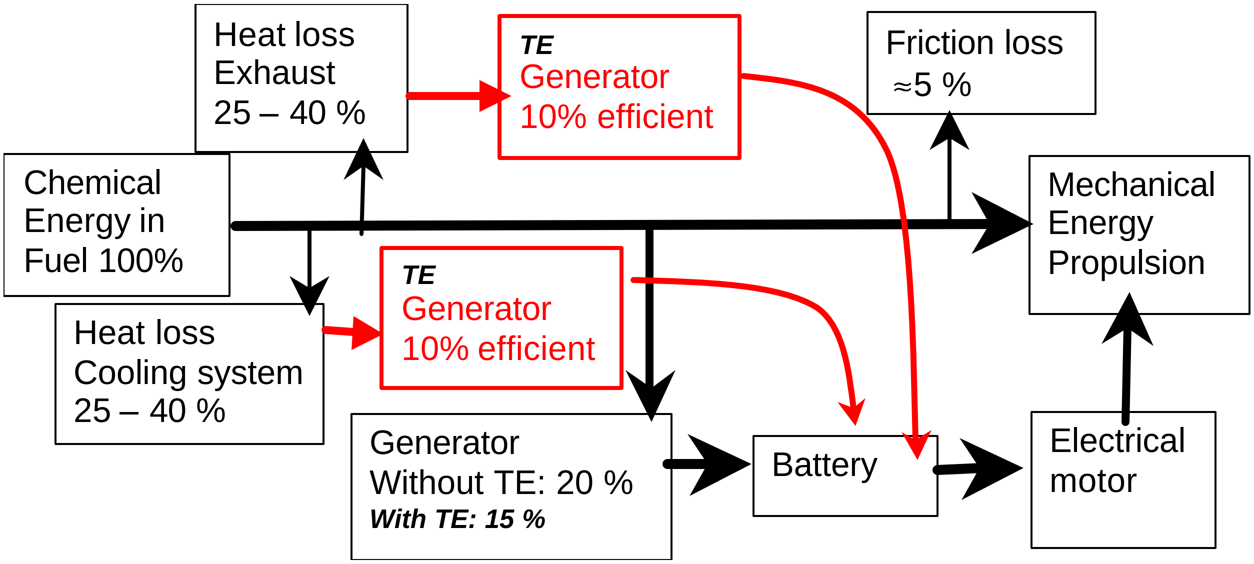


Figure 6-2. Energy use in a vehicle in which supplemental electrical propulsion is available (black lines). A thermoelectric generator (red line) can supplement the electrical generator, leading to a fuel economy improvement of up to 20%.

Climate Control. Thermoelectric climate control in automotive systems is attractive from the point of view of simplicity and environmental friendliness. In 1974 it was first suggested that chlorofluorocarbon compounds, principally R12, or freon (the refrigerant of choice in air conditioning systems for the last 50 years), were destroying the protective ozone layer in the stratosphere at an alarming rate. As a result, the Montreal protocol of 1987 has led to a gradual phasing out of these harmful chemicals. In their stead, non-chlorine-containing fluorocarbons, such as R134a, which do not possess the long-term stability of R12, have widespread use as refrigerants. It was not realized until quite recently, however, that all fluorocarbons, including R134a, can contribute to global warming. This is because these gases are capable of absorbing the infrared radiation the earth emits to stabilize its temperature. The infrared-absorbing capability of a gas is measured by its Global Warming Potential (GWP) index. The GWP index measures the absorption characteristics relative to that of CO_2, which is defined to have a GWP index of unity. The GWP indices of R12 and R134a are 8,500 and 1,300, respectively. In other words, 1 kg of R12 and R134a are equivalent to 8,500 and 1,300 kg of CO_2, respectively, in terms of their global warming impact. Thus even relatively small amounts of these chemicals released into the atmosphere (e.g., via leakage) can have serious consequences in the long term. In light of these sobering facts, it is natural to contemplate alternative cooling technologies, which might supplant vapor compression systems containing such chemicals. Thermoelectric cooling is one such alternative that presents many advantages, including all solid-state operation, electronic capacity control, reversibility to provide both heating and cooling, and high reliability. In spite of these many benefits, thermoelectric cooling has not enjoyed widespread or large-scale use due to the low efficiency relative to vapor compression systems [D. T. Morelli, *Proc. Mat. Res. Soc.* **478** 297, 1997, with permission].

Refrigeration is relevant to transportation as well as a number of other industries. Within DOE, the applied research in these areas is part of the EE/RE Program.

Estimated Time Scale

Applications in high-end industries are possible within the next 10 years. However, broader uses will require more significant advancements with a likely 20-year research horizon.

COMPLEX SYSTEMS SCIENCE FOR SUSTAINABLE TRANSPORTATION

EXECUTIVE SUMMARY

The transportation sector poses particularly formidable challenges from the perspectives of energy security and sustainability because of its strong reliance on petroleum-based fuels and the complexity of the overall transportation system. The emerging science of complex systems offers exciting possibilities for providing new insights and research tools to address these challenges in a broad multidisciplinary manner that balances the collective needs of society with those of individual stakeholders. With its emphasis on nonlinear, holistic, and dynamic behaviors and on organic, evolutionary models that highlight such issues as contingency, self-organization, adaptation, and robustness, the complex systems approach naturally incorporates many of the concepts that need to inform rational decision making on pathways to more energy-efficient and sustainable transportation (i.e., that meets future demands for mobility with minimal unintended ecological and socioeconomic consequences). Long-term basic research in this area is needed to develop the fundamental concepts, tools, and cross-disciplinary insights that will help to clarify the scientific criteria for sustainable transportation and effective strategies for addressing the multitude of challenges that may require more than purely technological advances. Shorter-term activities need to focus on accelerating the practical impact of more established complex systems tools (e.g., nonlinear systems dynamics, logistical optimization, agent-based modeling, network theory and game theory) and gaining experience in addressing complex transportation issues. One example of the type of important, but nontraditional, problem this approach may begin to address immediately is the planning of an efficient and robust strategy for transporting nuclear waste from distributed sources to the Yucca Mountain disposal site.

Summary of the Proposed Research

The Challenge of Sustainable Transportation. Modern transportation systems have given the industrialized world an unprecedented degree of mobility, which has been instrumental in improving the quality of life, fostering democratic values, and promoting economic prosperity. Ensuring the sustainability of these systems for the foreseeable future is a particularly formidable challenge. From a technological perspective, petroleum-based fuels are nearly ideally suited as a mobile energy carrier. Energy security concerns, however, (especially an increasing U.S. reliance on foreign oil and growing evidence for global climate implications of CO_2 emissions) have greatly accelerated the search for alternative decarbonized fuels and more efficient powertrain technologies. Furthermore, the transportation sector is increasingly challenged by a large number of other unintended environmental and socioeconomic consequences, such as air quality concerns, ozone depletion, landfill utilization, sprawl, congestion, noise, and vehicle-related fatalities and injuries, the costs of which are nearly all “externalized” to society at large.

Today’s global transportation “system” includes many different modes of transportation and their associated fuels, vehicles, infrastructure, policy issues, market pressures, and the needs, expectations and behaviors of end users. While impressive progress has often been made in dealing with various components and issues individually, that approach generally leads to suboptimal collective behavior and may be reaching a point of diminishing returns in terms of purely technological solutions to long-standing problems (e.g., close to 99% reductions in tailpipe CO, hydrocarbon, and NO_x emissions).

By themselves, traditional scientific disciplines and lines of inquiry are ill suited to address the full scope of the complex interdependencies and multiple time scales required to provide future generations with the same access to and benefits of mobility as we enjoy today, without undue economic, ecological, or sociological hardships. Intra-generational equity between the developed and developing world is also a critical and contentious issue, given that transportation represents the most rapidly growing sector in terms of energy demand, with most anticipated growth in currently undeveloped regions.

Opportunity for Complex Systems Science. There is clearly a need for a more integrated, multidisciplinary, scientific approach and new fundamental insights to help guide the development of and transition to more sustainable transportation systems. An exciting and promising research area in harmony with this challenge is the emerging science of complex systems. This field seeks novel regularities that cut across all fields of human knowledge and a balance between the prevailing scientific and industrial world view (with its emphasis on linearity, reductionism, and equilibrium) and a more nonlinear, holistic, and nonequilibrium perspective. Through mathematical models and computer simulations, complex systems research offers the potential to move away from mechanical analogies and their focus on predictability and optimization to more organic, evolutionary models that highlight such issues as contingency, diversity, robustness, and adaptation. The latter themes offer exciting opportunities to exploit biological insights into sustainability as a bridge between the physical and social sciences and to improve strategic decision making in the face of uncertainties associated with a coevolving environment, network effects, coupled time and length scales, and strong path dependencies.

Among the key questions pertaining to sustainable transportation that complex systems science can potentially address are:

- How do economic, cultural, institutional, and technological factors interact to shape transport patterns and their associated environmental and socioeconomic impacts?
- How do varied modalities of mobility (e.g., road vs. air, people vs. freight) complement and conflict with each other, and how do individual agents devise strategies and make choices as a result?
- What are the leverage points conducive to interventions toward more sustainable transportation systems and effective strategies for overcoming irrational systems archetypes (e.g., tragedy of the commons, shifting the burden) that might inhibit progress?

The degree to which answers to such questions may be reasonably independent of scale is itself an exciting opportunity for research. Lessons learned in local communities, for example, may translate into effective strategies at national and global levels. Smaller-scale problems also lend themselves to experimentation and to detailed investigation of the links between individual agent behaviors and the collective properties of the system. The complexity of the sustainable mobility challenge implies that there are unlikely to be any magic bullets, and that even the goal of seeking optimal solutions may be misguided. Instead, what research in this area promises is a process for creating a systematic approach to all relevant knowledge and for improving our ability to anticipate and avoid or mitigate non-intuitive unintended consequences of proposed actions.

New Scientific Opportunities

The proposed work divides naturally into two time-frames:

- Longer-Term Fundamental Research. The science of complex systems is largely in its infancy. Developing the requisite concepts, tools, and cross-disciplinary insights to address the multitude of sustainability challenges will clearly be an ongoing process, especially in light of still-to-be discovered environmental and socioeconomic concerns and technological options. Creative work of all kinds in this area needs to be encouraged.

- Shorter-Term Applications. In parallel with an ambitious long-term program, it would be beneficial to initiate shorter-term research to accelerate the practical impact of existing complex systems methodologies and to explore their implications for specific sustainable transportation challenges. Among the most fertile areas of current complex systems research are network theory (structure and dynamics), game theoretical studies of social behaviors (e.g., the evolution of cooperation), agent-based modeling, time-series analysis, evolutionary algorithms, and informatics and nonlinear dynamics in general. Traffic modeling as a nonlinear flow problem is already an active area of research that deserves further attention in all aspects from fundamental concepts to practical infrastructure planning and real-time traffic routing tools. A combination of existing tools might be useful for providing integrated assessments of technological and socioeconomic issues in the context of evaluating the practicality and robustness of proposed pathways to major infrastructure changes (e.g., from petroleum to hydrogen). Another application that needs immediate attention from an energy security perspective is the development of an efficient, safe, and socially-acceptable strategy for transporting nuclear waste from distributed sources to the Yucca Mountain disposal site.

Relevance and Potential Impact

This PRD is truly out-of-the-box and addresses some of the most critical, but most easily ignored, issues that inhibit progress in all DOE energy programs. The main themes here, of recognizing the systemic nature of problems and the desirability of considering environmental and socioeconomic aspects on the same footing as technological, are particularly relevant to the transportation sector. However, the insights and methodologies developed will also apply to problems in distributed energy, the diversity of renewable energy options, nuclear fuel systems, etc. The work proposed is high risk in the sense that complex systems science is still in its infancy and its practical impact is largely unproven. However, the potential societal benefits are enormous, and the research is sure to foster a great deal of exciting and important progress that will complement and leverage existing DOE initiatives at the scientific frontier of complexity.

Estimated Time Scale

In is understood that this type of research is not currently supportable by DOE.

Residential, Commercial, and Industrial Energy Consumption

Sensors

Solid State Lighting

Innovative Materials for New Energy Technologies

Multilayer Thin Film Materials and Deposition Processes

SENSORS

EXECUTIVE SUMMARY

Optimizing energy performance in residential and commercial buildings will require a new generation of smart controls whose function is driven by a new generation of sensors. Similarly, the application of smart sensors that monitor, control, and optimize production and manufacturing processes will also lead to efficient energy use in large-scale industrial processes. In many small-scale applications (e.g., appliances), sensors must be highly specific to an environmental parameter, robust, rugged, durable and low cost. In larger-scale building and industrial processes and applications, there is also the demand for a ubiquitous network of small, wireless, self-powered sensors with associated on-board signal processing, networking, and communications capabilities.

Summary of Research Direction

***Residential and Commercial Buildings*:** The operation of the current generation of buildings is characterized by a small number of simple sensors with fixed response modes. A room thermostat with a temperature sensor and simple feedback loop is a well-known example. In order to achieve significant breakthroughs in building energy efficiency, buildings must become dramatically more intelligent, self-aware, and dynamic in response to weather changes, energy use and changing occupant needs. Buildings should have the ability to sense and then control energy flows, temperatures, airflow, pollutant levels, and other specific physical parameters, both within the building structure and in its component elements and equipment.

A prototypical smart system will include four generic elements:

- self powered sensors,
- signal processing,
- wireless communication between sensors and to control systems, and
- intelligent response based on a sensed event.

***Industrial Sectors*:** Manufacturers today must continuously improve process operations, product quality, and productivity with fewer workers than ever before. Processing equipment must deliver unprecedented levels of reliability, availability, and maintainability as plant managers seek to reduce operational and support costs and minimize capital investments.

Advanced and wireless sensor systems will enable manufacturers to meet the demands of increased competitiveness by helping them to streamline process operations and to use energy and materials more efficiently. As in the case of buildings, industrial sensors should provide real-time, continuously sensitive monitoring of a specific function and provide diagnostics to continuously maintain the functionality and energy efficiency of operations. Sensor systems in industrial applications, however, face unique challenges: invulnerability to harsh environments and high reliability. Sensor systems must reliably perform mission-critical tasks over extended, pre-defined periods in environments characterized by

- extremely high (up to 2,600° F/1,430° C) and low operating temperatures,
- strong vibrations,

- airborne contaminants,
- excessive electromagnetic noise caused by large motors or conductors,
- exposure to harsh, corrosive chemicals,
- high humidity levels,
- potentially explosive situations, and
- mobile and stationary metal equipment affecting transmission pathways.

New Scientific Opportunities

Residential and Commercial Buildings. Two areas of scientific breakthroughs are needed to achieve the aforementioned vision.

The first needed breakthrough is a new generation of smart sensors that can detect and measure a wide range of physical and chemical parameters. The sensors should be small, self-powered, low cost, durable, and robust in order to work under a wide range of physical environments, with detection capabilities that are specific to the parameter of interest, such as chemical species, particle size and/or shape, etc. Very low cost sensors allow redundancy that will improve accuracy. Sensors would be available to respond to a full range of stimuli, such as optical and radiant measurements, surface acoustic waves, airflow, chemical species, biological agents, inorganic particles, energy flows, magnetic fields, current, voltage, temperature, stresses, etc. On board, integrated electronics provide signal processing, conditioning and data compression, if needed.

The second needed breakthrough is an information technology infrastructure that allows data from sensors to be collected, processed, and converted into useful information upon which action can be taken, thereby reducing energy use or providing other useful functionality. The same need is reflected in the industrial sector. The new paradigm is a dense network of ubiquitous, wireless, self-powered sensors that can be networked to provide a complete and reliable picture of energy use and related parameters throughout a building and its equipment. Wireless communications protocols that are energy efficient will allow very long battery life or will support stand-alone operation using scavenged energy. Open protocols that are standardized across many business sectors will ensure interoperability of sensor and network components. Neural networks and adaptive logic can be utilized to adjust and fine tune the operation of the building to meet changing occupant needs and external events, such as real time utility pricing.

Industrial Sector. Advanced industrial materials and control are needed to meet the challenges to sensor placement in the industrial sector. A list of proposed research directions is provided below:

- Improved Controls/Process Modeling – A process control system or algorithm that increases process stability, optimizes operations, or improves product quality. The system should use adaptive control, neural networks, or other advanced control technology. Development of the control system may require improved modeling or process simulation tools.

- Chemical Composition – Better understanding of spectroscopic techniques; more reliable and cheaper laser techniques to measure chemical composition; better understanding of chemo-metrics; ability to do chemical analysis of nanoscale samples.

- Physical Properties – Real-time sensors or techniques to measure a specific process condition(s), such as temperature, pressure, flow, web tension, or multiphase flow.

- Signal/Numerical Processing – Improved signal processing, especially for the purpose of predicting fouling, detecting equipment faults/failure, predicting process upsets, or correcting sensor drift. The signal processing algorithm should be used to process raw sensor data output into usable process information. This can be in the form of a "smart sensor" that detects failure or drift, and then self-calibrates.

- Imaging/Machine Vision – Real-time sensor or measurement technique for visual inspection of product, specifically looking for defects, inclusions, color, and cleanliness, as well as measuring product properties for quality.

- Emissions Measurement and Control – Measurement and control techniques for combustion emission control applications.

Relevance and Potential Impact

The potential impacts of smart sensors on energy savings in the residential, commercial, and industrial sectors are achievable on many different scales, ranging from single appliances, complete building systems, to large-scale industrial processes. They share the common objective of providing an "information rich environment" in which intelligent decision-making will greatly enhance energy efficiency, occupant health, comfort and operating efficiency.

Single building appliance. At the level of a single energy-consuming device, there are important energy savings to be achieved. For example, dishwashers typically employ a series of wash cycles based on the assumption that dishes will be dirty, even though many people prewash dishes. Energy consumption for hot water and energy to drive the dishwasher is based on this assumption. New machines use a novel optical sensor that directly monitors the turbidity of the wash water as a metric for cleanliness. Coupled with adaptive logic controls, the dishwasher provides clean dishes with less water and lower energy use. Sensors for consumer product applications must be robust, reliable and low cost, thus challenging designers to employ new technologies that meet performance needs.

Building systems. A broader vision of energy-efficient buildings assumes that buildings can be optimally operated as a wholistic mechanism that is more than the sum of its parts. Real-time, continuous monitoring and diagnostics allow the building to continuously maintain operations in a mode that provides the required functionality and energy efficiency, as well as meeting human comfort and health needs. In the event of unanticipated disturbances, either natural or man-made, the building can adapt and respond in a manner that enhances safety and security. Continuous monitoring allows routine and preventive maintenance to be cost-effectively scheduled.

Industrial processes. Many of our most energy-intensive industries have identified and highlighted their top needs in the development of sensor, control, and automation systems. Highest priority is placed on systems that can truly revolutionize manufacturing processes as, for example, by enabling replacement of a batch process with a continuous one. Such advances will result in major reductions in manufacturing cost and energy consumption. In addition, wireless industrial sensor systems offer manufacturers greater mobility and flexibility. Freed from the constraint of wires, plant managers can more easily track materials flow and reconfigure assembly lines in response to demand. An effective wireless sensor technology is envisioned as robust, reliable, cost-efficient, totally secure, and in many cases, integral to the measurement device.

Estimated Time Scale

The development and integration of wireless sensor networks could benefit from the advances in the semiconductor industries and could have some success in the next 1-3 years time frame. For all sectors, advanced materials research to enable smart materials design is a rather long-term goal with a development period of ~5-10 years needed. The length can be shortened by an aggressive program to ~3-5 years. To enable the discovery of new classes of materials for sensors with revolutionary selectivity, sensitivity, reliability, and durability in harsh environments, 10-15 years may be required.

SOLID STATE LIGHTING

EXECUTIVE SUMMARY

This year, about 20% of the U.S.'s electricity consumption will be due to lighting. Incandescent and fluorescent bulbs, old vacuum-tube-based technologies that have been around for decades, will provide the vast majority of that lighting. Incandescent light is quite inefficient, with only 5-6% of their electricity consumption being converted to visible light. The rest is converted to waste heat, which contributes significantly to building cooling loads. Fluorescent lighting is better, but still only converts about 25% of the electrical energy into visible light. This wasted electricity represents an enormous target for reducing energy consumption.

Solid-state lighting (i.e., the use of light-emitting diodes, or LEDs, for general illumination) is a new technology that has the potential to far exceed these energy efficiencies. Within the past few years, two innovative new semiconductor materials – wide bandgap semiconductors and organic light emitting materials – have enabled the development of the first LEDs with bright emission in the blue and near-ultraviolet (UV). With these colors, white LED light sources can now be realized based on the color mixing of different wavelength light from multiple LEDs, or the down conversion of UV or blue light to longer wavelengths (green, red) using phosphors. While tremendous progress has been made in the last decade – today's white LEDs are more efficient (25 lumens/Watt) than incandescent bulbs (15 lumens/Watt) – there is much fundamental materials science that must be done for further progress to be made. Ultimately, it should be possible to reach the stretch goal of 200 lumens/Watt in the next 1-2 decades, with an LED cost that is competitive with incandescent and fluorescent bulbs. The achievement of this goal would result in spectacular energy savings, a 50% reduction in electricity used for lighting and a 10% reduction in total electricity consumption. Globally, this corresponds to an 1100 billion kWh/year reduction in power consumption, worth $100 billion in reduced rate charges, and corresponding to reduced carbon emissions of roughly 200 Mtons/yr.

This proposed research direction seeks to increase fundamental understanding of basic physics issues, still poorly understood, in these relatively new solid-state lighting materials. Issues include charge transport, radiative and non-radiative electron-hole recombination, defect and impurity physics, growth chemistry and materials preparation physics, and aging and breakdown mechanisms. Three classes of materials are considered: (1) wide bandgap semiconductors (primarily nitride-based) for inorganic LEDs; (2) polymer-based materials for organic LEDs; and (3) new energy conversion and packaging materials to act as highly efficient phosphors and UV-stable, moisture-impermeable coatings for the LEDs.

Summary of Research Direction

At present, electricity is responsible for about 25% of the nation's total energy consumption. Of that, about 20% is due to lighting. Thus lighting represents a significant portion of energy consumption. However, conventional lighting technology, consisting primarily of incandescent bulbs and fluorescent tubes, is remarkably inefficient. Incandescent bulbs, which represent the major residential lighting source, convert only about 5-6% of their power consumption into visible light. Fluorescent lighting, which dominates industrial and commercial areas, is considerably better, with 25% energy efficiency, but nonetheless wastes a significant amount of energy as heat.

Recently, the development of new materials, both inorganic and organic, have enabled the production of white light using solid state technologies [i.e., light-emitting diodes (LEDs) and organic LEDs or OLEDs].

These new semiconductor-based lighting technologies promise to be more flexible, compact, robust, and longer lived than vacuum-tube-based technologies. LEDs and OLEDs offer the possibility of exceptional control over color, hue, and intensity, and can even be modulated at high rates, offering the possibility of simultaneous use for communications. But most importantly, LEDs and OLEDs offer opportunities for energy savings that are truly enormous.

Based on proof-of-principle demonstrations of lasers and LEDs in the red and infrared, it is believed that white LEDs operating at 50% efficiency might ultimately be produced. This corresponds roughly to an efficacy of 200 lumens/Watt. (By comparison, incandescent and fluorescent bulbs are typically 15 lumens/ Watt and 80 lumens/Watt, respectively.) Achieving the 200 lumens/Watt goal would have an immense impact on electricity consumption. It would decrease by 50% the amount of electricity used for lighting, and decrease by 10% the total consumption of electricity. The reduction in the U.S. alone would be equivalent to all the electricity consumed by residential homes in the states of California, Oregon, and Washington. Global reductions of power consumption would be about 1100 billion kWh/yr, or about \$100 billion/yr in rate charges. This corresponds to a reduction of about 200 million tons of carbon emissions per year.

The materials physics advances that have enabled the realization of white LEDs and OLEDs are different for the two technologies. For LEDs based on inorganic compound semiconductor materials, the enabling material is GaN and other related nitride-based III-V compounds including InN, AlN, and their ternary and quaternary alloys. This class of materials is generally referred to as wide bandgap semiconductor compounds. For organic LEDs, the enabling materials include Alq3 (a flexible, light emitting polymer), polyfluorene, and related polymers and small molecule organic materials. In both cases, the materials have become available only within the last ten years, and much of their fundamental physics is poorly understood at present. Progress has been rapid over the past decade, with inorganic white LEDs now producing 25 lumens/Watt, and organic OLEDs producing 6 lumens/Watt. However, much of this recent progress has been due to relatively uninformed phenomenological explorations of parameter space, and it is widely acknowledged that without detailed scientific understanding of these materials, further progress will be more difficult. Basic investigations of the physics of how these materials are synthesized, how electron transport occurs through them, how dislocations and other defects affect their properties, and fundamental questions about band structure, impurity levels, electron-impurity interactions, physics and chemistry of electrical contact formation, radiative and nonradiative electron-hole recombination mechanisms, spontaneously formed micro- and nanostructures, and degradation mechanisms at high current drive levels, are needed. With detailed knowledge of the fundamental science underlying these processes, it is expected that we will be able to specifically tailor the properties of these materials, so as to raise the overall efficiency with which they produce visible light, increase LED and OLED lifetime and reliability, and lower the cost by orders of magnitude.

New Scientific Opportunities

In order to achieve the 200 lumens/Watt goal for the LED/OLED devices, the following is a list of proposed scientific opportunities which are broken into three categories. These are (1) inorganic wide bandgap semiconductor LED materials, (2) organic OLED materials, and (3) energy conversion materials and associated UV-stable packaging materials.

Inorganic Wide Bandgap Semiconductor Materials. The nitride-based III-V compounds have a number of properties not seen in other III-V semiconductors. These include the lack of a native lattice-matched substrate (the large stresses that develop in heterostructures due to lattice mismatches between AlN, GaN, and InN) lack of a shallow level acceptor impurity for p-type doping; and poorly understood and poorly controlled chemical vapor deposition growth processes. In this area we propose research on:

- Innovative growth methods for reducing defects and tailoring residual stresses via innovative synthesis processes, as well as developing large area (diameter "2") lattice-matching substrates.

- Microscopic understanding of the role of doping, impurities, and their interactions with structural defects. Specifically, approaches to higher p-type doping levels, particularly for higher Al compositions.

- Investigations of fundamental processes involved in the chemical-vapor-deposition growth of nitride materials. Novel growth reactor designs with improved repeatability, temperature control, in-situ growth monitors, and more efficient use of precursor gases should proceed with further understanding of growth chemistry.

- Novel light emitting device designs to reduce parasitic resistances, increase internal quantum efficiency, and increase light extraction efficiency with the aim of tailoring the direction and amplitude of the photonic density of states.

Organics. Organic light-emitting diodes (OLEDs), although still in their infancy, hold tremendous promise as an energy saving light source, but continue to face deep and broad technical challenges. Performance limitations can be partly attributed to the very low carrier mobilities in these materials. At present, green OLEDs with efficiencies of 60 lumens/Watt have been demonstrated, but OLED lifetimes are observed to drop dramatically as drive current densities are increased to the levels needed for general illumination. Questions to be answered include:

- What is the chemical and electronic structure of the material interfaces?
- Why are luminescent efficiencies so high in some organic materials as opposed to others?
- What controls the singlet-triplet exciton formation ratio in conjugated materials?
- Why do shorter wavelength (blue, violet) devices tend to have lower luminous efficacy?
- Is it possible to modify materials to increase their stability in humid environments?
- What are the intrinsic mechanisms that lead to material degradation? How and why do these mechanisms depend on drive current?
- What is the chemical and electrical structure of the electrical contacts? What modifications can increase performance?

Energy conversion materials and UV-stable packaging. Phosphors are currently in use in fluorescent lamps, and a number of high-efficiency phosphors which can yield high-quality, high color rendering index (CRI) white light have been developed for fluorescents over the past several decades. However, the current fluorescent phosphors were optimized for the wavelength of the mercury vapor discharge in fluorescents, and are unsuitable for the >380 nm pump wavelength appropriate for white LEDs. In addition to new “conventional” phosphor materials, a number of other more novel approaches are possible. This topic considers basic physics investigations of a number of different materials approaches to energy conversion for solid state lighting, and the associated packaging material in which the phosphors will be distributed. Research is proposed on:

- Nanocrystalline quantum dots (CdSe, ZnS, etc.) for use as "phosphors," whereby the optoelectronic properties are controlled by quantum dot size and surface treatments.
- Novel inorganic semiconductor structures incorporating one or more near-surface quantum wells that act as phosphors, absorbing light from the nearby active region and re-emitting at a longer wavelength.
- "Nanophosphors," in which "conventional" phosphor material is produced on the particle size scale of a few tens of nanometers, eliminating backscattering of light into the LED and enabling highly efficient particle packing.
- Novel encapsulant materials that will withstand high flux UV irradiation and elevated temperature, block out moisture, and have small thermal expansion coefficients.

Relevance and Potential Impact

This PRD will be relevant to the programs at EE on (1) wide bandgap materials for photovoltaic power conversion and control, (2) wide bandgap materials for sensing and logic in high temperature, high pressure environments (e.g., down-hole sensing in oil wells), and (3) new polymers and other organic materials for cheap, large-area solar cells. The PRD will also serve the non-energy related DOE needs in the following aspects: (1) wide bandgap materials for high power electronics for synthetic aperture radar, and ultra-light imaging radar systems for Unmanned Aerial Vehicles (UAV), (2) solar blind UV-photodetectors, for detecting missile launch plumes, and (3) low power, compact UV sources for UV-fluorescence-based detection of chemical, biological, and nuclear weapons of mass destruction. A particularly appealing application is compact portable anthrax detectors.

Estimated Time Scale

More in-depth understanding on the device physics and degradation mechanisms in LED and OLED devices could be achieved in 10 years. It will require up to 20 years to integrate these findings into reaching the stretched performance goals of 200 lumens/Watt of LED/OLED devices that are cost competitive with incandescent and fluorescent light sources.

INNOVATIVE MATERIALS FOR NEW ENERGY TECHNOLOGIES

EXECUTIVE SUMMARY

The last decade has seen major advances in the fields of nanoscience and nanotechnology, advances that now enable scientists to control the chemistry and arrangement of matter at length scales 100,000 times smaller than the width of a human hair. Because of the fact that elementary energetic processes naturally occur at these same ultra-small length scales, these advances offer unprecedented opportunities to dramatically change the way we store, convert and use energy. Taking nature's construction of cells and tissues as our inspiration, it is now possible to imagine building, from the "bottom up," complex, hierarchical molecular organizations whose properties and functions reach far beyond those exhibited by their organic and inorganic building block components. The aim of this proposed research direction is thus towards the development of innovative materials for new energy-related technologies.

In the area of energy conversion, nanocomposite polymer/semiconductor assemblies are sought for next generation high-efficiency (~30%), low-cost solar cells for commercial and residential use in sunny geographical locales, as well as new thermoelectric materials for the conversion of waste heat to electricity and novel membranes and catalysts for stationary fuel cells. The transition to clean, renewable energy sources for mainstream commercial, residential and transportation applications further hinge upon substantial innovations in energy storage. The high interface per volume intrinsic to nanocomposite materials could open the path to a long-sought high-power, high-energy density, all solid-state rechargeable battery with performance, cost and ES&H (Environmental, Safety and Health) attributes that far surpass today's very best portable power storage devices. Looking even further into the future, chemical/molecular-based approaches that mimic the biological ATP-ADP engine would represent a revolutionary advance in energy storage. Finally, innovative materials can play a central role in reducing commercial and residential energy usage, which now accounts for ~37% of our total domestic energy consumption, through more efficient and durable building materials, and building elements that sense and respond to their environment. For example, replacement of today's less-efficient fluorescent and incandescent lighting with organic light-emitting devices would translate to a huge energy savings, with an associated reduction in carbon emissions from the energy points of origin, while "active" materials systems that could respond to climatic/lighting changes, such as phase-change building materials and smart electrochromic windows, could substantially reduce the energy spent on space heating and cooling (~35% of residential energy use).

Summary of Research Direction

The last decade has seen major advances in the fields of nanoscience and nanotechnology, advances that now enable scientists to control the chemistry and arrangement of matter at length scales 100,000 times smaller than the width of a human hair. These advances offer unprecedented opportunities to dramatically change the way we store, convert and use energy, because elementary and highly efficient energetic processes naturally occur at these same ultra-small length scales. Taking nature's construction of cells and tissues as our inspiration, it is now possible to imagine building, from the "bottom up," complex, hierarchical molecular organizations whose properties and functions reach far beyond those exhibited by their organic and inorganic building block components. The aim of this proposed research direction is thus towards the development of innovative materials for new energy-related technologies.

An example from energy conversion where nanostructured assemblies could favorably impact both energy security and the environment is in solar cell technology. Solar cells convert light to electricity by absorbing light of sufficient energy to excite electrons across the bandgap and into the conduction band of a semiconducting material. While silicon-based solar cells have been under commercial development for decades, their widespread use has been precluded by cost and efficiency considerations. Solar cells based on new materials, such as nanocomposite arrays of colloidal semiconductor nanorods embedded in a conductive polymer, hold promise as an inexpensive route to high-efficiency (30%) energy conversion devices for commercial and residential use in sunny geographical regions. Other advanced energy conversion strategies for these sectors similarly hinge upon materials developments, including thermoelectrics for the conversion of waste heat to electricity and membranes and catalysts for stationary fuel cells.

Beyond energy conversion, great fundamental research challenges must be addressed in the energy storage arena, particularly if clean, renewable energy sources are ever to graduate into mainstream use in the commercial and residential sectors, as well as transportation. Here again, recent progress in controlling materials structure and properties at the nanometer level can play an enabling role. For instance, the high interface per volume intrinsic to templated, nanocomposite materials could open the path to a long-sought high-power, high energy density, all solid-state rechargeable battery with performance, cost and ES&H attributes that far surpass today's very best portable power storage devices. Looking even further into the future, chemical/molecular energy storage approaches that mimic the biological ATP-ADP engine could revolutionize the very way we harness and use energy to such an extent that the full implications of an advance of this nature are difficult to project.

Finally, innovative materials can play a central role in energy security by reducing our commercial and residential energy usage, which now accounts for ~37% of our total domestic energy consumption, through more efficient and durable building materials and building elements that sense and respond to their environment. An example is in the area of lighting, which represents ~20% of the total U.S. electricity consumption. Through basic research advances in organic and inorganic light-emitting materials, solid-state LEDs with efficiencies nearing 50% may be attainable for large area diffuse illumination as well as local, high brightness sources. Replacement of today's less efficient fluorescent and incandescent lighting would translate into a huge energy savings, with an associated reduction in carbon emissions from the energy points of origin. Other relevant examples where innovative materials could lower energy consumption include phase-change materials as structural building elements and smart electrochromic windows. Such "active" materials systems would respond to climatic/lighting changes to substantially reduce the energy spent on space heating and cooling (~35% of residential energy use).

New Scientific Opportunities

The undisputed need for new approaches to harness, manipulate and conserve energy in the commercial, residential and industrial sectors dictates that basic research on innovative functional materials for energy technologies be adopted as a high priority element of the BES portfolio. This is because, almost invariably, the path to commercial realization of visionary energy technologies is obstructed by materials limitations. Application of powerful, state-of-the-art synthesis, molecular level processing, and computational modeling methods to address these key materials challenges affords exciting opportunities for future basic research within DOE. Specific examples of energy technologies that might be enabled through such basic science efforts include:

- high efficiency (~50%) organic LEDs for solid-state lighting,
- high efficiency (~30%) nanocomposite solar cells for electricity generation,

- low cost catalysts & high selectivity membranes for stationary fuel cells,
- thermoelectrics for waste heat utilization, self-powered thermal sensors and spot cooling,
- high energy density, high power density solid-state rechargeable batteries,
- reinforced lightweight composites for load-bearing applications,
- high sensitivity/selectivity sensors for optimizing energy usage,
- functional materials for high temperature/highly corrosive environments,
- membranes for high efficiency chemical phase separation,
- phase change materials for thermal energy storage in building envelopes,
- flexible, transparent, thin film conductors for organic LEDs, organic photovoltaics, and electrochromic windows,
- nanocomposite hard and soft magnets for sensors, electric motors, actuators, transformers, and magnetic refrigeration, and
- biomimetic molecularly-based energy storage.

Below, more detail is provided for several of the above technological examples, emphasizing how a new generation of materials, constructed in a bottom up fashion from molecular- and colloidal-scale building blocks, allows for independent tuning of different materials properties that might normally be coupled or otherwise difficult to realize.

As one illustrative example, self-assembled nanocomposite materials incorporating semiconducting nanorods and a hole-conducting polymer offer great promise for achieving low-cost, high-efficiency solar cells, wherein the rod diameters and lengths could be adjusted to match the bandgap to the solar spectrum, while the rod location and orientation could be controlled in the organic hole-conducting polymer matrix to deliver electrons and holes to their respective electrodes. By combining rods suitably, it may be possible to make multibandgap tandem cells with efficiencies rivaling those of the high end solar cells currently used in satellites, but instead manufactured by very high volume methods, such as roll-to-roll processing. Tandem cells of nanorod arrays with varying rod diameters, for instance, could allow efficient capture of low energy photons, while transmitting the high-energy end of the solar spectrum that could then be efficiently harvested using an array of shorter nanorods. Development of new processing technologies for rapid, large-scale manufacture of such devices, as well as low cost synthetic routes to the conductive organic and inorganic nanorod components, is paramount if the goal of affordable solar cells with conversion efficiencies of 30% or more is to be achieved.

Consider, as another example, a thermoelectric material that provides independent control of the thermopower, and of the electrical and thermal conductivity (a so called “phonon glass” but electron conductor). A quantum dot superlattice of isoelectronic materials with many interfaces could perhaps provide independent control of the electrical and thermal conductivity, while controlling the degree of doping to place the Fermi level near a peak in the electronic density of states could be used to enhance the thermopower. The tenability of such a material and the development of a low cost processing technology represent large materials development challenges.

High interface per volume materials offer other special advantages in the energy storage arena as well, particularly for advanced secondary battery technologies. For instance, nanoscale active electrode composites (Li-alloying metal nanoclusters, Li-insertion metal oxide or metal phosphate nanoparticles) self-assembled in a polymer ion-conducting matrix could enable all solid, thin film batteries capable of high current rates, while accessing the full theoretical capacity of the active electrode material. The use of nanoscale active components offers further promise to dramatically extend cycle life of rechargeable batteries by enhancing stability to volumetric excursions that cause decrepitation of bulk electrodes.

Molecularly designed organic or nanocomposite materials also hold new opportunities for building-integrated thermal storage based on solid-solid phase transitions. Here the challenge is to find inexpensive materials systems that exhibit inherently high heat storage capacity over a tunable temperature range with minimal cyclic expansion/contraction through the phase transition and no special isolation requirements. Despite the tremendous potential savings in energy such a technology could offer (space heating/cooling represents 35% of residential building energy use), materials studied to date for this application have been relatively primitive, off-the-shelf systems (e.g., paraffin). Bringing the full force of recent materials advances to bear on this technology challenge could yield a tremendous payoff in reduced energy consumption.

Finally, light weight reinforced composites could be envisaged where constituents could be added for control of special physical and mechanical properties. Such materials would have a combination of different functional properties in addition to providing load-bearing capacity.

In the development of such functional nanostructured materials, computer simulation will likely play an increasingly important role. Electronic structure calculations, for example, can be used to predict the electron and phonon energy states in nanocrystals and how they differ from their parent 3D bulk materials, thereby enabling the first-principles design of a material's optoelectronic properties. Similarly, recent years have seen great progress in describing the properties of systems of long chain molecules through computational approaches such as advanced Monte Carlo and molecular dynamics methods, self-consistent field models and phase-field calculations. Modeling the equilibrium and transient behavior of polymer/ inorganic nanocomposites of the types discussed above is made challenging by the enormous range of relevant length scales (angstroms to millimeters) and time scales (picoseconds to days) that characterize the structure and motion of the different components.

Relevance and Potential Impact

Much of the basic research in materials called for in this PRD could directly benefit existing applied energy programs under the DOE. Especially, specific efforts such as sensors, phase-change building materials and materials for solid-state lighting could feed into the DOE's Energy Efficiency program. Similarly, nanocomposite-based solar cells, materials for fuel cells and novel energy storage materials could nourish the DOE's program on Renewable Energy. For most of the innovative materials concepts discussed herein, the impact of each materials breakthrough would affect multiple energy technologies, and in some cases, extend well beyond the interests of DOE, such as for lightweight reinforced composites.

Estimated Time Scale

Experience in the materials industry has taught that commercial development of new materials is a long and often costly process, requiring typically about 10 years from the earliest development stages to full commercialization. One can project that a similar time frame might be needed to lay the basic scientific foundations underpinning the energy-related materials technologies described herein, given that sufficient, dedicated monetary resources were made available. This inherent lag time to payoff argues for immediate DOE investment, if energy security is to be effectively addressed within the next decade. It must be emphasized that the vision here is not incremental, but encourages the possibility of discovering entirely new ways of harnessing, manipulating, converting, or conserving energy. It is critical that appropriate long-term investments be made to guarantee advances in functional materials for future energy technologies.

MULTILAYER THIN FILM MATERIALS AND DEPOSITION PROCESSES

EXECUTIVE SUMMARY

Multilayer thin films consisting of nanoscale microstructures exhibit a wide range of superior physical properties, which have found many applications in the residential, commercial and industrial sectors. One example is the use of thin film multilayer coatings on glass, with the film thickness in the range of 5- 50 nm, to reduce heating energy use in buildings. These coatings can reduce heat loss in winter (up to 30%) and heat gain in summer through windows. (Windows in buildings account for about 4% of all U.S. energy consumption, at a cost of about $30 billion/yr.) Other applications based on multilayered structures include, but are not limited to, wear- and erosion-resistant coatings, magnetic recording media, and reflective x-ray mirrors. These applications are mainly driven by the significant improvement in properties derived from the manipulation of nanoscale structure. In order to propel new scientific revolutions in the application of multilayer thin film materials, significant advances in the design, synthesis, and deposition of these nanoscale multilayers need to be achieved. The major research directions proposed involve (1) development of a new generation of coating materials with optical, photochemical, and other functionalities; (2) creation of explicit mechanistic models that allow precise control and prediction of coating properties based on deposition conditions and film growth chemistry/kinetics; and (3) development of the next generation of thin-film deposition techniques and in-situ characterization tools.

Summary of Research Direction

The performance of many materials in buildings is influenced by surface optical and thermal properties. This is most readily apparent in surfaces that influence selective solar energy transmission, absorption and rejection. Conventional solutions for energy control are often based on manipulation of bulk materials properties. Modified surface properties can effectively control radiant energy flows. The ability to modify surface properties using specific coating structures and chemistry could provide exciting new energy control functions.

One important class of surface coatings is based on thin film multilayers. Historically multilayer coatings were applied in small areas at high cost (e.g., multilayer antireflection coatings on lenses at costs of >$1,000/m^2). Over the last 20 years a variety of new controllable, high rate, deposition technologies have been developed that are capable of producing very high performance multilayer coatings at low costs, $0.10-$10.00/m^2. Existing deposition processes include sol gel, evaporation, sputtering, chemical vapor deposition, etc. Coatings may range from 5-5000 nm in thickness, with stacks which may range up to 50 layers. Each deposition process has strengths and weaknesses with respect to available source materials, coating thickness and uniformity, deposition rate, film stoichiometry, morphology and microstructure, etc. Several of these production processes have been adopted on a very large scale. For example, low-emissivity coatings with 5-20 layers with a total thickness of 60-150 nm are manufactured in volume (50 Mm^2/yr) by reactive magnetron sputtering on sheets of glass 3 x 4 m and on plastic webs 2 m wide.

A new generation of products based on thin film coatings is currently being researched, including:

- electrochromic window coatings that dynamically control sunlight transmission;
- photovoltaic devices to convert sunlight to electricity;

- touch screens for input to computer systems; and
- organic light emitting diodes for energy efficient lighting.

Although commercially viable processes are available for some applications, there are seemingly fundamental limitations to each process that constrain its applicability. Most of the deposition processes involve complex chemical reactions (e.g., CVD) or energetic plasmas (e.g., sputtering). Current thin film process technology is based on semi-empirical experience in optimizing these complex deposition processes rather than a first principles model of the process that would allow a "materials-by-design" approach to new coating developments. Furthermore, optical properties of materials used in these coatings are often highly dependent on deposition conditions (e.g., substrate temperature, pressure, gas flow rates for reactive sputtering).

New Scientific Opportunities

Coating Materials and Systems. A first generation of static optical coatings (coatings that reflect long wave radiation, and spectrally selective coatings that reject solar infrared radiation) are well established in the marketplace. These are based largely on silver-based sputtered coatings that are antireflected to increase transmittance using dielectric layers. There are numerous additional energy efficiency applications for buildings that will benefit from an aggressive effort to develop and synthesize new materials systems for these applications. One of the more interesting but challenging opportunities is the development of a new generation of optically active electrochromic windows in which a small control voltage can induce a large change in optical density. First generation prototypes are emerging but do not yet meet functional and cost requirements. Novel materials systems could provide enhanced performance, longer life and lower production costs. Dynamic redirection of sunlight using optically active coatings is a challenge that has not yet been achieved. Holographic coatings or layers with controllable index of refraction might provide suitable control mechanisms. Transparent conductive coatings that meet functional objectives and other energy control functions, as well as cost objectives for organic LEDs, remain technical challenges.

Deposition Systems. A key breakthrough and enhancement of thin film deposition systems would extend industry's current large investment in these production facilities. A primary objective would be the creation of explicit mechanistic models that allow prediction of coating properties based on accurate models of deposition conditions and film growth chemistry and kinetics. Currently, process parameters are determined by empirical "tweak and look" approaches that offer little opportunity for breakthroughs in materials design. Understanding the close relation between manufacturing process parameters and the local thermophysical and chemical environment at the point of film nucleation and growth, and the resultant bulk and surface properties of materials, is crucial for a breakthrough in the progress in coating developments that could lead to the next generation of thin film technologies. Modifications to conventional deposition approaches can provide the ability to achieve new film properties using "conventional" materials. Energetic deposition by Filtered Arc or by Pulsed Magnetron sputtering with biasing techniques, for example, is an emerging technology for the formation of smooth, dense films that show improved adhesion, enhanced refractive index in the case of oxides, and diamond-like bonds in the case of carbon. Another example is the development and application of a plasma-assisted sputter source that can increase the deposition rate, thus reducing costs, and can improve the stoichiometry of compound films used in multilayers. Some deposition processes with these new capabilities might be inherently unstable and require real time process control to achieve and maintain optimal deposition conditions. A new generation of sensors that provide real time, in-situ optical, chemical and spectroscopic information may be required.

Relevance and Potential Impact

The combination of novel materials produced using these more versatile deposition systems could provide revolutionary advances in optical coatings for energy efficiency in buildings. Because they build on existing industry experience with related technologies they have the potential to be widely adopted by industry, once the basic R&D problems have been solved.

There are numerous opportunities to use high performance thin film coatings to reduce energy use in buildings. For example, heat loss and heat gain through opaque building surfaces occur in part because of the surface radiative properties which can be readily controlled using thin film coatings. Energy flows through glazed openings are even larger and can also be controlled using coatings on glazed surfaces. One example is control of cooling loads through windows. Approximately 1 quad of resource energy worth about $10 billion/yr is directly associated with cooling performance of windows. An equivalent amount of energy could also be captured if daylighting systems displaced electric lighting in the perimeter zones of buildings.

Estimated Time Scale

Initial useful results could be achieved by an aggressive program in 3-5 years. To further improve coating performance and processes that will increase durability and manufacturability as well as enhance the required energy control properties, 5-10 years might be required.

Cross-Cutting Research and Education

Nanomaterials

Preparing Tomorrow's Workforce for the Energy Challenge and Heightening the Public's Awareness

NANOMATERIALS

EXECUTIVE SUMMARY

New materials engineered on the 1-100 nanometer length scale will play a vital role in future energy technologies. It is on this length scale that the electrical, thermal, mechanical, optical, and chemical properties of materials have always been determined. As nanoscale science and technology are developed, new materials of revolutionary capabilities will emerge. High temperature superconductors and strained-layer superlattices are two current examples of nanoengineered materials of great energy relevance. Single-walled carbon nanotubes in their various forms are among the leading candidates for future examples. They have properties that could lead to transforming advances in fuel cells, batteries, capacitors, nanoelectronics, sensors, photovoltaics, thermal management, super-strong lightweight materials, hydrogen storage, and electrical power transmission. Continuous fibers composed of single-walled carbon nanotubes of a specific type (the so-called “armchair” tubes) are expected to have an electrical conductivity similar to copper, thermal conductivity similar to diamond, and a tensile strength 10-100 times higher than steel while having only 1/6th the weight. Since the carbon nanotubes behave as individual, ballistic quantum conductors along the tube axis, but have much less conductivity perpendicular to this axis, eddy current losses in the macroscopic spun carbon nanotube wire may be vanishingly small. When a practical scheme is developed to produce these nanotube “quantum wires” at a large scale and low cost, they may replace the copper windings in electric motors, and enable electric power transmission lines of much greater length and efficiency than currently possible. Support of the underlying basic science that leads to such new nanomaterials should be a prime objective of basic energy research.

Summary of Research Direction

Basic research within the DOE Office of Science has always concentrated heavily on the challenge of discovering new materials and understanding their behavior at a fundamental level. Over the years this research has concentrated increasingly on the nanometer length scale, to the point that now it is hard to find an important materials research topic that does not qualify at least broadly as nanoscale science. During the course of this workshop it became abundantly clear that nanoscale materials science continues to be of critical importance in the future of all energy technologies. In many cases it is the single most limiting issue.

Rather than summarizing the vast range of new opportunities in nanomaterials, this cross-cutting PRD will focus on just one: single-walled carbon nanotubes. The possibilities with just this one line of research are enough to occupy researchers for decades to come.

New Scientific Opportunities

Single-walled carbon nanotubes (swnt) can be visualized as sort of nanoscale soda straws formed from a single atomic layer of graphite cut into a long strip, then curled up and sealed seamlessly along its length to form a long hollow tube about one nanometer in diameter. The ends of the tube can either be open or closed with a hemispherical dome of carbon to form a closed hollow molecule that is a member of the fullerene family – it is an elongated “buckyball”. These swnt molecules can, in principal, have any length from a few nanometers to many meters in length, although typical methods now make them a few microns long. The longest ones prepared thus far by any method are no more than a few millimeters in length. Since the graphene sheet has the highest Young’s modulus of any material, these carbon nanotubes have both a high longitudinal extensional modulus (~ 1GPa), and an extremely high bending stiffness. When forced to bend or twist the tubes buckle, much like a soda straw. But when the stress is relaxed they are found to snap back straight with no damage. In addition to this extremely high bending toughness, the tubes are predicted to have an exceedingly high tensile strength in the range of 10-100 times higher than steel, but with a density of only 1.3 g cm^{-3}.

It is perhaps best to think of these tubes as a new polymer, a follow-on to nylon, polyethylene, or Kevlar. Like these earlier feats of polymer engineering (which are themselves marvelous examples of nanotechnology), the new single-walled carbon nanotubes can be made from cheap gas phase carbon feed stocks such as methane or carbon monoxide, using a catalyst that stays attached to the "live" end of the growing polymer. Over the past decade methods have been developed to produce these tubes with good quality in gram amounts, and thus far with slightly lesser quality in kilograms. With intense research it is reasonable to expect that large-scale industrial production of this new all-carbon polymer will be possible at low cost, and that over time revolutionary new catalysts and processes will be found to produce swnt with precise control of length, diameter, and type, similar to the revolutions that have occurred in polyolefin production in the last century.

Each swnt "buckytube" is uniquely specified by a pair of small integers (n,m) which define just how the strip of hexagonal graphite is cut. The diameter of the tube ranges from 0.6 to 3 nm depending on the sum of the two integers, n+m, while the electrical properties of the tube depend on the difference, n-m. If n-m=0 the nanotube is a one-dimensional metallic conductor. If n-m = 3, 6, or some higher multiple of 3, it is a semi-metal. Otherwise, if |n-m| mod 3 > 0 the tube is a direct bandgap semiconductor with a bandgap in the range of 0.8-1.4 eV, depending on the exact values of n and m. Just as with more traditional direct bandgap semiconductors, such as GaAs, these semiconducting nanotubes have been found to be good light emitters directly across the bandgap, except here they do this on a nanometer scale. The semiconducting tubes have been used to produce the world's first single molecule transistor, operating in air at room temperature.

The n=m metallic tubes, which are termed the "armchair" tubes because their open ends resemble the arms and seat of a chair, are now known to be sensational electrical conductors, rivaling copper. They are such good conductors because they are quantum "light pipes" for electrons, and they have extremely long coherence lengths. Current calculations indicate that an electron traveling in a ballistic quantum wave packet down one armchair tube can hop onto an adjacent armchair tube with no loss. If this turns out to be true in practice, we may find that a fiber spun from all armchair swnt tubes will have an electrical conductivity similar to copper while having only 1/6th the weight. Such a bucktube quantum wire should have extremely small eddy current losses since the transport properties are good only as long as the longitudinal momentum of the electron is conserved. Experiments have already shown that swnt can be spun into continuous highly aligned fibers from a sulfuric acid spinning medium, much like Kevlar. It may be possible to develop such a technology on a mass scale. These armchair quantum wires may someday be the logical replacement for copper and aluminum wiring throughout commercial and domestic applications

Relevance and Potential Impact

The fact that these swnt buckytubes are the best electrical conducting polymers that we have ever discovered suggests they may be involved in revolutionary improvements in nearly every technology where electrons flow (e.g., fuel cells, batteries, capacitors, photovoltaic devices, memories, logic, and interconnects in computers and sensors). If the armchair quantum wire has the properties projected above, and if it can be made in large amounts at low cost, it may enable a truly worldwide electrical energy grid.

Space Based Solar Power. NASA has recently taken a fresh look at the notion of solar power satellites, and this notion has been the focus of an NRC study. There is plenty of power to be had from space in geosynchronous orbit, easily the additional 10 TWe that is expected to be needed by the year 2050. However, to make this economically feasible breakthroughs must be made in a wide range of technologies. Nearly all of which could be facilitated by nanomaterials; especially those made with single-walled carbon nanotubes.

Carbon-nanotube-based materials may enable dramatic reductions in the weight of rockets and aerospace vehicles. They may enable construction of huge structures in space, including the structural support, the PV arrays, transport of waste heat to thermal radiators, and the field emitters used in the high power microwave generators. Through their use in nanoelectronic computers, memories, and sensors they may enable dramatic developments in autonomous robots that, with artificial intelligence, are able to construct and repair these huge, complex, orbiting structures. The swnt will be useful as well in construction of the necessary rectenna arrays on earth, and the electrical power transmission grid and local energy storage that handle the power beamed down from above. Also enabled will be the notion of Lunar-based solar power. This may very well be the way the world's energy challenge is finally met by the year 2100.

Estimated Time Scale

Major developments in the first commercial swnt applications may be expected within the next few years. Applications in fuel cells, supercapacitors, lithium ion batteries, flat panel field emission displays, and electromagnetic interference (EMI) shielding will likely happen within the next 10 years. Continuously spun swnt fibers and "quantum wires" may also be available within this time period. Full realization of the opportunities afforded by swnt could still be unfolding decades in the future.

PREPARING TOMORROW'S WORKFORCE FOR THE ENERGY CHALLENGE AND HEIGHTENING THE PUBLIC'S AWARENESS

EXECUTIVE SUMMARY

This proposed research direction aims at attracting a critical mass of students in physical sciences and engineering to take up the energy challenge, and at raising the awareness of the public, including scientists, in today and future challenges and opportunities in energy.

There is an urgent need to cultivate basic research in energy and to redress the balance of the number of students in physical sciences and engineering. The proposed research direction offers the opportunity to achieve world class education and technical training by communicating the joy and excitement of the energy challenge to young adults, thereby raising the pupils' awareness and inspiring them with unique and exciting missions that will meet their life idealism and career ambitions.

To achieve these goals, it is suggested that DOE compile background material on the theme "In Search of Terawatts." Background material includes, for example, PowerPoint slides highlighting the grand challenges in energy for this century, both from a scientific/technological and societal perspectives. This background material will be prepared by DOE staff and will be distributed to DOE-supported scientists. It will constitute the basis for public talks intended for primary and secondary schools, universities, and other public places.

Though it is acknowledged that the National Science Foundation already invests massively in educational programs, it is believed that the paramount magnitude of the energy problem and its urgency justifies that DOE undertakes this proposed research direction.

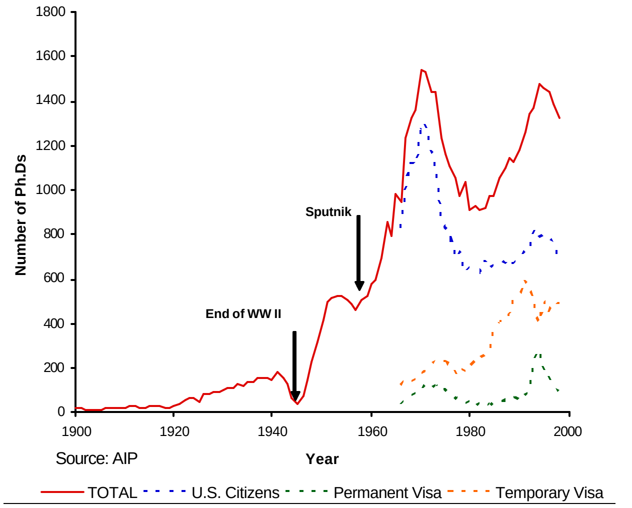
Summary of Research Direction, Relevance and Potential Impact

The challenge in securing clean, cheap and abundant energy for this century has long been overlooked. Responding to this challenge is both time-critical and complex.

Today, globally energy consumption is 13 TW per year, 25% of which is consumed by the American population. Experts and scholars agree that annually 50 TW of energy will have to be produced to supply enough energy to the 10-12 billions worldwide population expected in the year 2050. None of today's technologies or a combination of them can fulfill this demand. In fact, meeting the Terawatt Challenge, while complying with environmental requirements, will necessitate not only revolutionary scientific breakthroughs but also the mobilization of a critical mass of high skilled researchers, scholars, and students, as well as the continuous support from the general public. Preparing tomorrow's workforce to the energy challenge and educating the public are two enabling forces that support and complement research and development in energy.

In other words, strong human capital and outstanding technical talent are some of the many potential game-changers for securing our energy future and strengthening U.S. international competitiveness and leadership. The success in achieving this goal relies heavily on our ability to attract the best students in physical sciences and engineering and to attract them in a large enough quantity.

During the 20th century, massive federal investments in basic and applied research after World War II and the Sputnik mission have greatly contributed to the growth of the number of scientists and engineers, as illustrated in Figure 8-1. In the mid-1990s though, the growth was mostly due to the influx of foreign-born students, mostly from China. Today, nearly half of the total number of U.S. Ph.D. degrees awarded every year in physics is earned by students coming from overseas.

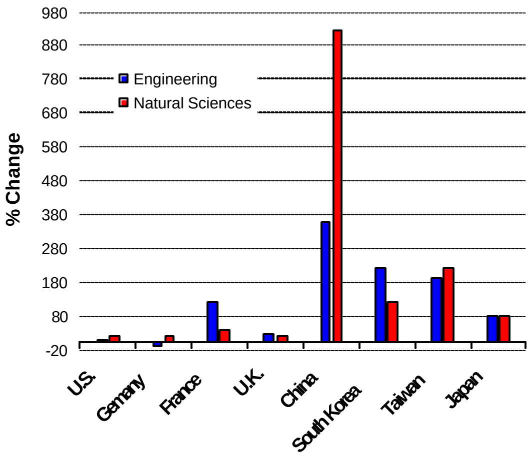


Source: AIP

Figure 8-1. Physics Ph.D. degrees awarded in the U.S.

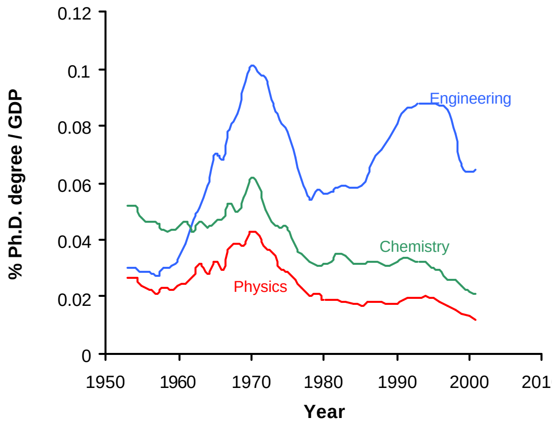
The American higher education system is loosing its edge in educating scientists and engineers. Figure 8-2 indicates that the U.S. has had one of the lowest growths of Ph.D. degrees in engineering and natural sciences between 1990 and 1999. China is greatly contributing to the worldwide growth of scientists and engineers. The same trend is observed at the undergraduate level. In fact, the number of students in engineering and natural sciences at the bachelor level increased by a factor of 1.4 in the U.S. between 1975 and 1998, while that of Pacific Rim tripled over the same period of time. For the first time, the pool of scientists and engineers worldwide is expanding faster in the Pacific Rim than in the U.S.

Clearly, the production of U.S. Ph.D. degrees in engineering, physics and chemistry (including U.S. and non-U.S. citizens), normalized to the gross of domestic product, has drastically decreased since the 1970s, reaching ever-lowest levels in 2001 (Figure 8-3). During the past decade only, the number of U.S. graduate students has decreased by 26% in physics, 19% in mathematics, and 10% in chemistry. Engineering though experienced a modest growth between 1885 and 1992, but has fallen since then.



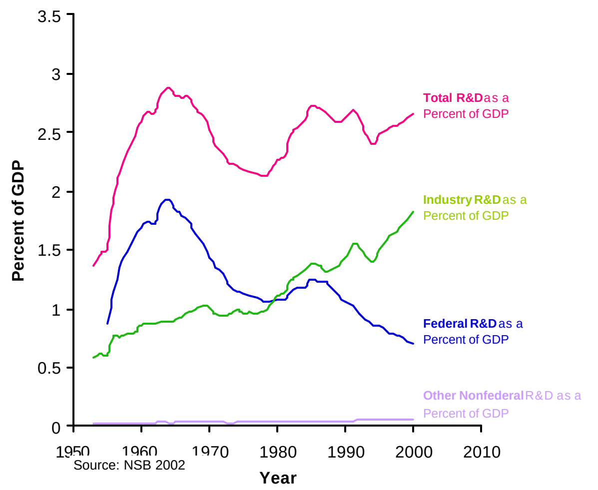
Natural sciences include physics, chemistry, astronomy, and biological, earth, atmospheric, and ocean sciences. Source: National Science Board, 2002. For France, Japan, and South Korea, % change corresponds to 1990-1998.

Figure 8-2. Trends in Ph.D. degrees granted between 1990 and 1999.



GDP is expressed in 1996 constant dollars (in million)
Source: AIP, ACS, AAES, and NSB

Figure 8-3. Production of U.S. Ph.D. degrees as percentage of GDP.



Source: NSB 2002

Figure 8-4. U.S. R&D funding as a percentage of GDP, by source.

The decline in the number of the U.S. graduate students in physical sciences and engineering is directly linked to the disinvestment of the federal government in research and development (Figure 8-4). The federal share of total U.S. R&D funding has decreased from 65% in 1965 down to 26% in the year 2000. Today, more than half of the U.S. R&D funding comes from the industrial sector, emphasizing the development of new products at the expense of basic discoveries.

The same trend applies for public investment in energy. The federal government has drastically disinvested in energy R&D during the 1980s. In the year 2000, the energy share of the total federal R&D budget was 1.4%, compared to12% in 1980.

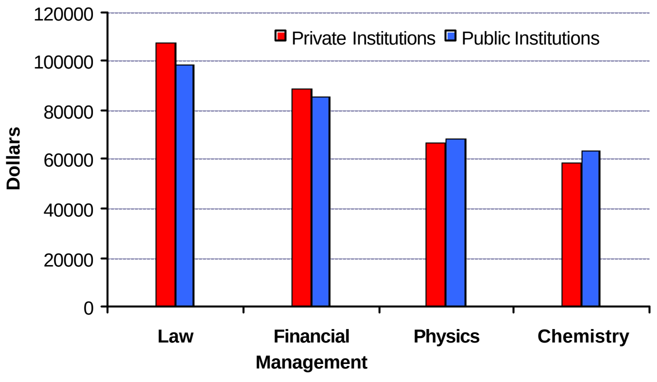
In addition to the burdensome decline in the number of American students in physical sciences and engineering, the U.S. will soon experience difficulties in renewing its highly qualified technical workforce. The energy industry has long experienced difficulties in recruiting trained workforce. Moreover, the scientist/researcher labor pool is ageing. The total number of retirements among workers holding degrees in science and engineering will increase significantly over the next 20 years. Meanwhile, the demand for physical scientists and engineers by the year 2010 will increase by 18% and 9%, respectively, according to the U.S. Bureau of Labor Statistics.

The decline of student enrollment and the relatively low attractiveness of scientific careers will make it difficult to renew the U.S. skilled workforce. For example, academic positions in physics and chemistry are financially poorly rewarded, as illustrated in Figure 8-5. The average faculty salaries in chemistry and physics departments is 20-46% lower than those in law and business schools.

In summary, federal disinvestment in science and engineering basic research, skills shortage and low attractiveness of scientific careers are weaknesses that are likely to hamper the rate of innovation, thereby undermining U.S. competitiveness over the coming decades.

There is a pressing need to reverse these trends: Strong human capital and skilled workforce are key assets to maintaining U.S. leadership in a knowledge-driven world economy.

It is recommended that DOE play a key role in raising the awareness of scientists, students, and the general public in the energy challenge



Source: College and University Professional Association for Human Resources

Figure 8-5. Average faculty salaries at 4-year institutions, 2001-2002.

and education issues. This can be achieved by compiling some background material in forms of PowerPoint slides on the theme: "In Search of Terawatts." This background material will include data and facts on energy that will reflect the needs for today and tomorrow's scientific grand challenges, both at the academic and industrial level. It will include, for example, data on funding research in physical science, energy consumption, production cost of electricity by source (coal, nuclear, gas, oil, wind, solar, and geothermal), energy reserves, energy costs versus efficiency, energy conversion, storage and distribution, population growth, and environmental issues. This background material will be distributed to DOE-supported scientists to help them build public talks for K-12 students, undergraduate students, teachers, scientists, and the general public.

Mass communication of the energy challenge to a broad audience will likely generate informed interest among the public and, more importantly, among the student community.

This proposed research direction, "Preparing Tomorrow's Workforce for the Energy Challenge," will have unprecedented impact on the realization of the scientific endeavor for solving the single most important challenge of this century: producing annually 50 TW of clean, cheap, sustainable and abundant energy by the year 2050.

Such an initiative will captivate the imagination of children, students, teachers, researchers and the public, and therefore contribute to developing the garden of science. If appropriately funded and supported by federal agencies, this could have a similar impact as that of the Sputnik mission.

Sources

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College and University Professional Association for Human Resources

Energy Biosciences Research

Energy Biotechnology: Metabolic Engineering of Plants and Microbes for Renewable Production of Fuels and Chemicals

Genomic Tools for the Development of Designer Energy and Chemical Crops

Nanoscale Hybrid Assemblies for the Photo-Induced Generation of Fuels and Chemicals

ENERGY BIOTECHNOLOGY: METABOLIC ENGINEERING OF PLANTS AND MICROBES FOR RENEWABLE PRODUCTION OF FUELS AND CHEMICALS*

EXECUTIVE SUMMARY

Emerging knowledge in functional genomics and molecular technologies provides new opportunities for the rational genetic improvement of plants and microorganisms to produce renewable sources of fuel and chemicals.

Plants are the primary producers of fixed carbon. During the past 10,000 years, plants have been extensively modified by humans to improve the production of food, feed, and fiber. An understanding of fundamental mechanisms that govern plant growth and development will allow the design of plants that can contribute to future energy security. This will require the ability to control plant architecture and composition (lignin, cellulose, hemicellulose, starch, and oils), along with improvements in the energy-efficiency of plant production (reduced nutrients, water, and land requirements) and an expansion in the range of environments that can be used for cultivation (salt tolerance and stress resistance). Improved genetic control of plants will allow production of novel biomaterials and increased efficiencies in renewable fuel production. Further advances in the fractionation of biomass into individual components using physical, enzymatic, and chemical treatments offer major opportunities for cost savings.

Metabolic engineering of new microbial biocatalysts offers the potential to produce novel biomaterials and chemicals that will serve as renewable alternatives to materials currently produced from petrochemicals. These improved microbial biocatalysts are required to expand the range of useful conditions for industrial fermentations and reduce costs through process simplification. Substantial cost savings can also be realized by the development of biocatalysts that produce enzymes (e.g., cellulase, xylanase, etc.) for carbohydrate depolymerization as coproducts during fermentation, eliminating the need for separate enzyme production facilities. Application of biochemical and genetic principles provide mechanisms for the rational design of improved enzymes concerned with the depolymerization of plant constituents and production of useful chemicals. Recent expansion in genomic sequences from microbes and plants provides a vast toolkit of genes and enzymes that can now be recombined and used to provide clean and sustainable solutions to our current dependence on imported petroleum.

Summary of Research Direction

Fossil fuel is the residue of ancient plants and microalgae that formed vast deposits of petroleum, coal, and natural gas. The ancient photosynthetic processes that produced these reservoirs of fossil energy also shaped our climate and the composition of our atmosphere. Storage of carbon in relatively inert fossil forms reduced atmospheric carbon dioxide and other compounds associated with planetary heating, and produced our oxygen-rich atmosphere. The vast scale of contemporary photosynthetic processes offers the opportunity to replace part of our dependence on fossil residues for energy and chemical feedstocks

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*This document incorporates portions of the Renewable and Solar Energy Team's Proposed Research Direction entitled "To Displace Imported Petroleum by Increasing the Cost-Competitive Production of Fuels and Chemicals from Renewable Biomass by a Hundred Fold."

with contemporary sources of renewable biomass. Biological transformations of renewable biomass materials also offer the opportunity to displace current petroleum-based chemicals and plastics using renewable and environmentally-friendly processes.

Approximately 0.2% of the current U.S. energy needs are supplied by renewable biomass, principally direct combustion (heating or electricity) or ethanol as a fuel extender and oxygenate (providing 2 billion gal/yr or 1.3% of total automotive fuel). Because of advances in genetic technologies, there are major new opportunities to increase the primary production of fuel and chemical feedstocks by genetic modification of plants for increased yield of useful constituents. In addition, there are important opportunities to improve technologies for the solubilization and conversion of plant constituents by the application of our emerging knowledge of microbial genomics. Broad implementation of biomass as a primary energy source in the U.S. and elsewhere will depend upon the genetic modification of plants to expand the range of soil environments for productive cultivation, to minimize nutrient requirements, and to increase crop productivity (tons/acre per year). These improved plants will become the feedstocks of the future. This is a long-term goal where sustained investment in fundamental research is essential. Results from these investigations will serve as a guide for the rational design of future improvements using a combination of traditional and molecular approaches.

To realize significant increases in primary biomass production, a systematic research program on plant metabolic engineering is imperative. An important objective should be to understand the mechanisms involved in the synthesis of cell wall polymers that are the principal constituents of biomass. Additionally, a focus on metabolomics, enzyme design and engineering, and metabolic modeling will be integral to achieving improved primary productivity of biomass and chemical feedstocks derived from carbohydrates or lipids. Understanding the factors that control plant adaptation to the environment and disease will also be important to maximizing yield and allowing the utilization of marginal land for biomass production. Areas of particular interest include salt tolerance, metal tolerance, and more efficient use of water and nutrients.

Research on microbial systems should focus on the development of improved bioconversion processes to produce chemicals (ethanol, longer chain alcohols, fatty esters, etc.) that can be blended with currently used automotive fuels (gasoline, diesel) and on the development of microbial processes for higher value coproducts (commodity chemicals, bio-based plastics) that displace petroleum and increase revenues. Under-utilized residues from agriculture and forestry, with little or no current value, represent a potential source of feedstocks for this area of application. Approximately 30 million tons of corn is currently converted to fuel ethanol in the U.S. by a mature industry using very efficient processes that take advantage of the highly digestible nature of starch by microbial enzymes. While this can continue to expand and make an important contribution to the energy security of our nation, the energy intensive nature of corn farming and competing uses of corn as food and feed will prevent the substantial replacement of automotive fuel by ethanol from corn alone. In contrast, the use of inexpensive lignocellulosic residues as feedstocks should have minimal impact on consumer costs for the primary products from agriculture (food, feed, and fiber). This new use represents an expanded benefit with minimal investment of additional energy. Additional fuels from lignocellulosics can be blended with gasoline to reduce petroleum imports while maintaining the benefits of corn-based ethanol production.

The high capital cost and increased risk associated with process complexity have thus far blocked the industrial implementation of many promising new technologies for production of biofuels and chemicals. Much of this process complexity can be reduced through the genetic engineering of improved microbial biocatalysts, the genetic improvement of plants for specific applications, and by improvements in plant fractionation technologies that increase efficiency and reduce costs.

New Scientific Opportunities

Many aspects of process complexity can be improved by the application of knowledge from microbial and plant genomics. Genomic sequences provide a catalogue of genes that can be used to alter cellular structure, composition, and function. These sequences provide a starting point for our understanding of integrated processes that limit the growth of plants, efficiency of water and nutrient use, the partitioning of photosynthate among cellular constituents, tolerances to extreme environments, and bioconversion processes by microorganisms. An exciting opportunity is to build on this knowledge base by discovering the corresponding gene functions and physiological activities. Our increasing knowledge of plants should also support the genetic modification of plant composition for specific bioconversion processes. Understanding the fundamental mechanisms that regulate the partitioning of photosynthate between carbohydrate polymers (cellulose, hemicellulose, starch), protein, lipid, and lignin should now allow rapid improvements in modifying plant composition for fuels and chemicals. For instance, increasing the lignin content with reduction in carbohydrate content would increase the energy density of plant residues intended for use in combustion.

Cellulose depolymerization by enzymes is arguably the single most expensive step associated with the bioconversion of lignocellulose to fuels and chemicals. Increased understanding of the molecular mechanism of glycohydrolases may lead to creation of more efficient enzymes that resist product inhibition. Additional approaches include the co-production of glycohydrolases by the microbial biocatalysts during fermentation and the co-production of glycohydrolases in the tissues of plants prior to harvesting for bioconversion. Significant reductions in added cellulase will also be achieved by improved understanding of the fundamental chemical and physical processes involved in the fractionation and solubilization of biomass.

Relevance and Potential Impact

The efficiency with which we have converted fossil biological energy sources into fuels and chemicals has allowed a tremendous expansion in population and improvement in the quality of life throughout the industrialized world. As we look toward a future that must rely upon alternative energy sources, the same fundamental biological processes that created fossil deposits and our oxygen-rich atmosphere can be harnessed to provide a renewable source of energy and chemicals. Traditional plant breeding coupled with chemical and microbial conversion processes has allowed tremendous increases in the production of food and food products over the past century. The application of the emerging field of metabolic engineering together with new advances in other areas of science and technology offer the opportunity for even greater improvements in bio-based products over the next 50 years. We envision that the application of knowledge-based methods to improvement of energy crops will provide similar gains in productivity to those realized in improvement of food crops by breeding. Increased productivity will improve the economic feasibility of growing and processing energy crops and will lead to expanded acreage of plants for energy production. We believe that a reasonable goal is to obtain a hundred-fold increase in contribution of renewable biomass (20% of energy needs) to our national security.

Estimated Time Scale

50 years

GENOMIC TOOLS FOR THE DEVELOPMENT OF DESIGNER ENERGY AND CHEMICAL CROPS

EXECUTIVE SUMMARY

Yields of usable energy per hectare of cultivated land must increase 3- to 5-fold if energy crops are to play a significant role in securing our energy future. There are no fundamental barriers to achieving the necessary gains, given a focused effort to genetically improve energy crops -- crops that will have efficient conversion of the CO_2, which is initially fixed by photosynthesis, into the specific chemical energy stores that are necessary for a particular utilization process.

Examples of the envisioned improvements in yields are as follows: from today's 3-5 dry tons/acre/yr to 12-15 dry tons/acre/yr in the upper Midwest, and from 4-5 dry tons/acre/yr to 15-20 dry tons/acre/yr in the Southeast. While yield of biomass dry matter is the single most important factor in a breakthrough to large and inexpensive supplies of biomass energy from energy crop production, other factors will also have key parts to play. These factors involve crop properties such as energy density, yield of liquid fuels (e.g., oils), and compatibility with other steps in the processes that lead from the crop as grown in the field to the final product. Reduction of the environmental impact of the entire energy cropping/energy production process is also an important goal that can be achieved through selective improvement of the feedstock plants.

Achieving these important goals will require research to dramatically improve the throughput, availability and cost-effectiveness of the genomic and informatics tools that are used to identify, functionally analyze and manipulate genetic combinations of the many genes that control critical plant properties. Recent advances in single molecule studies on DNA, including single molecule genomic mapping and single molecule sequencing, suggest that the necessary tools are within reach. These advances will both require and enable powerful new genome-centered informatics tools that have the potential to revolutionize the speed and precision of energy crop (and other plant) improvement.

Summary of Research Direction

Research in this area should: (1) develop molecular biological and other biotechnical means and databases to support efforts to aggressively increase energy crop yields; (2) emphasize especially the development of information and techniques that will speed and improve breeding and selection for high energy yields in crops (i.e., annual energy produced in the crop per unit of land area); (3) develop highly capable genomic tools for assisting the rapid development and improvement of novel energy/chemical crops and for the identification/characterization of key gene functions; and (4) map genes to guide breeding of plants with high yields and with other desired properties such as high oil content or ease of conversion to liquid fuels or high-value chemicals (e.g., chemical structures well suited for liquid fuels for the transportation sector).

This effort has four main components:

- Conduct a broad search for plants with both general and regional promise for development into energy crops;
- Develop highly capable genomic tools to accelerate the rapid improvement of these crops through conventional breeding;

- Develop tools for directed genetic engineering of critical crop properties; and
- Integrate goals for the genetic improvement of energy crops directly into the process engineering of the utilization/conversion systems that they feed.

New Scientific Opportunities

A partial listing of opportunities for scientific contributions is shown below. Elaboration of a select number of these opportunities follows in the remainder of this section.

- Genome mapping of candidate energy crops: poplar, eucalyptus, sugar-cane-like grasses, switchgrass, arondo donax (giant reed), other grasses, etc. (about 10 to 20 species)
- Bio-physical chemistry: correlating the physical and chemical processes/structures in plants to yields and to energy content or energy density, and to readiness to convert to liquid fuels or hydrogen, etc.
- Computational biology to go from basic structure to physical/chemical/biological properties to the complex factors that determine yield and energy content
- Microcalorimetry or other measurement techniques for early and fast correlation of genes to desired properties
- Extensions and correlations to and among trees, grasses, algae, bacteria, etc. on both macro and micro scales of living organisms (flora and fauna)
- Artificial chromosomes
- Genome-scale marker-assisted breeding
- Optical mapping of whole genomes
- Direct sequencing of single DNA molecules

While certain plants, such as poplar and switchgrass, have been identified as likely candidate biomass energy crops, it is not obvious which of these or other essentially wild species have the greatest potential for net solar energy conversion efficiency in a particular utilization scheme once subjected to intensive genetic improvement. This is especially true given wide variations in environmental conditions from location to location where energy crops will be needed. It is important that a number of candidate species be explored and developed in parallel and that they be differentially tailored for a set of different utilization schemes. Development programs must be conducted over the range of different environmental zones where energy crops will be needed.

The current productivity of established crop improvement programs depends upon a range of molecular tools for “marker-assisted breeding” and upon computer analyses that reveal the identity of genes that make even subtle but important contributions to plant qualities. The application of similar genomic and computational tools to the development and improvement of novel energy crops will be essential in order to obtain improvements at a pace that matches the need for developing renewable energy resources.

However, the analytic capacity of current genomic analysis tools is inadequate to support the development of multiple new species with multiple improvement program goals at multiple sites. To support the goals of energy crop improvement, these tools must become much less expensive (100-1000 fold less expensive for complete genome sequencing), have higher throughput (complete genome characterization in hours instead of years), and be more accessible (distributed in local labs instead of concentrated in centers). Genomic analysis in breeding programs must provide sufficient detail to identify the specific genes that contribute to critical plant characteristics and to manipulate their recombination at the resolution of individual genes. Recent developments such as methods for optical mapping of whole genomes and for direct sequencing of single DNA molecules offer the promise that a focused research effort can develop the necessary tools over the next half decade.

The worldwide genomics effort directed toward understanding the roles of specific genes in regulating vital characteristics of model and crop plants is continuing to identify genes that could contribute in important ways to the improvement of novel energy crop varieties. In some cases, it will be appropriate to move genes from one species to another in order to achieve specific goals. Tools for transferring genes, including groups of genes, into energy crops will be needed. For the purposes of assuring predictable outcomes and of easing the combination of transgenic with traditional breeding methods, the development of artificial chromosome vectors for energy crop species is important.

The net efficiency of energy cropping systems depends not only on the internal conversion efficiencies of the plant but also on the efficiency with which its constituents are used by the downstream processes that it feeds. In many cases it may be possible to solve difficult engineering problems in the utilization process by instead engineering genetically-controlled properties of the feedstock plants themselves. Genetic modification of feedstocks also has the capacity for minimizing the environmental impacts of the overall process. An understanding of how plant properties contribute to net energy efficiency and to environmental impacts requires a new level of integration of genetic and process engineering.

Relevance and Potential Impact

Yields of up to 3 to 5 times those now achieved in mid-scale plantings of energy crops – plantings of about 20 to 2000 acres – are needed to make energy crop fuels or feedstocks production and cost competitive with those of conventional fuels. Energy crop fuels at these higher yields would enable biomass energy to rise to a potential of 10-20% of U.S. energy, instead of the 2% role that could well be the upper bound if residues and wastes are the only feasible fuels/feedstocks. Examples of the envisioned improvements in yields are as follows: from today’s 3-5 dry tons/acre/yr to 12-15 dry tons/acre/yr in the upper Midwest (Missouri, Iowa, Illinois, Wisconsin, Minnesota, and the Dakotas), and from 4-5 dry tons/acre/yr to 15-20 dry tons/acre/yr in the Southeast.

Yields of usable energy per hectare of cultivated land that is captured from solar radiation and conserved by plant photosynthesis must increase 3- to 5-fold if energy crops are to play a significant role in securing our energy future. An important element of the challenge involved in achieving these improvements is that transportation factors limit the scope of energy cropping to relatively local utilization. Another important element is that the measure of "usable energy" will depend upon whether the crop is used directly for local heat or electricity generation or is converted first to liquid fuels, methane or hydrogen. It will also depend upon details of the specific process that is involved in the utilization scheme. Different plants have different value in different processes. There are no fundamental barriers to achieving the necessary gains, given a focused effort to develop improved "designer" energy crops with efficient conversion of the CO_2 that is initially fixed by photosynthesis into the specific chemical energy stores that are necessary for a particular utilization process.

However, all biomass energy processes incur a fuel cost – usually called fuel cost for a power plant, but feedstock cost for an industrial plant that is making a fuel, chemical or fertilizer product. The fuel or feedstock is a raw biomass material that, in the case considered here, is harvested from an energy crop. The gain of 3 to 5 required is what can bring the feedstock cost down to the low levels that can be economic for the power plant or processing plant. Therefore, the achievement of much higher yields of energy harvested per unit of farmland area is what can do the most to change the economics.

High yields are also the key to making biomass a 10-20% energy source, rather than one that is constrained by economics and by available land to a 1-5% energy role.

The number of processing steps and the difficulty of feedstock handling are also factors in the economics, and often as important or more important than the feedstock cost. Therefore the improved energy density and the improved ease of processing to final product are also important. These fuel or feedstock properties are also capable of improvement by genomic tools. The precedent of food crops today that are unrecognizable versus their wild type origins show the promise of genomic improvement via information, even without any manipulation, i.e., without genetic engineering and creation of genetically modified organisms. This research direction is the path to such productivity of desired products. It continues the normal "domestication" process and applies it to new crops and new products. The fact that the technical tools are so much improved today makes the prospect for great enhancement and true breakthroughs all the much greater.

This section includes relevance to applied energy programs (e.g., Fossil, Nuclear, Energy Efficiency, Renewable Energy, Fusion). In this case these applications are to all of the biomass energy technologies and uses within DOE's Office of the Biomass Program. Applied to improved environmental performance and environmental remediation efforts, many of DOE's environmental missions may also benefit from application of this research direction.

Estimated Time Scale

5-10 years: Development of genomic analysis tools with sufficient capacity to support aggressive energy crop improvement.

10-20 years: Exploitation of these genomic analysis tools in the production of 3-5 fold increases of energy crop process yields.

NANOSCALE HYBRID ASSEMBLIES FOR THE PHOTO-INDUCED GENERATION OF FUELS AND CHEMICALS

EXECUTIVE SUMMARY

Efficient synthesis of fuels like hydrogen and carbon-based chemicals from renewable sources (e.g., water and CO_2) using sunlight as the energy source, is a major opportunity for securing our energy future. The main obstacle to realizing this opportunity in direct solar conversion systems is the lack of photoactive materials that accomplish the combined task of light harvesting, charge separation, and chemical transformation with the required efficiency. Approaches based on inorganic or organic materials have many promising features, but some of the components lack the efficiency and specificity of natural systems. New discoveries over the past ten years of nanoporous inorganic, organic, and inorganic/organic hybrid structures with pore or cavity sizes in the 10-300 Angstrom range show promise for overcoming these limitations. These materials allow robust covalent anchoring of metals, organic, and biological moieties inside the pores. The potential for unprecedented efficiency lies in the tight control of the chemical reactivity through design of the reactant binding site, the controlled spatial arrangement of the active components, the traffic control of chemical intermediates imposed by the pore environment, and efficient ways to separate primary products. Substantial advances have also been made in recent years in the understanding of design principles and mechanisms of natural systems that accomplish demanding energy-related transformations, notably bacterial and plant photosynthesis. The confluence of the emerging nanoscale hybrid materials and advances in the understanding of nature's design rules of its photosynthetic and catalytic systems opens up opportunities for combining biological and inorganic/organic components in engineered assemblies for the direct photo-induced conversion of renewable substrates to fuels and chemicals at unprecedented efficiencies. A major research task involves the elucidation and understanding of the dynamics of biological components in the natural environment, which will provide a guide for the design of hybrid materials that retain the full activity of the natural component. Biological principles of chemical recognition provide insights into technologies for the nanoscale self-assembly of these hybrid structures. Another important challenge is the development of strategies for organizing the nanoscale assemblies relative to one another in order to achieve concerted, macro-scale effects.

Summary of Research Direction

The discovery over the past 10 years of novel nanoporous inorganic, organic, and inorganic/organic hybrid structures with pore or cavity sizes in the 10-300 Angstrom range and a variety of topologies has opened up new materials for efficiently accomplishing demanding chemical transformations. Key ingredients are transition metal centers or organic moieties attached to pore walls that act as active sites with specific reactivity. Controlled spatial arrangement of these sites, coupled with the molecular traffic control imposed by the pore environment on chemical intermediates, allows steering of reactions to desired products. In principle, functionalization of these porous structures can be expanded to include active biological entities, thus offering opportunities for hybrid reactors that feature the highly efficient and product-specific components of natural systems. Substantial advances have also been made in recent years in the understanding of design principles and mechanisms of natural systems that accomplish demanding energy-related transformations, notably bacterial and plant photosynthesis. Specifically, the use of novel spectroscopic, diffractometric, advanced computational, and molecular genetics tools has led to detailed insights into structural and dynamic aspects of light harvesting, energy and electron transfer, and chemical transformations at the catalytic sites of photosynthetic systems.

New Scientific Opportunities

The confluence of the emerging nanoscale hybrid materials and advances in the understanding of nature's design rules of its photosynthetic and catalytic systems opens up opportunities for combining biological and inorganic/organic components in engineered assemblies with unprecedented efficiencies for the conversion of solar photons to fuels and chemicals. Hybrid assemblies for the efficient photo-induced conversion of renewable substrates to fuels, like water splitting to H_2 and O_2, and the conversion of CO_2 and H_2O to methanol or other C-based fuels are a top priority. Such materials are equally expected to lead to efficiency breakthroughs in a broad range of photon harvesting, storage and conversion chemistries. This holds especially for efficient catalytic multi-electron transfer assemblies, the current lack of which constitutes a major obstacle to progress in photon energy conversion and storage, and fuel-reforming systems in direct photon conversion, photo-electrochemical, or fuel cell systems. Assemblies could range from predominantly inorganic/organic structures featuring metallic or organic active sites and just one or two biological functionalities, to essentially biological structures with only a few engineered components. Examples of current possibilities for the former include dendritic light harvesting assemblies coupled to biological or engineered transition metal centers, or mesoporous inorganic (e.g., silicate) frameworks that afford controlled spatial arrangement of covalently-anchored light-absorbing chromophores and engineered or biological transition metal redox sites. With the anticipated vigorous development of new types of nanoscale materials, new opportunities will emerge for improved coupling of light harvesting moieties with catalytic sites, channeling of sequences of reactions, and efficient ways of separating primary products. Near term examples of the predominantly biological assemblies are the generation of hydrogen by genetically engineered green algae and the use of photosynthetic reaction centers modified to produce alternative chemicals. In both cases, the separation of desired products from undesirable co-products poses challenges in the purely biological system that may be overcome by the incorporation of non-biological elements. In the case of photosynthetic hydrogen production, H_2 and O_2 are intermixed in the gas released by the algae. Hybrid systems that incorporate the unique compartmentalization properties of nanoporous supports may provide methods for separating the two gases that do not also catalyze their recombination into water.

Exploration of such hybrid assemblies will be guided by design concepts derived from natural systems, and a vigorous effort for further development of spectroscopic, diffractometric, computational, and molecular genetics tools is required for a mechanistic and dynamical understanding of the chemical transformations of natural and emerging hybrid systems. In particular, structural aspects of the matrix environment of the biological component in hybrid materials are expected to critically affect its function by influencing product release or the dynamics of substrate binding to the catalytic site. Furthermore, the conformational response of surrounding protein or membrane molecules may be critical for the activity of the natural system and, hence, an important factor to consider when incorporating biological components into artificial assemblies. Elucidation of the dynamics is still at an early stage in natural systems, and a major sustained effort is required to improve the understanding of these factors. This knowledge will be crucial for the design of hybrid assemblies.

The function of complex systems of nanoscale catalysts depends very strongly on their organization. The extremely specific molecular recognition properties of biological macromolecules suggest that they may provide solutions to the problem of assembling these complexes. As one example, a designed sequence DNA molecule could provide the scaffold for the self-assembly of catalytic domains (biological, organic or inorganic) that are attached to sequence-specific DNA binding proteins, such as transcription factors or synthetic analogs. An important challenge is the development of strategies for organizing these nanoscale assemblies relative to one another in order to achieve concerted, macro-scale effects. For instance, a nanoscale assembly capable of catalyzing direct water photolysis may be inserted into a membrane such that H_2 is produced on one side and O_2 on the other. All of the assemblies must be inserted into the membrane in the same direction in order to achieve a large-scale production of pure H_2.

Relevance and Potential Impact

The direct use of sunlight for the synthesis of fuels or the storage of solar energy in the form of other high-energy chemicals has the potential of playing a major role in replacing fossil fuels as an energy source. In light of the extreme variety of hybrid materials expected from this research effort, fueled by the anticipated continued rapid pace of discovery of new nanoscale structures and advances in the understanding of natural systems, the likelihood of artificial photosynthetic materials that are efficient, durable, and economically feasible is high.

Estimated Time Scale

10-20 years

APPENDIX B

FACTUAL DOCUMENT

INTRODUCTION

This document consists of a series of white papers providing data and background on key energy sources and applications that sustain the U.S. and international economies. These papers have been prepared to support the Office of Basic Energy Sciences (BES) and their Advisory Committee (BESAC) in their evaluation of energy research needs and options for the future. Based on the panel structure established for this evaluation, these white papers address the following energy options:

- fossil energy (including coal, gas, and oil)
- nuclear fission energy
- renewable and solar energy
- nuclear fusion energy
- distributed power generation, fuel cells, and hydrogen
- transportation energy consumption
- residential, commercial, and industrial consumption

Standalone papers have been prepared for each of these panel topic areas. As a result, some repetition exists among the topics. For example, fuel cells are discussed briefly in several papers, but covered in detail under distributed generation.

In addition to background information, the papers also include some discussion of relevant research activities and opportunities. It is important to mention that much energy technology research is more applied than typical for BES. Such research is likely funded by private industry or the DOE applied program offices (e.g., Energy Efficiency or Nuclear Energy). The discussion of applied research can clarify the range of issues that must be dealt with before a given technology can be successfully implemented, and may be helpful in defining the research components of interest to BES. Each of the white papers includes a list of references or resource materials. In addition, most of the data was obtained from the *Annual Energy Review, Annual Energy Outlook,* and the *International Energy Outlook* .

To provide a common base of comparison, the energy data was converted from traditional units such as Quad (10^{15} Btu) and kWh to SI units. For example, the closest equivalent to the Quad is an Exa-Joule (EJ) (10^{18} J), where 1 Quad = 1.055 EJ. A list of conversion factors for common energy units is contained in Table 1.1.

Table 1.1. Energy conversion factors for common units

Conversion factors	Metric prefixes
1 Watt (W) = 1 Joule/second (J/s)	milli = m = 10^{-3}
1 Quad = 1 x 10^{15} Btu = 1.055 x 10^{18} J = 1.055 EJ	pico = p = 10^{-12}
1 barrel oil = 5.63 x 10^{9} Joule = 5.63 GJ	Kilo = k = 10^{3}
1 cubic ft gas = 1.08 MJ	Mega = M = 10^{6}
1 ton coal = 22.2 GJ	Giga = G = 10^{9}
1 kWh = 3.6 MJ	Tera = T = 10^{12}
10^{9} kWh = 3.6 x 10^{15} J = 3.6 x 10^{-3} EJ	Peta = P = 10^{15}
	Exa = E = 10^{18}

Although this document focuses on U.S. energy research needs, the issues of U.S. energy production and consumption can not be divorced from international energy issues. Therefore, this introduction will be presented in three parts. First, some aspects of the current global energy picture will be summarized. This will be followed by a section that presents recent U.S. energy supply and consumption data. A comparison of U.S. and international energy consumption data will comprise the final segment.

Global Energy Issues

To properly assess future U.S. energy needs, it is necessary to compare current energy consumption with the anticipated future global energy picture. The mean global energy consumption rate was 13 TW in the year 2000, with the U.S. consuming about a quarter of that amount. Of this, oil accounted for 4.5 TW, coal for 3 TW, natural gas for 2.7 TW, hydro for 0.3 TW, biomass for 1.2 TW, and other sources 1.8 TW. Note that a mean energy consumption rate of 1 TW= 31.5 EJ/yr.

The world population is expected to grow to 10-11 billion people by the year 2050, and this growth will be concentrated in the developing counties. This population growth, together with the standard of living goals for these developing countries, will have a substantial impact on energy consumption patterns if reduced emission of greenhouse gases becomes an important goal. Meeting these emerging energy needs without increasing greenhouse gas levels will limit the use of fossil fuels everywhere in the world, including the U.S., and require huge amounts of carbon-free energy.

The required quantities of energy are quite staggering, and have been summarized in recent publications [Hoffert, 1998; Hoffert, et al., 2002]. Energy projections are strongly dependent on the assumptions made in extrapolating current trends. The essence of the analysis by Hoffert and coworkers is based on three reasonable assumptions:

1. an expected population of 10-11 billion by the year 2050,
2. an increase in the average world Gross Domestic Product (GDP) of 1.6%/yr (historical average),
3. energy growth is counterbalanced by a decrease of 1%/yr in the energy consumption per unit of GDP because of expected increases in the efficiency of energy utilization.

These assumptions result in an expected energy consumption in the year 2050 of 28 TW, which is more than double the present world energy consumption rate of 13 TW. Although fossil fuel resources and proven reserves are huge (40,000 EJ for oil plus gas and 180,000 EJ for coal, enabling their possible use for about 50 years for oil and gas and 275 years for coal), their use may be severely restricted by the problems of CO_2 emissions.

The present CO_2 concentration in the atmosphere is 325 ppm, compared with a pre-industrial value of ~275 ppm. If the CO_2 concentration in the atmosphere is to be restricted to 550 ppm in the year 2050 (which is twice the pre-industrial value), about 20 TW of carbon-free power will be required. This is appreciably more than the total world energy consumption today. Furthermore, even if no restrictions on CO_2 emissions were implemented, just to maintain the present rate of decrease in carbon intensity of energy utilization (at a rate of –0.56 kg C/yr/watt) will require 10 TW of carbon-free energy by year 2050. This is also a huge and daunting requirement. A similar case for the need for daunting amounts of carbon-free power can be advanced based on sustainability arguments even in the absence of greenhouse gas effects.

Global electricity production amounted to about 1.3 TW in 1998. Of this, nuclear power provided 0.83 TW. Hydroelectric power produced 0.29 TW as the largest renewable power source. The 1.2 TW of biomass power produced in 1998 was unsustainably burned biomass, as opposed to renewably-farmed biomass. Other renewable energy, including renewable biomass, provided only 0.29 TW of power. Sustainable biomass power production, which can be broken down into electrical power, heat, and ethanol, contributed a total of 10^{-1} TW out of the 12-13 TW of total primary power produced globally in 1998. Wind produced $2x10^{-3}$ TW of power. Solar electric power production is growing rapidly, but from a very small base, providing about one-millionth of the total global primary power. Solar thermal and other renewable resources are also currently small fractions of the overall primary energy supply.

The available global renewable resources are estimated to be: (1) hydro: 4.6 TW total, 0.9 TW practical, and 0.7 TW already installed; (2) wind: 50 TW total on land, 2 TW practical on land (higher if oceans are utilized); (3) biomass: 5-10 TW total (not considering land required for food production and utilizing 100% of the cultivatable cropland for energy production); (4) solar: 1.2×10^5 TW total; practical: 600 TW (60 TW at 10% conversion efficiency) (to generate 12 TW of solar power at 10% efficiency would require 0.1% of the worlds land mass). Nuclear energy from fission can provide substantial amounts of carbon-free electricity and process heat from known uranium resources for about 50 to 100 years at current levels of consumption. The implementation of known breeder reactor technology would significantly extend the time over which fission could contribute.

These numbers suggest that among the energy sources traditionally considered to be “renewable,” only solar could provide the required carbon-free energy. This could be implemented as biomass or as photovoltaic or advanced solar conversion technology. However, breakthroughs and disruptive technology are required to achieve such a level of implementation. Similarly, nuclear fusion remains a promising long-term energy source, with substantial research and development required before it can contribute to global energy production.

U.S. energy supplies and consumption

Figures 1.1 to 1.5 represent energy sources and energy consumption in the U.S. for the year 2000. The data in Figures 1.1 to 1.4 emphasize both relative and absolute values in each case.

Figure 1.1 shows sources of energy used. Values are for domestically produced supplies, except for net imports. Net imports include oil (25.8 EJ), gas (4.1 EJ), and other (0.8 EJ) imports, minus oil (2.3 EJ), gas (0.3 EJ) and coal (1.6 EJ) exports.

U.S. energy consumption values shown in Figure 1.2 include both end-use consumption by the major sectors of the economy plus the energy lost as heat through generating electricity at power plants. Electricity generation on average was 32% efficient, with 68% of energy lost in conversion. Each sector includes both electricity end-use and primary energy use (i.e., oil or gas).

The primary energy sources used in generating electricity are compared in Figure 1.3. This includes co-generated electricity sold on the grid, but does not include electricity generated by industrial firms and used on-site. Coal represents the major contributing source for generation.

Both electricity and non-electricity generating sources of renewable energy are shown in Figure 1.4. Starting clockwise in Figure 1.4, Hydro through Wind represents the renewable energy used for electrical generation available on the power grid. Hydro-Industrial through all Biomass uses represents energy used directly in the sector. Biomass-Residential represents wood burning sources. Ethanol production is used in gasoline blending.

As shown in Figure 1.5, use of electricity is almost evenly split among residential, commercial, and industrial sectors. Electricity represents only 13% (3.9/29) of overall energy use for the industrial sector versus 36% for residential and 46% for commercial use. Electricity use in transportation is negligible.

The categories of proven fossil energy reserves for both the U.S. and international communities are shown in Figure 1.6. The data does not include nonproven reserves such as oil shale or tar sands. Coal dominates the fossil reserves. The U.S. has a significant fraction of the total coal supplies but much smaller proportions of the oil and gas supplies.

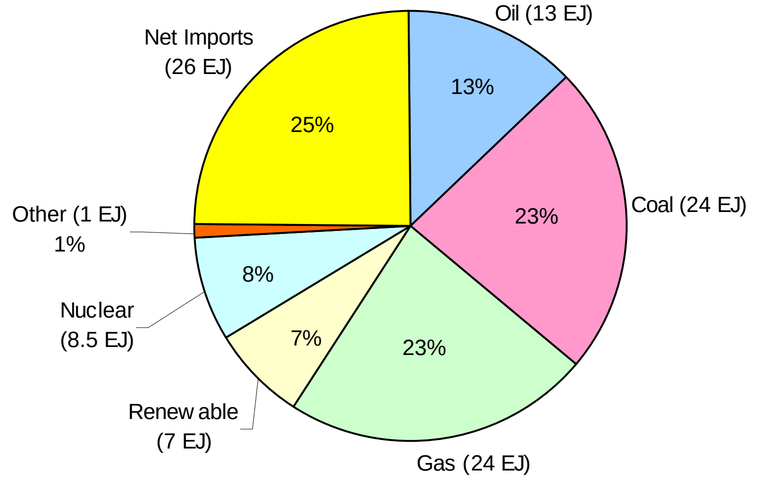

Figure 1.1. Year 2000 U.S. Energy Supply (EJ)
Source: EIA 2002

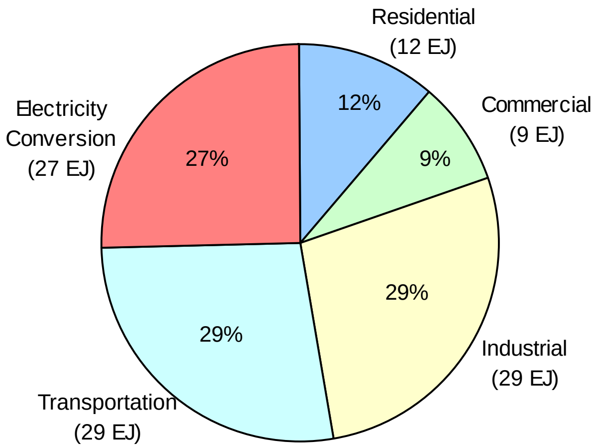

Figure 1.2. Year 2000 U.S. Energy Consumption (EJ)
Source: EIA 2002

Comparison of U.S. energy and international energy consumption

Figure 1.7 compares U.S. and international consumption of primary energy sources in the year 1999. Energy consumption data for individual countries, along with their GDP expressed in 1997 U.S. dollars, is listed in Table 1.2. The U.S. is characterized by both high-energy consumption and high GDP. The third column in the table lists the energy consumption per unit GDP. Based on this parameter, the U.S. appears less efficient than many industrialized nations, but much more efficient than most developing nations.

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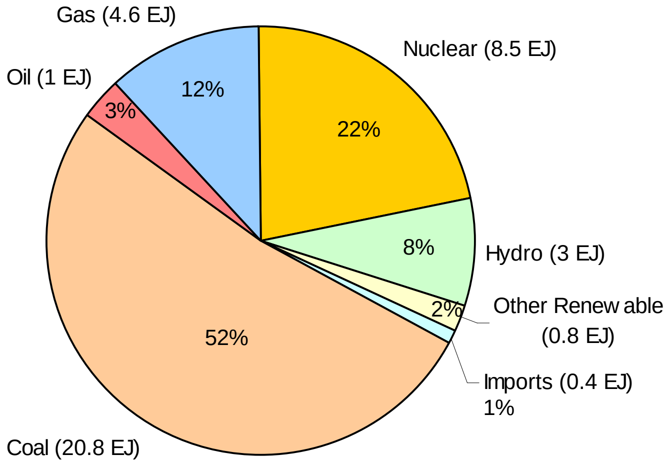

Figure 1.3. Year 2000 U.S. Electricity Generation (EJ)
Source: EIA 2002

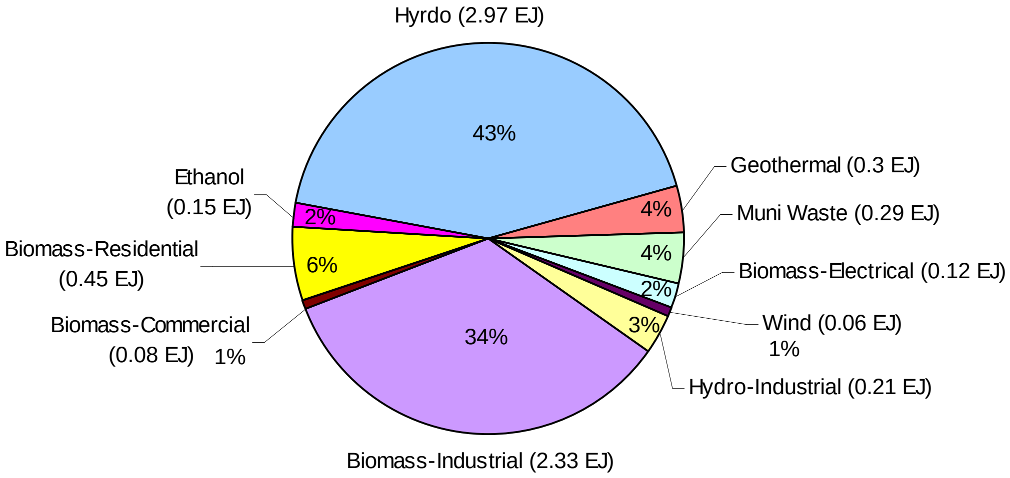

Figure 1.4. Relative Contribution of Various Renewable Energy Sources in Year 2000 (EJ)
Source: EIA 2002

Other Resources

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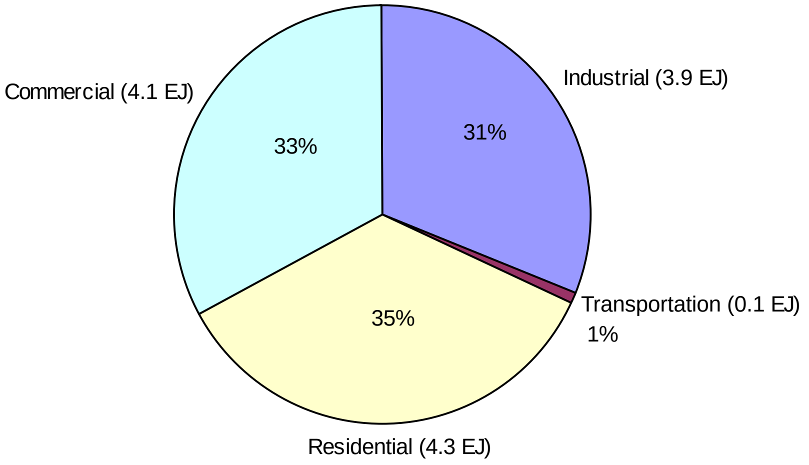

Figure 1.5. Year 2000 U.S. Electricity Consumption (EJ)
Source: EIA 2002

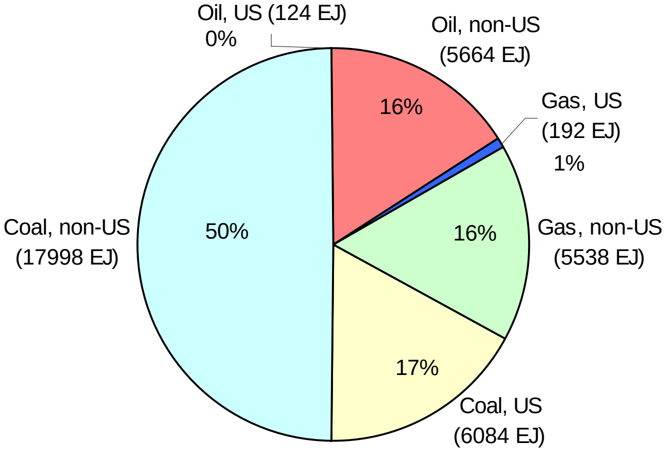

Figure 1.6. World Fossil Energy Proven Reserves (EJ)
Source: EIA 2002

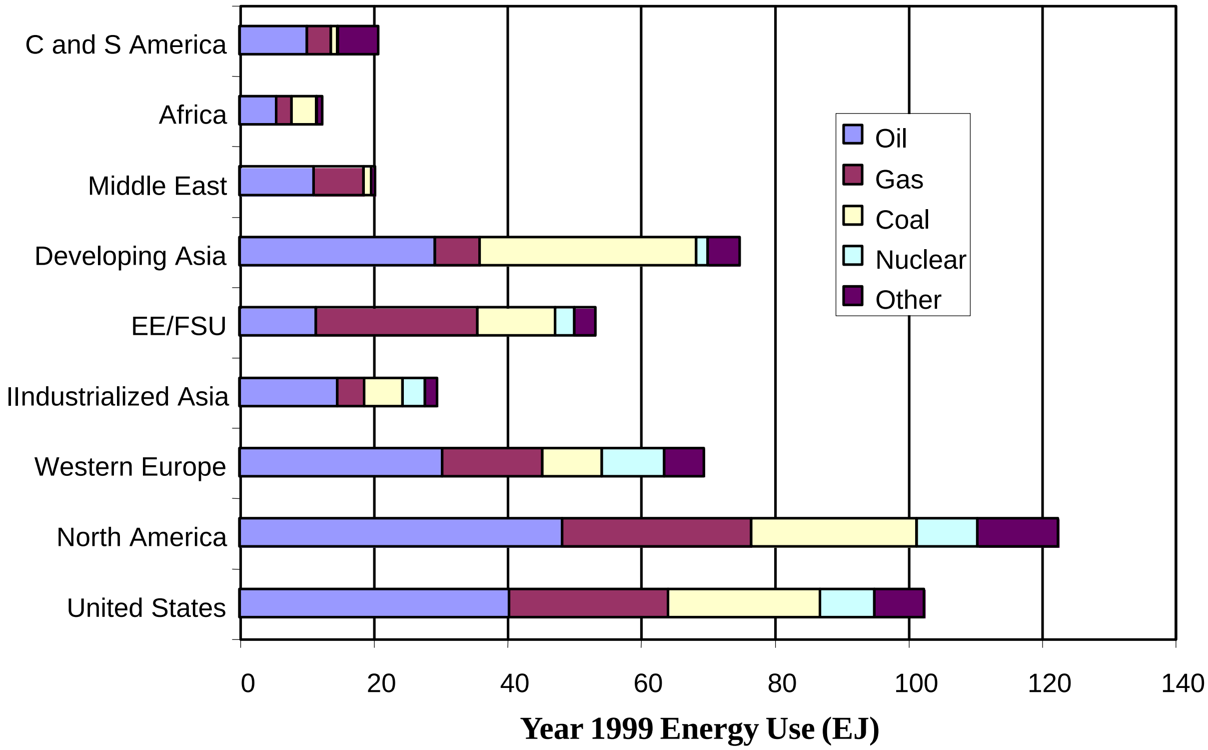

Figure 1.7. Year 1999 International Energy Use by Region and Fuel Source
Source: IEO-2002

Table 1.2. Year 1999 World Energy Use and GDP by Country and Region

	GDP (Billion 1997 $)	Energy (EJ)	MJ per $ GDP
North America	10,165	122	12.0
United States	9,029	102	11.3
Canada	699	13	18.9
Mexico	437	6	14.7
Western Europe	8,944	70	7.8
United Kingdom	1,384	10	7.5
France	1,499	11	7.2
Germany	2,187	15	6.8
Italy	1,207	8	7.0
Netherlands	407	4	9.9
Other Western Europe	2,260	21	9.3
Industrialized Asia	4,821	29	6.1
Japan	4,304	23	5.3
Australasia	516	7	12.7
Total Industrialized	23,930	221	9.2
Former Soviet Union	569	41	72.7
Eastern Europe	363	12	32.6
Total EE/FSU	932	53	57.1
Developing Asia	3,165	75	23.6
China	1,037	34	32.5
India	473	13	27.2
South Korea	493	8	15.6
Other Asia	1,162	21	17.7
Middle East	577	20	35.3
Turkey	186	3	17.0
Other Middle East	391	17	44.3
Africa	499	12	25.0
Central and South America	1,452	21	14.4
Brazil	816	9	11.0
Other Central/South America	636	12	18.6
Total Developing	5,693	129	22.6
Total World	30,555	403	13.2

FOSSIL ENERGY

Introduction

Fossil energy resources are currently the backbone of the U.S. energy system, both for stationary (power plant and industrial), and non-stationary (transportation) applications. Their continued availability in the short term is critical to the health and growth of the U.S. economy. Their reasonable prices establish the ground rules for the competition among different fuels. The different fossil fuels will not always fill the same roles in the future that they do in the current economy because they have highly variable resources bases, but there will be critical select applications for which each of the fossil fuels will always remain the best among all of the alternatives. Ensuring energy security requires making the needed fuels available in quantities (and therefore at prices) that will maintain U.S. economic security.

This section outlines the current situation with respect to the major fossil fuel groupings, and provides information on current applied research priorities within DOE's Office of Fossil Energy. Reviewing the situation and the midterm applied program objectives is important in order to understand what we are currently doing. This helps focus attention on the many unknowns that will be the objectives of any fundamental research program.

Coal

Supply and Demand

Of the three main fossil fuels used today (coal, petroleum, natural gas), coal has the largest reserves, both domestically and worldwide (Table 2.1). Domestic use totaled 24 EJ (23 Quads) [EIA 2001], while domestic recoverable reserves totaled 6,100 EJ (275 billion short tons) [EIA 2002]. At current rates, the U.S. has over 250 years of existing recoverable coal reserves.

There are several varieties of coal (lignite, subbituminous, bituminous, and anthracite) with varying qualities, such as heat and ash content. Bituminous and subbituminous coals are most often used for electricity production, while some power plants use lignite. Anthracite is of higher quality and used more for coking operations or other industrial needs. Over 89% of coal in the U.S. is consumed by electric generators, with 3% by coking plants and 8% by other industrial users.

Table 2.1. Fossil Fuel Reserves (EJ)

	U.S.	Global
Coal	6,084	24, 082
Petroleum	124	5,788
Natural Gas	192	5,731

Source: EIA 1999

Coal is mined from the surface or underground, depending on the geology and topography of the coal seam. Each mining process has its advantages and disadvantages. Surface mining is generally more disruptive to the environment. Underground mining is more dangerous and expensive. The country can be divided into three main coal regions: Appalachia, the Interior, and the West (Figure 2.1). The largest production of coal is through surface mining in the West (Figure 2.2).

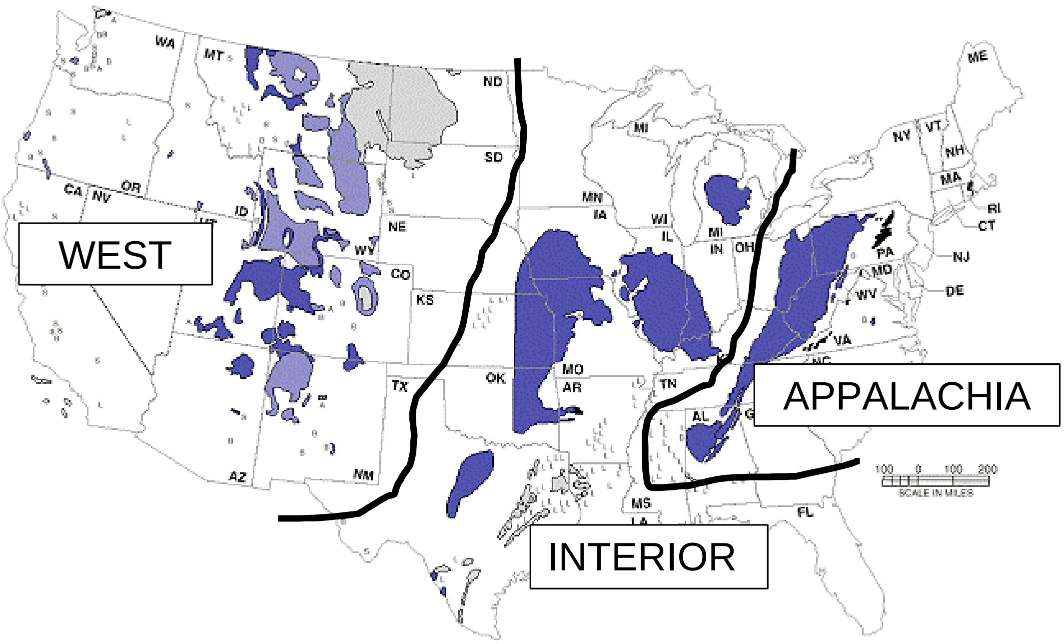

Figure 2.1. U.S. Coal Regions
Source: EIA 1999

Sulfur content is a key parameter for coal (Table 2.2); the quality varies with regional location. High-sulfur coal is found largely in the Interior and Appalachia and low-sulfur in the West (Figure 2.3). While this figure shows recoverable reserves, the demonstrated reserve base is roughly double this amount.

Because of emissions regulations and mining costs, the move towards the use of western low-sulfur, surface-mined coal has increased greatly. Between the years 1989 and 2001, western coal production increased 71%, while Appalachian coal production declined 8% and Interior production declined 25% [EIA 2002].

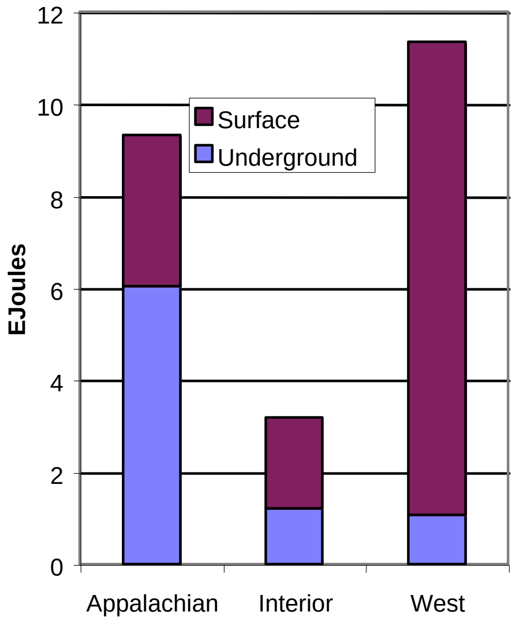

Figure 2.2. Year 2000 U.S. Coal Production by Region and Mining Type
Source: EIA 1999

Table 2.2. Average SO_2 Content of Different Classes of Coal

	lb/MBtu	g/MJ
Low Sulfur	0.6	0.26
Med Sulfur	1.9	0.81
High Sulfur	4.5	1.93

Source: EIA 1999

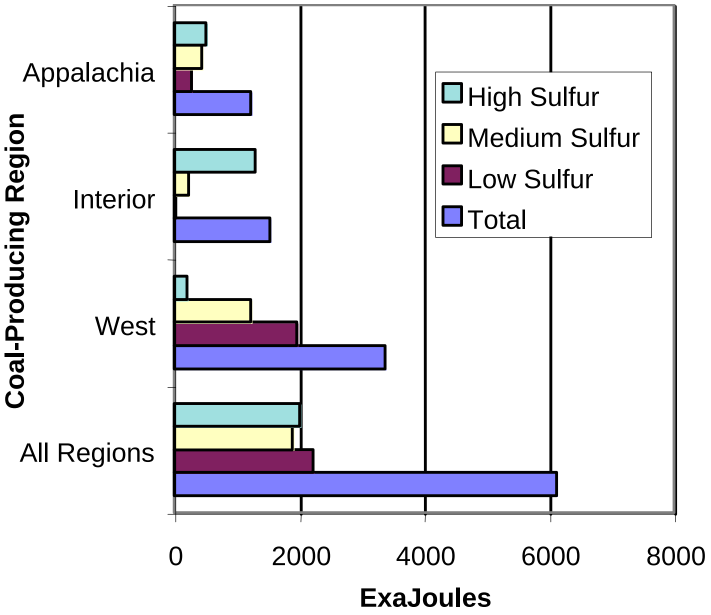

Figure 2.3. U.S. Estimated Recoverable Coal Reserves
Source: EIA 1999

Issues

The key long-term issue for use of coal is the nature and volume of emissions. These include SO_2, NO_X and the amount of greenhouse gas emitted. Coal contains 24.4 g Carbon/MJ, while natural gas emits just 13.7 g C/MJ. Nuclear or renewable sources release essentially net zero greenhouse gases (depending on the amount of fossil fuel used in their production).

Other contaminants in coal are also a major issue. Sulfur emissions from all fuels have been regulated for years, with recent proposals from the U.S. government to lower the limits by 73% by the year 2018. Mercury is another air pollutant, deriving largely from the use of coal. The U.S. government's "Clear Skies" proposal will reduce mercury emissions 69%, from the current 48 tons to 15 tons. Though coal combustion produces significant amounts of nitrogen oxides, it is not the major source of NO_X within the U.S. All fossil fuels produce NO_X, especially petroleum from motor vehicles. However, within the electricity sector, coal is a significant source of emission of NO_X, especially if power plants have no treatment equipment. Current regulations and lawsuits are forcing utilities to install selective catalytic reduction (SCR) or other equipment to reduce NO_X emissions.

With large domestic reserves and low cost, coal could contribute much more to our nation's energy supply, if emissions issues are resolved. However, since coal is a solid, it is more difficult to use for transportation or distributed energy.

Research Areas

Since carbon oxidation is the major source of energy derived from coal, and greenhouse gas production is of greater concern, significant mechanisms to reduce or eliminate the emissions of gaseous CO_2 is worthy of long-term research. According to *Clean Energy Futures* [Interlaboratory Working Group 2000], there are numerous ways of removing CO_2 from the atmosphere and of storing it or keeping anthropogenic carbon emissions from reaching the atmosphere. Six carbon sequestration methods were described in a recent report [DOE SC/FE 1999]:

- Separation and capture of CO_2 from the energy system before combustion
- Sequestration in the oceans post-combustion
- Sequestration in terrestrial ecosystems post-combustion
- Sequestration in geological formations post-combustion
- Advanced biological processes post-combustion
- Advanced chemical approaches post-combustion

Some of these options are available today. CO_2 injection into geological formations as part of enhanced oil recovery has been practiced for decades, although the long-term performance of these formations at retaining CO_2 for longer periods has never been tested. Oil and gas fields that retained gaseous hydrocarbons for thousands of years may be expected to retain CO_2 equally well. Deep aquifers without documented caprock containment may be abundant but of uncertain capacity to retain CO_2. Since 1996, Statoil in Norway has sequestered annually about 1 million tonnes of CO_2 in sandstone 1000 meters beneath the North Sea, which is equivalent to about 3% of Norway's emissions [Herzog 2001]. Other near-term options are available because they can provide important secondary benefits, such as improving ecosystems during reforestation. However, most options involve long-term carbon management, requiring considerable research to ensure their successful development and acceptance. Because carbon capture and sequestration will require additional energy use, additional power use will be needed, perhaps provided by additional coal. David and Herzog show a 9-15% energy penalty for carbon capture and sequestration from coal-fired power plants in the year 2012, with an increase in cost of \$2.9 to \$6/GJ (1.04 to 2.16¢/kWh) [David and Herzog 2000]. These costs translate into \$18 to \$32 per tonne of CO_2 avoided. While promising, deep sea and geological storage options have constraints, including environmental impacts, safety, and duration of storage.

Continued improvements in efficiency and environmental acceptability could enable coal to establish a growing role in both the U.S. and worldwide energy portfolios, while still pursuing the goals of a clean energy future. The DOE Office of Fossil Energy has developed an applied research agenda "Vision 21 EnergyPlex" [FETC 1999], a new approach to 21st century energy production from fossil fuel-based systems. This vision integrates advanced concepts for high-efficiency power generation and pollution control into a new class of fuel-flexible facilities capable of co-producing electric power, industrial-grade heat, high-value fuels, chemicals and hydrogen, with virtually no resulting emissions of air pollutants. Improvements in combustion, filtration, gas separation, and chemical conversion will all play a role. These technologies will build on current research in integrated-gasification combined-cycle power plants and fuel cell advances to create tertiary cycle systems incorporating fuel cells, gas turbines, and steam turbines. If successful, this multi-product approach may achieve efficiencies approaching 60-80% after the year 2015. This increase is well above the typical 33-35% efficiencies from today's conventional coal-fired power plants.

Gas

Supply and Demand

Natural gas is relatively abundant, both in the U.S. and worldwide and relatively inexpensive. Domestic proven reserves stand at 192 EJ, while consumption in the year 2000 was 25 EJ (23.4 Quads). Global supplies are also large, with estimated reserves at 5,700 EJ (5,300 TcF). Compared with use of other fossil fuels, natural gas consumption is growing the fastest (Figure 2.4), increasing 21% between the years 1990 and 2000. Overall, production of electricity is the fastest growing use of natural gas, increasing 52% from the years 1990 to 2000.

Beyond proven reserves of 192 EJ (177 TcF), conventional gas has a domestic resource base of 670 EJ (616 TcF). Non-conventional sources, such as tight sands, coal-bed methane and Devonian shale, also have large resource bases and could become more widely used depending on prices of other competing

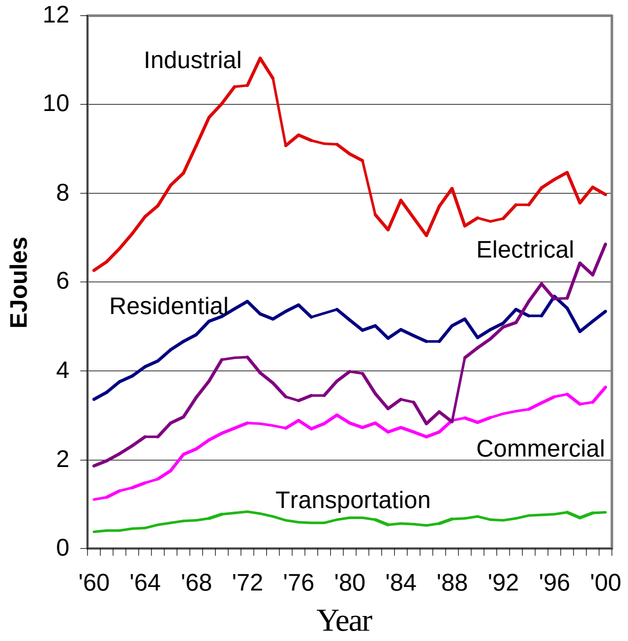

Figure 2.4. U.S. Natural Gas Consumption (EJ)
*1989-2000 Electrical includes non-utility generation.
Source: EIA 2002a

energy sources. Other non-conventional sources show even more potential. Methane hydrates, found in permafrost regions and the seafloor, are believed to have massive potential (Table 2.3).

According to the *National Energy Policy* [NEPDG 2001], while the resource base that supplies today's natural gas is vast, U.S. conventional production is projected to peak as early as the year 2015. Increasingly, the nation may have to rely on natural gas from non-conventional sources, such as tight sands, deep formations, deep water, and gas hydrates. Also, many resources are in environmentally sensitive areas requiring use of less intrusive technologies.

Most gas is transported and delivered through pipelines. Offshore and onshore wells deliver gas through systems that span the country (Figure 2.5). A small amount of gas is delivered to the U.S. by liquid natural gas (LNG) ships.

Prices for natural gas were fairly steady through the year 2000 (Figure 2.6). However, prices were extremely volatile in the years 2000 and 2001, returning to historical levels in the year 2002. High prices were attributed partly to the low prices for gas and oil in the year 1998, which reduced the amount of new drilling. Once prices rose, drilling accelerated. There is some question whether this market volatility will be ongoing or an aberration.

Table 2.3. U.S. Natural Gas Resource Base

	EJoules
Conventional (High and Low Quality)	670*
Unconventional (Coalbeds, Tight Gas, Devonian Shales)	560*
Gas Hydrates	350,000**

* Technically recoverable domestic resource base
** Mean estimate of U.S. hydrate resource base
Source: IWG 2000

Issues

Natural gas is relatively clean, emitting only 13.7 g C/MJ and essentially no SO_2. The main concern is the amount of NO_x that is emitted during combustion with air, although recent improvements in technology have greatly reduced these amounts. Natural gas is not as easily stored as a liquid and has contributed only a small role in the transportation sector.

Since natural gas is the cleanest of the fossil fuels and relatively available domestically, it is expected to be the preferential fuel for new growth. To increase gas consumption significantly, the infrastructure (pipelines, storage fields, and distribution systems) to support this growth will need to be built.

Natural gas could become more widely used as a transportation fuel. If fuel cells are to be used, hydrogen must be separated from the other components of fuel. This is easier generally with natural gas. (Natural gas is already used in hydrogen manufacturing for oil refining.) However, advances in reformers may increase the feasibility of liquid fuels, lessening the advantage of natural gas. Alternatively, if liquid fuels remain preferable for transportation (either in conventional engines or fuel cells) and petroleum supplies diminish, then natural gas could be converted to liquids. Conversion of gas to liquid is available, although the process is not as economically feasible as current use of oil.

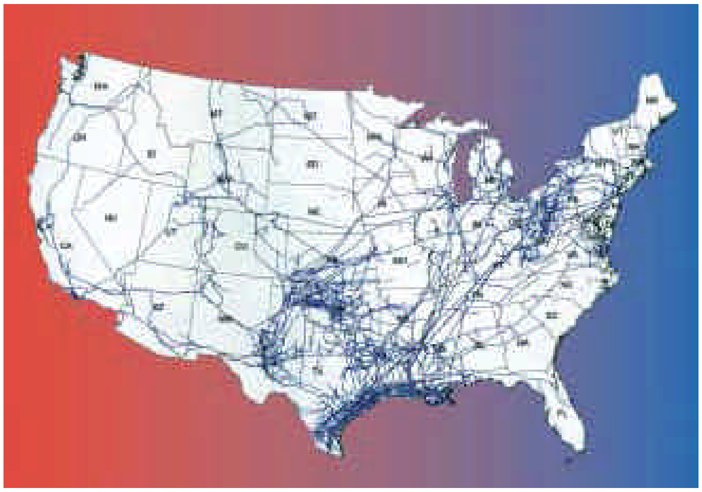

Figure 2.5. Gas Pipeline Infrastructure
Source: NEPDG 2001

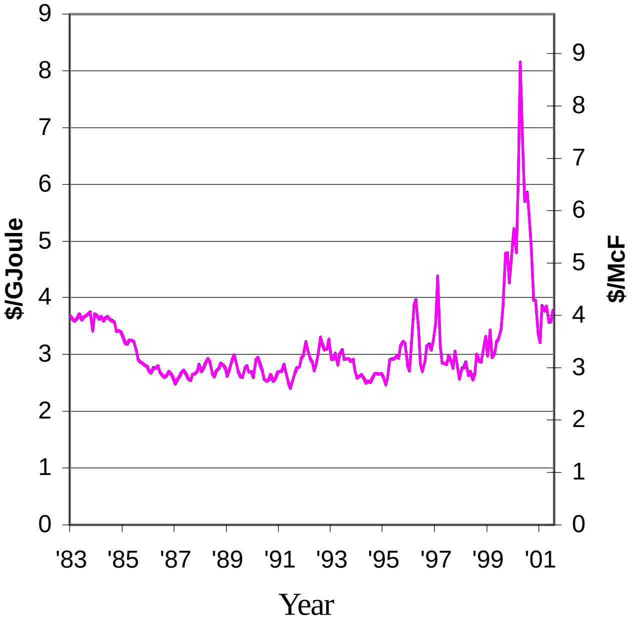

Figure 2.6. U.S. Average Citygate Gas Prices
Source: EIA 2002b

Research areas

Natural gas and oil will both benefit from advanced exploration, drilling, and recovery methods. The *National Energy Policy* [NEPDG 2001] outlines many of the applied research areas that will enhance oil and gas discovery, drilling, and recovery:

- advanced, more energy-efficient drilling and production methods;
- 3-D seismic technology, to increase greatly the success rate by enabling geologists to use computers to better determine the location of oil and gas before drilling begins;

- deep-water drilling technology, to enable exploration and production of oil and gas beneath the ocean's surface, at depths over two miles;
- high-powered lasers, to drill for oil and gas; and
- highly sophisticated directional drilling, to enable drilling of wells at long horizontal distances from the drilling site.

Recent Office of Fossil Energy applied oil and gas program workshops identified detailed basic research needs, applicable to both the oil and gas sectors.

The workshop on fundamental applied research identified the following areas that require additional research:

- enhanced oil recovery - methods to modify oil in-situ, fundamental physical and chemical properties of reservoir fluids and rock, dynamic process characterization and monitoring, and multifunctional chemicals;
- reservoir characterization - improved interwell imaging, integrate core, logging and seismic data, improve capability for processing real-time datasets;
- drilling, completion and stimulation - smaller drilling systems, improved fluid-flow identification, downhole separation technology, and diagnostics of tight/unconventional gas.

The diagnostic and imaging workshop recommended four applied research and development (R&D) topics:

- understand and overcome the limits on seismic resolution, including acquisition and processing, hardware, and sampling theory;
- data fusion or integration, both static and dynamic data at multiple scales and from multiple sources, including knowledge management and visualization;
- pre-stack and elastic inversion, including 3-component data and processing framework; and
- shear wave imaging, integrated seismic-electromagnetic, and single well imaging system.

The workshop on accessing deep formations defined applied R&D needs for deep drilling:

- advanced smart drilling systems - real time data transfer and real time data instrumentation, and rig operator decision support system;
- drilling diagnostics and sensor systems - downhole diagnostics drilling parameters including data validation, weight torque on bit, and state of bore hole analysis; and
- drilling and completion fluids - economic tests and simulators to determine drill fluid contribution to well-bore stability.

According to *Clean Energy Future*s [Interlaboratory Working Group 2000], a significant amount of undiscovered domestic conventional and non-conventional (see Table 2.3) gas sources are accumulated deeper than 15,000 feet in widely differing geologic settings. Several technology challenges must be overcome to exploit deep resources, including better ways to detect commercial volumes of gas using surface-based sensing and use of advanced materials for drilling at high temperatures and pressures at extreme depths. Domestic methane hydrates are found on land in permafrost regions (such as much of Alaska) and within ocean floor sediments. To achieve safe and environmentally acceptable production, the location, sedimentary relationships, and physical characteristics of methane hydrates must be determined. In addition, production approaches for disassociating the methane from the cage of water ice molecules in the hydrates must be developed. Hydrates are quasi-stable, so releasing the methane requires either reducing the pressure or increasing the temperature (or both) of the material. Among other methods of gas production, the feasibility of using depressurization by a drilling well in hydrate reservoirs [Ji et al. 2001] is being studied.

Hydrogen production, along with capture and sequestration of the carbon from natural gas, would enable natural gas to be a long-term source of energy for the U.S. and worldwide. Sequestration and separation technology must become more economically feasible, and the political will to reduce carbon emissions must occur on a broad scale.

Gas-to-liquid research may lower the cost for natural gas to be used as a liquid fuel for critical sectors such as transportation. This will open up domestic resources to replace petroleum if supplies tighten. Also, it can allow distant natural gas fields, such as on the Alaska North Slope, to use existing oil pipelines.

Oil

Supply and Demand

Domestic supplies of petroleum are small compared with the large annual use. Current domestic reserves stand at 124 EJ (22 GBarrels), while consumption in the year 2000 was 41 EJ (39 Quads or 7.2 billion barrel or 20 million barrel per day) [EIA 2001]. The current worldwide availability of oil reserves (5,800 EJ) compared to the rate of consumption (158 EJ) suggests only 35 years worth of remaining supply. This is a misleadingly small number since reserve growth has consistently paralleled consumption over the last century related, to improved technology and thus recovery rates. Unquestionably, much of the future oil supply is located in politically volatile areas (Figure 2.7 and Figure 2.8). In addition to the reserves already identified, the U.S. Geological Service (USGS) estimates undiscovered resources of another 4,000 EJ (720 billion barrels) [USGS 2002] worldwide.

Crude oil production has declined in the U.S. for years. OPEC (Organization of the Petroleum Exporting Countries) was the dominant supplier through the 1970's, reducing production in the 1980's to maintain higher prices. Other suppliers entered the market after prices increased in the 1970's. Their production has grown at a slower pace in the 1990's (Figure 2.9).

In addition, other potential sources (such as heavy oil, tar sands, or gas-to-liquids) are available at current or higher prices and through advances in technology. Over 3 trillion barrels of these non-conventional fuels are estimated as available (17,000 EJ), with the most significant deposits in Canada and Venezuela. In addition, coal-to-liquid technologies and oil shale deposits dwarf conventional oil resources [EIA 2002].

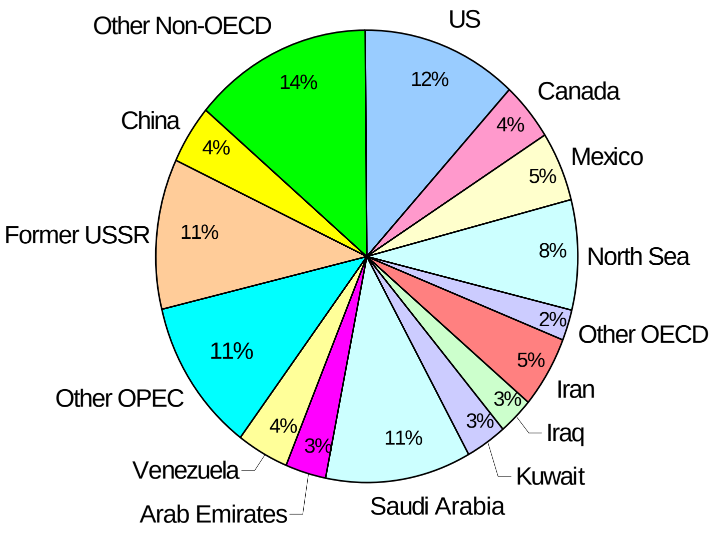

Figure 2.7. Year 2000 Crude Oil Supply (158 EJ or 77 million barrels per day)
Source: EIA 2002

Oil is currently the dominant fuel for transportation, providing over 96% of the energy used in that sector. The current transportation infrastructure supports a liquid fuel supply. Any change in supply source would require a major transformation in the transportation industry. Oil is also used to a smaller extent in other sectors (Table 2.4) Distillate fuel is used for home heating and industrial combustion turbines, while residual fuel is used for industrial and electrical boilers. Oil is also used as a feedstock to petrochemicals and plastics.

Issues

Domestic conventional supplies have been insufficient to meet U.S. consumption for several decades. The U.S. must import over half of the total oil supply needed, challenging national security and jeopardizing the trade balance. In the year 2000, the U.S. imported 58% of the oil consumed, costing $116 billion. The major suppliers are shown in Figure 2.7. U.S. production has been declining since 1970, and a turnaround is not expected. Oil must be recovered from more complex and inaccessible fields, with the depletion in more accessible locations. Technology improvements (such as steam injection, horizontal drilling, and 3-D seismography) have extended the life of many oil fields. Some fields within the U.S. have not been exploited, but their use is very controversial (e.g., Arctic National Wildlife Refuge).

As with all fossil fuels, CO_2 (20.4 g C/MJ) is emitted during combustion. Since most oil products are used in nonstationary applications, capturing these at the source is difficult. Rather, CO_2 may need to be se-

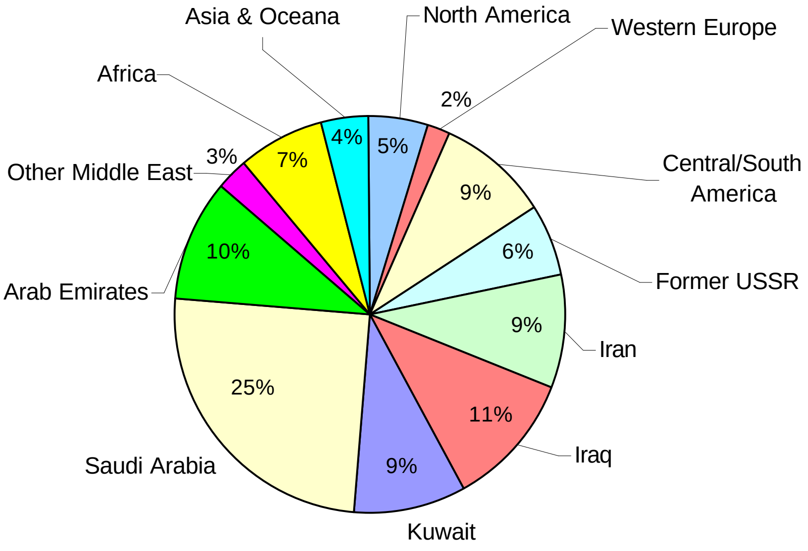

Figure 2.8. Global Petroleum Reserves (5,800 EJ)
Source: EIA 2002

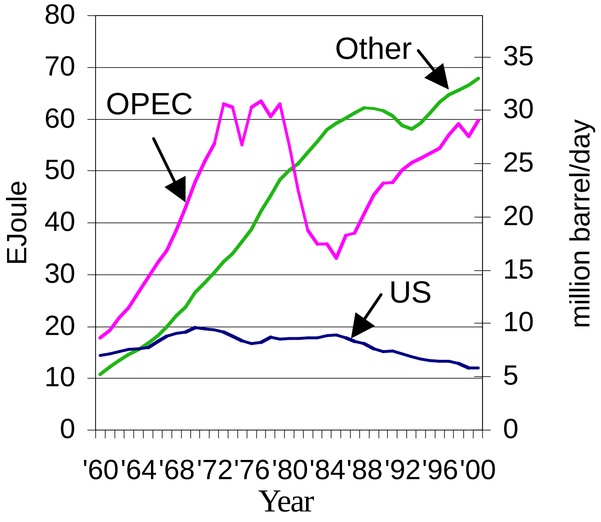

Figure 2.9. Crude Oil Production
Source: EIA 2002

questrated through withdrawal from the general atmosphere. Other notable pollutants from oil combustion include NO_X, which contributes to low-level ozone formation. Specific fuels (e.g., diesel fuel) also produce pollution as particulates.

With all forms of transportation heavily dependent on oil, disruption of the supply may create broad economic problems. The Strategic Petroleum Reserve provides short-term oil supplies, but longer-term relief may require more diverse sources of transportation fuels.

Research areas

Many of the opportunities for research in oil production are the same as described earlier for natural gas. In addition, there is research ongoing in improvements to refinery operations that lower the energy usage, such as use of inorganic membranes for improved separation of gases and recycle of waste streams. Advanced research and development (R&D) includes computational methods to improve catalyst development and experimental evaluation. Such improvements and R&D can increase the use of domestic, low-quality oils that are difficult or expensive to refine today.

Table 2.4. Year 2000 U.S. Refined Petroleum Products Consumption

	EJ	Million Barrel/Day
Motor Gasoline	17	8.5
Jet Fuel	4	1.7
Distillate Fuel	8	3.7
Residual Fuel	2	1.0
Other	10	4.8
Total	41	19.7

Source: EIA 2001

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NUCLEAR FISSION ENERGY

Current Status

The U.S. has 104 commercial reactors operating at the present time. All are one of two variations of light-water reactors (LWR)s. There are 69 pressurized water reactors of the type produced by the former Babcock and Wilcox, Combustion Engineering, and Westinghouse Corporations and 35 boiling water reactors produced by General Electric. Commercial nuclear reactors currently produce about 20% (8.5 EJ in the year 2000) of the electricity generated by American utilities. As shown in Figure 3-1, this fraction increased dramatically in the latter part of the 20th century, but has been relatively constant in recent years. Nuclear fission accounted for 1.44% of electrical generation in 1970, 11.0% in 1980, and 20.5% in 1990. For purposes of comparison, the nuclear electric fraction in 2001 for several other industrialized nations was: United Kingdom - 23%, France - 77%, Belgium - 58%, Germany - 31%, and Japan - 34%.

The most recently commissioned nuclear plant began commercial operation in 1993. The modest further increases in U.S. nuclear generation shown in Figure 3-1 since that time have arisen primarily from two factors: (1) improved plant capacity factors, as shown in Figure 3-2, and (2) small power upgrades at existing plants. Power upgrades ranging from 1.4 to 6.3% at 57 reactors were approved by the U.S. Nuclear Regulatory Commission (NRC) between 1977 and 2001. These upgrades added approximately 2000 MJ/s (MW) electrical (MJ/s_e) capacity equivalent, roughly the equivalent of two new nuclear power plants. The upgrades were made possible largely through the application of state-of-the-art instrumentation, and auxiliary equipment upgrades. Upgrades comprising another 1600 MJ/s_e are expected to be approved during the next 5 years. During this same period, the Tennessee Valley Authority is planning to carry out the necessary work to restart Watts Bar Unit 1, which has been shutdown since 1985. This project will add another 1065 MJ/s_e nuclear capacity. Thus, in the absence of either orders for new

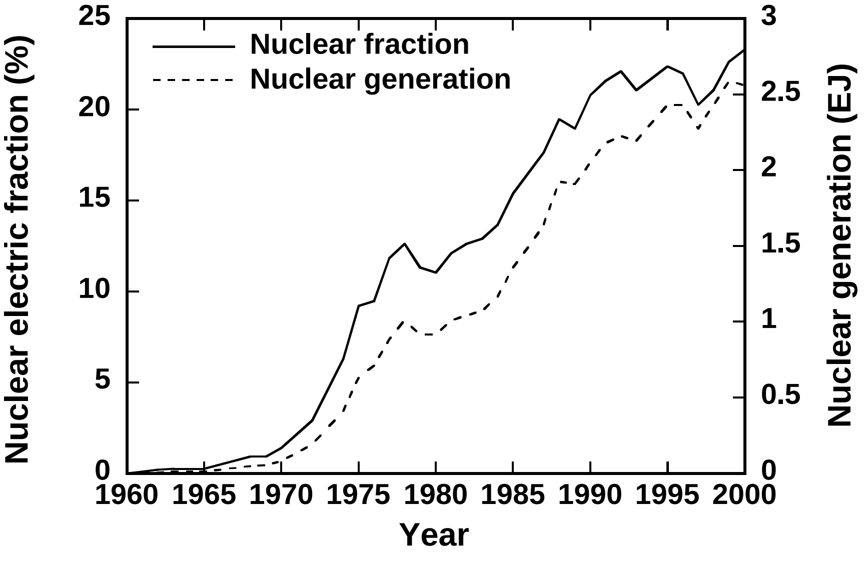

Figure 3.1. Nuclear power contribution to electrical generation in the U.S. Both the fraction of utility-generated electricity and the total nuclear electric generation is shown.

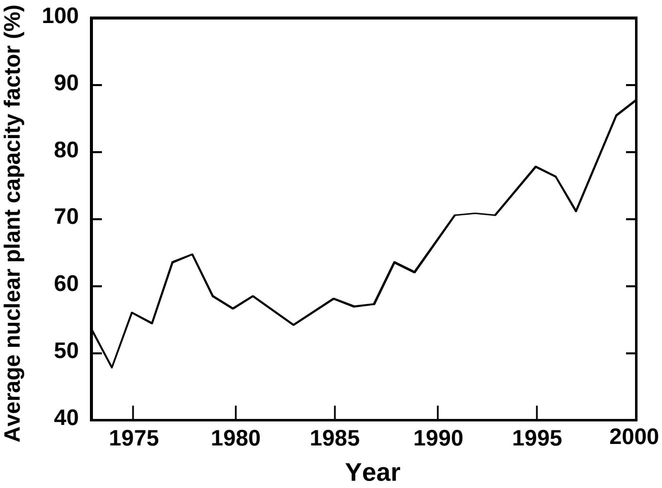

Figure 3.2. Average nuclear power plant capacity factor for units in the U.S.

construction or unexpected difficulties, nuclear electrical capacity is expected to increase by 2.5 to 3% over the next 5 years. In this case, the proportion of electricity produced by nuclear fission is likely to remain slightly above 20%.

Future growth of nuclear energy is a goal of the present administration and the Department of Energy. A program called NE-2010 (http://www.ne.doe.gov/planning/NucPwr2010.html) , the Nuclear Power 2010 Initiative, was announced in February 2002 to facilitate the building of a new nuclear electric generating station by 2010. Such a plant likely would incorporate one of the standardized designs that have already been reviewed by the NRC and as such will involve only modest extension of current technology. These designs provide major improvements in safety and in system simplification by reducing dependence on power-driven complex equipment for emergency core and containment cooling. Direct-cycle high temperature gas-cooled reactor (HTGR) designs are also candidates. They are extensions of HTGR technology that have predicted major improvements in reliability and simplification through elimination of the intermediate cooling systems and the potential for water-graphite interactions.

The DOE also has led a long-term international program intended to lead to the design of the next generation of nuclear reactors, the so-called Fourth Generation designs. The Generation-IV (http://gen-iv.ne.doe.gov/) effort is primarily defined by several technological and economic goals, notably including, higher reliability and efficiency, a high level of inherent safety, financial life-cycle advantages over other technologies, low financial risk, and waste minimization. The intent is to reduce the net cost of nuclear-generated electricity while improving public acceptance of nuclear reactors. The *Generation-IV Technology Roadmap* has recently defined the most promising reactor concepts for long-term development under this program, and has defined the research and development required to commercialize those concepts.

The *Generation IV Roadmap* has a major fuel cycle component that is likely to be incorporated into the Advanced Fuel Cycle Initiative now being developed by DOE's Office of Nuclear Energy, Science and Technology (NE). Processing of fuel is a large element in this part of the Generation-IV program. The *Generation-IV Roadmap* also indicated the desirability of developing technology that is sufficiently flexible to be used for multiple purposes, such as production of hydrogen, providing process heat, and desalination.

Many of the issues preventing the expansion of nuclear energy are social and political. The Generation-IV framework is designed to identify and address many of these issues with respect to reactors to be deployed after 2020. An additional and often major objection to even continuation of nuclear power has been concern about the need for long-term storage of spent fuel in the absence of a designated permanent disposal site. In 2002, the Congress and the President approved the Department of Energy developing a license application for the Yucca Mountain waste disposal site. The successful implementation of this decision may improve the acceptance of nuclear power. The major technological issues related to spent fuel storage have been investigated, and ongoing research in this area is being funded by DOE primarily in the Office of Civilian Radioactive Waste Management, although some will be done in the Environmental Management Science Program, being transferred to OS, and BES presently does support some basic research on issues relating to radioactive waste isolation.

The other major impediment to the expansion of nuclear energy in the U.S. is economic, probably the major reason no new U.S. plants have been built for decades and perhaps the highest hurdle for new designs to overcome. A recent study by the International Energy Agency (IEA) on the relative competitiveness of natural gas, nuclear power, and coal among members of the Organization for Economic Cooperation and Development (OECD) examined various operating costs, capital costs, plant decommissioning costs, and the costs of waste disposal. The IEA concluded that in terms of operating costs, nuclear power plants are competitive against coal and natural-gas-fired generation units. Natural-gas-fired units averaged 2.2-4.1 cents/kWh, coal plants 1.9-3.3 cents/kWh, and nuclear 0.8-3.2 cents/kWh. The fuel costs for a nuclear power plant are significantly lower than those for coal or natural gas plants. However, construction costs, which are strongly dependent on the cost of capital, are another matter. In capital-intensive industries such as electricity generation, interest rates play a key role in determining the relative economics of different generation fuel sources. The capital cost of a new nuclear unit is substantially higher than that for a comparable fossil unit. In addition, due to their higher construction costs, the relative cost of nuclear power plants is more sensitive to interest rates than are the costs of coal or natural gas plants. Using recent values for French-built pressurized-water reactors, capital costs averaged \$1,636/kW at 0%, \$1,988/kW at 5% interest, and \$2,280/kW at 10% interest. Care must be taken when using costs, as well as construction times, in other countries. Government roles, as well as financing approaches, differ significantly and therefore these numbers are not directly transferable to the U.S.

Construction costs are also sensitive to the time of construction. Although nuclear power plants have been built in as little as 4 years, the IEA study noted that the average construction time for U.S. plants completed after the Three Mile Island accident was 12 years. The increased construction time resulted from the need to incorporate improvements in safety identified by the accident, inefficient management of the construction, as well as to cope with the drastic drop in the rate of increase in electricity demand following the OPEC (Organization of the Petroleum Exporting Countries) embargo. In recent years, new plants have been constructed in Japan and Korea to regulatory standards somewhat similar to U.S. requirements in a 4 to 4 1/2 year time frame. The IEA study concluded that nuclear energy was competitive in more than one-half of the OECD (Organization for Economic Cooperation and Development) countries analyzed at the 5% rate, but was not competitive at 10%. Currently approved and certified reactor concepts hold promise of shorter construction times, and expedited construction is a goal of the Generation-IV design concepts. However, until new reactors can be shown to meet these expectations and are constructed and begin operation there will remain considerable hesitancy and skepticism by the electric utility industry as to whether the environment and legal structure in the U.S. will allow such expedited construction.

The major resource issue associated with nuclear power is the supply of uranium. Current best estimates of proven uranium reserves are adequate for more than 50 years at the current rate of consumption, with about three times that amount in so-called speculative reserves. There is also an extensive potential uranium resource available in seawater if the technology can be developed to economically extract it. In addition, weapons-grade uranium and plutonium from military stockpiles in the U.S. and Russia is being made available for use as reactor fuel. This material is highly enriched, at over 90% U-235. Similarly enriched plutonium (93% Pu-239) can also be used in mixed-oxide fuel. Conversion of just the highly enriched uranium will provide about 15% of world reactor requirements for more than 20 years. The spent-fuel reprocessing that is being carried out in Europe and Japan provides further feedstock by recycling unburned U-235 and Pu-239, although this is being done on a very limited basis. If the level of reprocessing was expanded, all these sources might provide adequate feedstock for nuclear reactor fuel for at least 100 years, although the economics of reprocessing are not currently favorable.

If reprocessing and other technologies mentioned above do not expand, but nuclear power does, then more uranium must be utilized. Significant levels of uranium enrichment capacity exist in the U.S., France, Germany, Netherlands, United Kingdom, Japan, Russia, and China. The commercial technologies used are gaseous diffusion and gas centrifuge. The gaseous diffusion process was developed during World War II, and plants using this process tend to be older, but still account for about 60% of installed capacity. The more recent gas centrifuge process is more efficient. Compared to gaseous diffusion, it consumes only about 20% of the electricity per unit of uranium enriched. Excess capacity has worked to keep the cost of enrichment relatively stable in recent years, with the U.S. closing down some of its oldest, World War II vintage gaseous diffusion plants. The remaining U.S. enrichment capacity is adequate for almost twice the current nuclear fuel demand in the U.S.

Future Research Needs

The IEA economic study evaluated and compared existing, not future technologies. Expectations are that future nuclear power plants will see significant efficiency gains through programs like the Generation-IV effort. Of course, some gains may also be expected for competing technologies. The most significant gains could be achieved by nuclear power if the safety features of new designs increase social acceptance, and if the predicted lower construction costs also can be realized. Design safety issues are heavily addressed in each of the Generation-IV design studies.

Another major focus of the Generation-IV designs is increased thermal efficiency in the nuclear steam supply system (i.e., obtaining more electrical energy per unit thermal energy). As a result, higher operating temperatures are desired, which increases the demands on structural material performance. In March of this year, DOE Office of Nuclear Energy, Science, and Technology (NE) and the Office of Basic Energy Sciences (BES) sponsored a workshop to bring together experts from the reactor materials and design community with fundamental materials scientists to identify research and development needs and opportunities to provide optimum high temperature nuclear energy system structural materials. The format of the workshop was structured around the reactor concepts proposed as part of the *Generation-IV Nuclear Energy System Roadmap* in order to define relevant research needs, while at the same time making an effort to identify research needs that cut across designs.

Among the many materials R&D areas identified at the workshop, the following areas appear to be the most critical for advancing Generation-IV concepts:

- Research on advanced ferritic-martensitic and martensitic steels that allow for increased temperature of operation for liquid-metal and supercritical water concepts while improving toughness at lower temperatures. Issues include stability of oxides in oxide-dispersion-strengthened materials, basic microstructural and microchemical changes, and phase stability at high temperatures. This will require the use of irradiation facilities, which are few in the U.S. and may require going overseas. This first area should identify the work necessary to develop a limited number of the most promising candidates for the irradiation research in the following five areas.

- Development and fundamental understanding of radiation performance of refractory alloys, ceramic composites, and coatings for high and very high temperature concepts.

- Research to improve radiation performance of austenitic stainless alloys including resistance to void swelling, embrittlement and stress corrosion cracking. This research should also examine other alloys employed in present and near-term deployment plants, as well as consider non-radiation environments for these materials.

- Development of new high-temperature superalloys that are tailored for radiation environments (e.g., low nickel contents and controlled phase stability)

- Fundamental and applied understanding of the complexity of radiation damage in engineering alloys, including austenitic, ferritic, ferritic-martensitic, refractory metals, and ceramic materials.

- Developing a more detailed understanding of the radiation-induced complex, non-equilibrium microstructural and chemical evolution which occurs at the nanoscale, leading to changes in plasticity, corrosion and fracture processes.

All six of these areas could benefit from basic research and all six of them could equally benefit from applied and developmental research. The responsibility for basic research that underpins these six areas properly belongs to BES.

Some additional basic research areas that warrant consideration include:

- irradiation assisted stress corrosion cracking and aqueous corrosion
- irradiation induced embrittlement
- mechanisms and modeling for the degradation of radioactive waste packages
- welding and joining (Temperbead repair, laser welding, underwater welding)
- nondestructive evaluation and condition monitoring
- mechanical behavior, predictive modeling and computer simulation
- radiation effects
- heat transfer
- complex multiphase fluid flow
- human performance
- neutronics
- reprocessing methods

A final issue related to both safety and efficiency is reactor fuel performance. In order to minimize refueling frequency, some advanced designs have proposed exposing fuels to higher burnups. In addition to reducing the downtime for refueling, these schemes also reduce the amount of high-level waste created. Some of these designs involve fuels more highly enriched in U-235 than current LWR fuels (possibly increasing concern about diversion of nuclear materials). Achieving higher burnup will increase the effects of radiation damage to the fuel (e.g. swelling and cracking) and higher operating temperatures will further challenge the stability of the fuel. In order to reach the desired fuel performance goals, advanced oxide or carbide fuels may be required. There is limited experience with the coated-particle fuel form used in advanced gas-cooled reactor designs. German-fabricated fuel has performed well in irradiation tests, but experience with U.S.-fabricated fuel has been mixed. Thus, issues related to fuel performance also warrant further research. Higher fuel burnup and higher fuel temperatures will also increase the demands placed on fuel cladding or fuel coatings that constitute the engineered barriers to fission product escape. Significant improvements in fuel performance may not be possible without concomitant improvements in the radiation resistance of the structural materials mentioned above.

Summary

Nuclear energy provides somewhat more than 20% of electricity in the U.S., 35% in the European Union, 24% in all OECD countries - about 16% of electricity worldwide. The importance of this power source may increase due to concerns of greenhouse gas emissions from fossil-fired (coal, oil and natural gas) plants used to produce 65% of the world’s electricity. For example, according to a recent OECD report, OECD power plant emissions of carbon dioxide without nuclear power would be about one-third higher than they are at present. This is an annual savings of 1.2 billion tons of carbon dioxide, or about 10% of total CO_2 emissions from energy use in the OECD.

It is difficult to envision a scenario in which the Kyoto Protocol emission target of a 700 million ton reduction in carbon dioxide emissions in OECD countries by 2008-2012 (relative to 1990 levels) can be achieved without either a significant reduction in electrical production or an increase in the use of nuclear-generated electricity. This realization is part of the basis for the current debate on nuclear power in countries such as Germany and Sweden that have initiated plans to shut down their nuclear plants, and for plans in the U.S. and elsewhere to increase nuclear capacity by reviving the nuclear industry. The initial steps in that revival are the extension of useful life of the present generation of nuclear plants and the deployment of new plants in the near term. Similar efforts to extend the lives of existing plants are being pursued overseas and an International Near Term Deployment plan has been formulated to achieve goals similar to the U.S. NE-2010 program as an adjunct to the International Generation-IV planning. For the longer term, the Generation-IV International Forum (http://gen-iv.ne.doe.gov/intl.html), with the U.S. DOE in a lead role, is identifying the reactor designs, and accompanying research needs for the next generation of reactors that will further improve reactor safety, reliability, thermal efficiency, and waste management.

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RENEWABLE AND SOLAR ENERGY

Energy sources that are replenished by nature, with human intervention, and within a relatively short time period after their use are defined as "renewable energy." Their replenishment can range from being instantaneous to requiring decades. In contrast, fossil-based energy resources require millions of years for their formation and cannot be effectively replenished. The U.S. Energy Information Administration generally includes the following sources as "renewable": conventional hydroelectric, geothermal, wind, solar, biomass, and waste. To further define these categories, the following information is offered:

- Conventional hydroelectric power is distinguished from pumped storage hydroelectric power since the latter is a net energy consumer.
- Solar includes both solar thermal and photovoltaic (PV) sources.
- Biomass includes organic matter produced by biological photosynthesis (lignocellulose from trees, corn and other energy crops, wood and woody plants, algae and other photosynthetic organisms, food by-products, etc.) that can be converted to fuels and chemicals by fermentation or thermal processing.
- The waste energy stream includes methane and other flammable gases recovered from landfills, and various solid waste forms that are burned to produce electricity or thermal energy.

Hydroelectric, wind and solar power do not produce any greenhouse gases at the point of energy generation, whereas combustion of biomass and waste and fermentation of biomass produces CO_2. As long as an equivalent amount of biomass is regrown through photosynthesis, there is no net increase of CO_2 in the atmosphere as a result of burning or fermenting biomass. Depending on the source and application, geothermal sources may also release greenhouse gases, as well as other noxious gases such as hydrogen sulfide.

Renewable energy resources can contribute to all the major energy sectors in the U.S., including electricity (25%), transportation fuels (28%), residential and commercial space heating (19%), and industrial process heat (28%). The central goal for renewable energy is to become competitive with fossil energy.

Global Energy Issues

To properly discuss the role of renewable energy for future U.S. energy needs it is necessary to discuss the future global energy picture. The world population is expected to grow to 10-11 billion people by the year 2050, and this growth will be concentrated in the developing counties. This population growth, together with the standard of living goals for these developing countries, will impact the emission of greenhouse gases to an extent that will limit the use of fossil fuels everywhere in the world, including the U.S., and require huge amounts of carbon-free energy. The numbers are quite staggering, and have been summarized by M.I. Hoffert [Hoffert 1998, Hoffert et al. 2002]. The essence of this analysis is that a population of 10-11 billion by year 2050, an increase in the average world GDP of 1.6%/yr (historical average), counterbalanced by a decrease of 1%/yr in the energy consumption per unit of GDP because of expected increases in the efficiency of energy utilization, produces an expected energy consumption in year 2050 of 28 TW (or 888 EJ/yr) (1 TW = 31.7 EJ/yr). The present world energy consumption rate is about 13 TW (412 EJ/yr). Although fossil fuel resources and proven reserves are huge (40,000 EJ for oil plus gas and 180,000 EJ for coal, enabling their possible use for about 50 years for oil and gas and 275 years for coal), their use will possibly be severely restricted by the problems of CO_2 emissions. If the CO_2 concentration in the atmosphere is to be restricted to 550 ppm in 2050 (twice the pre-industrial value; the present level is 325 ppm), then by 2050 this will require the availability of 20-30 TW of carbon-free power. This is appreciably more than the total world energy consumption today! Furthermore, even if no restrictions on CO_2 emissions were implemented, but rather the present rate of decrease in carbon intensity of energy utilization continues (at a rate of -0.56 kg C/yr/watt), then 10 TW of carbon-free energy will be required in 2050 - also a huge and daunting requirement.

The available global renewable resources are estimated to be: (1) hydro: 4.6 TW total, 0.9 TW practical, and 0.7 TW already installed; (2) wind: 50 TW total on land, 2-4 TW practical on land; higher if oceans are utilized; (3) biomass: 5-10 TW total (not considering land required for food production and utilizing 100% of the cultivatable crop land for energy production), practical: unknown possible restriction due to water supply; (4) solar: 1.2 x 10^5 TW total; practical: 600 TW (60 TW at 10% conversion efficiency) (to generate 12 TW of solar power at 10% efficiency would require 0.1% of the worlds land mass). These numbers suggest that the best long range renewable resource that could provide the required carbon-free energy is solar, whether implemented as biomass or as photovoltaic or advanced solar conversion technology. However, breakthroughs and disruptive technology are required to achieve such a level of implementation. A similar case for the need for daunting amounts of carbon-free power can be advanced based on sustainability arguments even in the absence of greenhouse gas effects.

Electricity from Renewable Energy Sources

As shown in Figure 4.1, the total net electrical production by electrical utilities from renewable energy sources has remained essentially constant since about the year 1975, with hydroelectric power accounting for nearly 99% of the renewable contribution. Values for the various renewable components in the year 2000 were: hydroelectric, 0.91 EJ; geothermal, 7.2 x 10^{-4} EJ; wind, <1.8 x 10^{-4} EJ; solar, <1.8 x 10^{-4} EJ; wood, 2.52 x 10^{-3} EJ; and waste, 4.7 x 10^{-3} EJ. Since the consumption of electricity has increased by about 57% since the year 1975, the fractional contribution of renewable energy sources to electricity production by utilities has been declining, as shown in Figure 4.2.

As shown in Tables 4.1 and 4.2, nonutility power producers utilize renewable energy sources to a greater extent. In the year 2000, electrical utilities generated 10.8 EJ and nonutility producers 2.82 EJ of electricity. The absolute and relative contribution for all sources is shown in Table 4.1, and the renewable sources are compared in Table 4.2. Since the nonutility producers have less hydropower and little nuclear power, their relative use of both fossil fuels and other renewables is higher than the utilities.

Increasing hydroelectric generation is the most rapid way to grow the renewable component of electricity production. It is estimated that 60 GJ/s of undeveloped hydroelectric power is available in the U.S. Assuming a 50% capacity factor, 60 GJ/s of hydropower would add 0.95 EJ of energy annually, more than doubling the current contribution. Tapping into this potential capacity would involve three approaches: upgrading equipment at existing hydropower facilities, adding generating equipment at existing dams that are not so equipped, and developing new projects. The development of new hydroelectric projects may involve a trade-off between the potential elimination of generating facilities that produce greenhouse gases and the impact of new dams on waterways and marine life.

As shown in Figures 4.1 and 4.2, other renewable energy sources have not yet made a significant contribution to electricity production by U.S. utilities, despite substantial R&D efforts initiated after the oil shocks

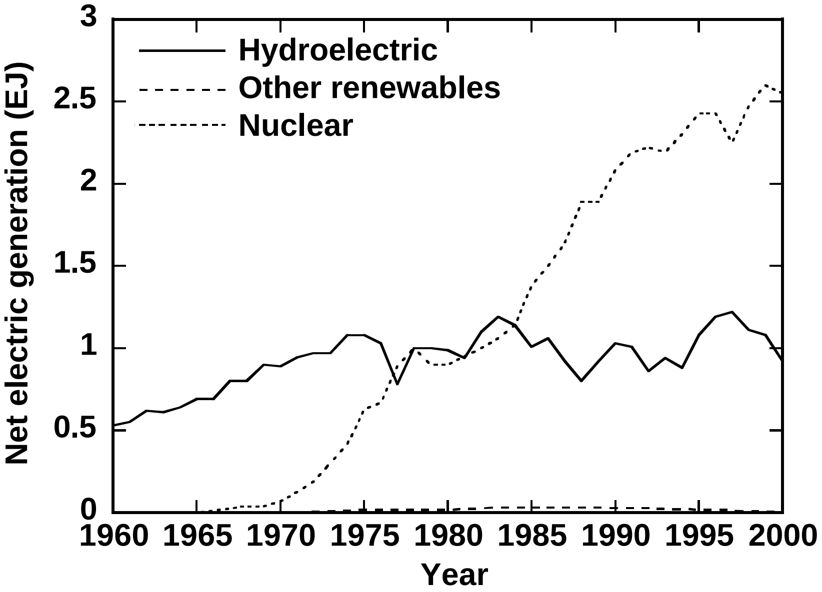


Figure 4.1. Electrical production by utilities from all renewable energy sources with conventional hydroelectric shown separately from other renewable sources. Nuclear energy, the other CO_2-free electric source is included for comparison.

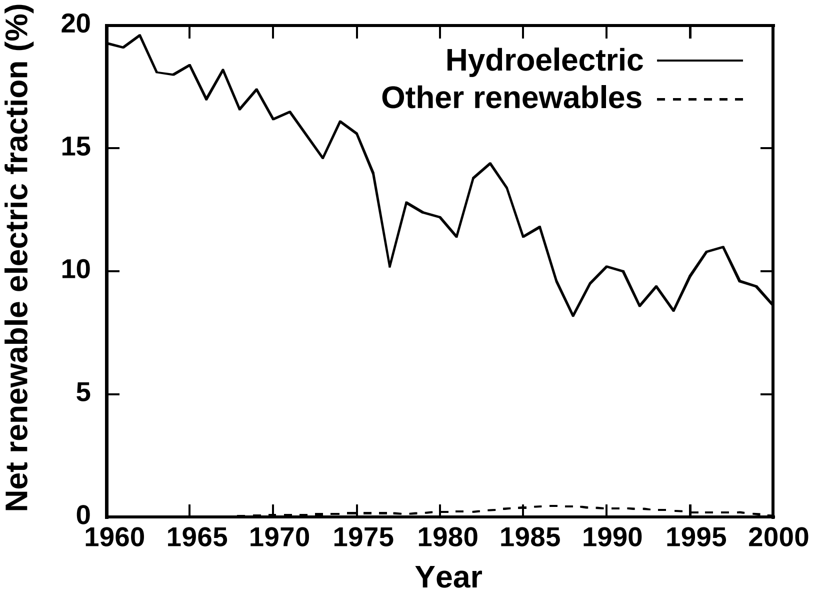


Figure 4.2. Fractional contribution of conventional hydroelectric power and other renewable energy sources to total electrical production by utilities.

Table 4.1. Electrical Energy Production and Fractional Contribution from Various Sources for Utility and Nonutility Power Producers

Electrical energy source	Electrical utilities Energy (EJ)	Electrical utilities Fraction (%)	Nonutility producers Energy (EJ)	Nonutility producers Fraction (%)	Fraction of total electricity (%)
coal	6.09228	56.129	0.98064	34.803	47.107
oil	0.26028	2.398	0.13176	4.676	2.246
natural and other gas	1.04328	9.612	1.15812	41.101	10.637
total fossil	7.39584	68.139	2.27016	80.567	59.989
nuclear	2.53944	23.396	0.1746	6.196	19.028
hydroelectric	0.91044	8.388	0.07812	2.772	6.862
geothermal	0.00072	0.007	0.0504	1.789	0.136
wood	0.00252	0.023	0.13968	4.957	0.381
waste	0.00468	0.043	0.08388	2.977	0.252
wind	0.00018	0.002	0.01764	0.626	0.047
solar	0.00018	0.002	0.00288	0.102	0.009

Table 4.2. Relative Fraction of Various Renewable Sources to Total Electrical Production from Renewable Sources for Utility and Nonutility Producers

Electricity source	Electrical utilities (%)	Nonutility producers (%)
hydroelectric	99.091	18.428
wood and waste	0.758	52.498
geothermal	0.114	24.161
solar	0.019	0.737
wind	0.019	4.177

of the early 1970s. This research reduced substantially the cost of some renewable power sources (currently, 3-5 cents/kWh for wind and 25-30 cents/kWh for PV) . A major limiting factor for adoption of these sources is the cost and practicality of electrical energy storage and integration into the power grid.

The peak in the utilities renewable energy production curves in the year 1987 is due to a peak in geothermal power that year. The total non-hydro renewable contribution to electricity production in the year 2000 was less than 1%. A very substantial increase in these values is required if they are to contribute significantly to the reduction in greenhouse gas production in the near future. A combination of technical and natural obstacles must be overcome to make this a reality.

The present relative importance of renewable energy sources increases when total energy production is considered. Total geothermal energy production includes geothermal heat pumps and direct thermal energy use. Similarly, the solar energy component includes space and water heating. Wood burned for space heating is the largest single component. In the year 2000, renewable energy consumption (without hydroelectric) was 3.50 EJ, or 5.2% of total energy production. Of this, wood, waste and alcohol was 3.09 EJ; geothermal was 0.30 EJ; solar was 0.066 EJ; and wind was 0.048 EJ. The alcohol was that blended with gasoline for use as a motor vehicle fuel.

Research and Development Issues

Wind

Due to ongoing improvements, wind is the renewable energy technology closest to being economically competitive today. In the year 1999 worldwide wind capacity increased by 36% to 13,400 MJ/s, with Germany, the U.S., and Spain contributing over 40% of the increase. Some projections indicate that the local contribution of wind to electrical capacity could reach up to 10-20% in some regions. Such a significant market penetration would require addressing the impact of the intermittent output of wind through modification of systems operation, hybrids with other technologies (e.g., gas turbines), and energy storage. Near-term R&D is needed for higher towers, lightweight blades with advanced airfoil designs, direct-drive systems, advanced power conversion devices, and durable and lightweight structural components. Overall, the greatest impediment to widespread use of wind power is a lack of sites that offer consistent and adequate volume and velocity of winds. If high reliability is needed from the wind generation site, the cost of a backup system such as a gas turbine adds significantly to the net cost of electricity.

Studies at the National Renewable Energy Laboratory (NREL) have shown that, if windmills are sited at 5% spacing, which is about the optimal spacing of windmills so that they do not obscure one another, and if no excluded, environmentally-sensitive lands or urban areas are covered, then approximately 0.4 TW of wind power can be produced in the U.S. This amount of energy, though small compared to the 3 TW that is currently consumed domestically from all energy sources, is comparable to the entire current U.S. electricity consumption.

With respect to electric wind power potential, 27% of the earth's land surface is rated as class three, representing lower available velocity. A class four rating represents land where sited windmills are economical (~3-5 cents/kWh of electricity production) by having a mean wind speed at a certain height above ground. The proposed use of class-three-rated land for windmill siting requires advances in wind turbine technology to make these lower wind velocity areas economical in the next 50 years. Adding up all class three and four land surfaces, and considering practical siting constraints, results in approximately 2 TW of electrical power potential from terrestrial wind.

The offshore electrical power potential of wind is larger than 2 TW and, in some cases, such installations make geopolitical sense. However, going far offshore would be required to realize a needed demand of 10-20 TW of carbon-free power primarily through wind-generated electricity. Getting the power generated offshore to the land-based regions where it is needed to meet demand can result in transmission losses. In addition, the impact of removing energy from the atmosphere through the number of windmills necessary to produce the level of power needed might have a negative impact on weather and other atmospheric conditions. For example, to produce the 0.4 TW of domestic electricity needed from the available class four wind resource areas in North Dakota, a state with high potential for using wind energy, 50% of the energy in the atmosphere would have to be removed through an exhaustive installation of windmills. It is not clear what the impact of such a drastic measure would be.

Exploitation of wind-generated electricity on a large scale is challenging in the U.S. for another set of important reasons. The wind resource is not located where the power demand is. Most of the U.S. population resides outside of major wind producing areas. The grid cannot currently handle the level of power that might be produced by wind. Furthermore, wind is a relatively mature technology, but as an intermittent source demands an accompanying energy storage system. The use of compressed air storage in the windfarm is probably the best way, from a physics point of view, to provide the storage capacity and thereby convert an intermittent resource into baseload power. The penalty of including storage is about 1 cent/kWh, so such an approach becomes interesting when wind electricity is about a factor of two lower in cost than it is now. Hence large scale use of wind power poses challenges in assessing possible limitations that might arise due to extracting significant amounts of energy locally out of the natural atmospheric circulation, in handling the potential load with the structure of the grid, and in finding effective storage methods to convert intermittent power to baseload power.

The effectiveness of wind turbines depends on the interaction of the blade with the air flow at its surface, a challenging problem in basic fluid dynamics. Turbulence at the surface deforms the blade locally as it turns, which in turn disturbs the local air flow. Advanced numerical methods in computational fluid dynamics are needed to accurately predict the fluctuation aerodynamic forces, blade deformations, and vibratory responses. A second basic research problem is the structural performance of the turbine blade. New blade materials and composite fabrication techniques are needed that combine light weight, high stiffness, and long lifetime (> 10^9 cycles) with low manufacturing costs. These goals can be achieved through improved understanding of composite materials behavior and fatigue mechanisms. Finally, the variability in local wind conditions leads to intermittent power production that can be accommodated if it is known a few days in advance. A better understanding of mesoscale atmospheric processes is needed to forecast average and turbulent wind flow fields over complex terrain in the lower 200 meters of the atmospheric boundary layer with high accuracy three days in advance.

Geothermal

Geothermal power is cost competitive at good quality sites, and the installed geothermal electrical capacity has increased from 500 MJ/s in the year 1973 to the current 2800 MJ/s. However, the number of such sites is limited, with most being located in the western U.S., Alaska, and Hawaii. Geothermal wells are a versatile energy source that are currently being used to produce electricity, to heat greenhouses through direct thermal use applications for geothermal heat pumps, and in aquaculture. The geothermal resource in the U.S. is huge, with over 40,000 Quads of energy potential. However, 90% of this potential is at low temperatures (<150°C or <300° F) and much is inaccessible as a result of lack of water, low permeability soils, and environmental concerns. To access these less attractive resources, basic research is needed in exploration technologies, drilling, reservoir engineering, and conversion technologies. While much technology has been borrowed from the petroleum industry, geothermal resources require new technology for higher temperatures, hard rock drilling, reservoir estimation, fracturing and other geothermal-specific requirements. Materials performance problems exist due to the corrosive nature of steam at some locations.

Geothermal energy makes important contributions to the energy mix in certain regions, including the western U.S. and regions of the Asian-Pacific and central Europe. Some nations, such as the Philippines, produce a significant portion of their electricity from geothermal sources. Other nations, such as Iceland, use geothermal heat directly for space heating and industrial processes. The use of geothermal heat pumps in the U.S. has increased significantly in recent years and, in fact, holds the largest potential for increasing the geothermal component of the total energy mix because the development is not dependent on special high-temperature geothermal regions. Nonetheless, large expansion of geothermal utilization is likely to be dependent on reducing both development costs and uncertainty. Major costs involved in finding and developing geothermal energy are associated with exploration and drilling. Reduction of drilling costs is an important target for applied research. However, the better location of drilling targets would be another way to reduce costs and requires advancement of the basic sciences involved in exploration. Uncertainty in resource size and performance acts as a hindrance to development, since developers prefer surer targets. Improving the understanding of reservoir performance mechanisms through basic research would be useful to lower this uncertainty and thereby increase the rate of development.

Photovoltaics

The solar constant is 1.76 x 10^5 TW, hence, there is ample solar energy potential. From the 1.2 x 10^5 TW of solar energy that strikes the earth's surface, a practical siting-constrained terrestrial solar power potential value is about 600 TW. The numbers range from very conservative estimates of 50 TW to optimistic estimates of 1500 TW, depending on the land fraction devoted to power generation. A good number to use for onshore electricity generation potential is probably 600 TW. Thus, for a 10% efficient solar farm, at least 60 TW of power could be supplied from terrestrial solar energy resources. For calibration, photosynthesis currently supplies 90 TW globally to make the biosphere run, so the amount of power available from the sun is very large (see Fig. 4-3).

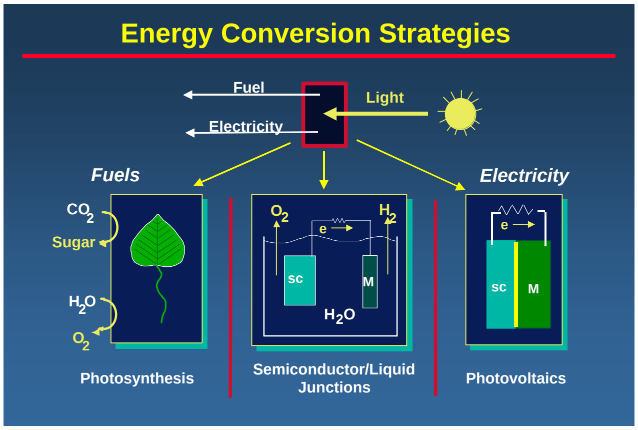


Figure 4-3. Energy conversion strategies for converting solar energy to usable energy.

The land area that is required to produce 20 TW of carbon-free power from solar energy is 0.16% of the earth's surface, or 5 x 10^{11} m^2. Producing 3 TW with a 10% efficiency solar cell farm would require covering 1.7% of the land in the U.S. The size of even this project (comparable to the land devoted to the nation's interstate highways) should not be underestimated (see Fig. 4-4). For example, if a 10% efficient solar energy conversion unit was installed on every home rooftop in the entire U.S., only 0.25 TW of power would be generated. Nevertheless, this requires about a factor of 100 less land than current biomass technology and similarly less land than using wind to generate equivalent amounts of power.

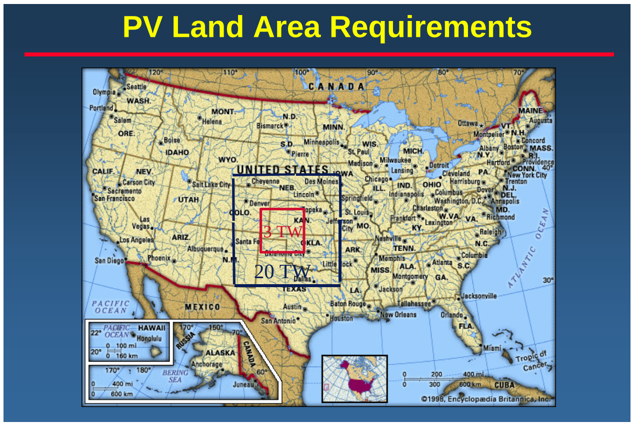


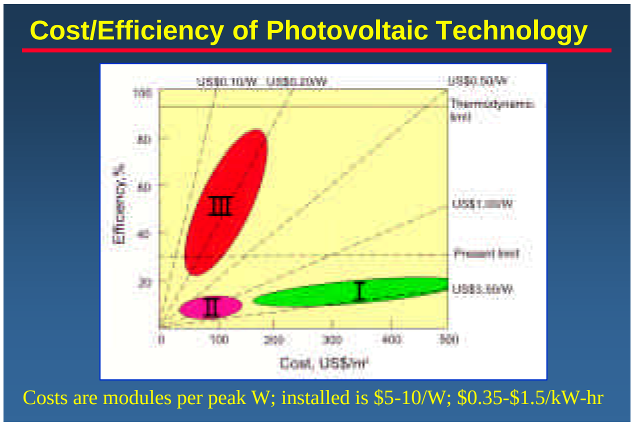
Figure 4-4. Boxes showing land area requirements to produce 3 TW or 20 TW of photovoltaic energy at 10% efficiency.

The efficiency of photovoltaic devices has been increasing steadily. Nevertheless, current technologies all lie on a relatively common cost/watt scale. The underlying reason for this roughly equal cost/watt trade-off is that the photovoltaic materials now available suffer from the same fundamental physical limitations. Large-grain, pure materials, with a long lifetime capable of making efficient solar cells, are costly to produce. Alternatively, cheaper materials with smaller grain sizes have grain boundaries that act as recombination sites, resulting in inefficient solar cells. A similar trade-off is found for organic ("plastic") photovoltaics. If pure inorganic single-crystal materials, like silicon and GaAs, are replaced with much cheaper organic materials, the materials are inherently disordered and therefore are cheaper but more inefficient. The net result is that one can ride anywhere on this cost/watt trade-off scale, but nevertheless end within a factor of 20%.

Use of disruptive technologies is one approach to reducing the cost/watt trade-off. Further discussion on these approaches is found at the end of the next section on advanced direct solar photoconversion.

Advanced Direct Solar Photoconversion

Direct solar photoconversion is the process whereby the energy of solar photons is either converted directly into fuels, chemicals, or materials starting from simple and renewable substrates such as water, CO_2, and N_2, or the photons are converted directly to electricity. These processes require photoactive organic, inorganic, or biological molecules or materials that can absorb a large fraction of the solar irradiance and drive the chemical reactions that produce the fuels, chemical, materials, or electricity. The latter photoconversion process that produces electricity can be distinguished from photovoltaic conversion based on solid state semiconductor p-n junctions by the fact that molecular photochemical and/or electrochemical processes are involved in photoconversion.


Cost/Efficiency of Photovoltaic Technology

Costs are modules per peak W; installed is $5-10/W; $0.35-$1.5/kW-hr

Figure 4-5. Cost/efficiency of photovoltaic technology.

Three branches of science and technology can be defined for solar photoconversion: photoelectrochemistry, photochemistry, and photobiology. They all depend upon photoinduced charge generation (i.e., electrons and positive holes) followed by efficient positive and negative charge separation at various types of interfaces that ultimately produce oxidation-reduction (redox) chemistry. Photoelectrochemistry involves semiconductor-molecule interfaces, photochemistry involves molecule-molecule interfaces, and photobiology involves biological interfaces with other biological and non-biological molecules.

Fuels produced by solar photoconversion are derived from endoergic reactions wherein the photon energy is stored as chemical free energy in the reaction products. Extremely important examples of this process are hydrogen from photolytic water splitting, and methane, methanol, or ethanol from the reduction of CO_2 by water. The later can be termed "artificial photosynthesis" since biological photosynthesis uses the same reactants of CO_2 and H_2O to form biomass and O_2. However, the term "artificial photosynthesis" is also applied more generally to all fuels and chemical products produced via solar photochemistry. The photoactive molecules and materials used to create and separate electrons and holes and to drive the appropriate redox chemistry are semiconductors (inorganic or organic) in photoelectrochemistry, molecular structures in photochemistry, and biological structures (e.g. *in vivo* water-splitting blue-green algae or *in vitro* reaction centers) in photobiology. Some photoconversion reactions can also be exoergic, such as photooxidation of organic molecules to make higher value products or to destroy organic pollutants and the formation of hydrogen from organics or biomass using photosynthetic bacteria.

The best reported conversion efficiency (rate of H_2 free energy produced/solar power in) for the photolytic splitting of water by semiconductor structures is about 12%. It was achieved using a monolithic tandem cell structure consisting of two series-connected p-n junctions of GaAs and $GaInP_2$ with metal catalysts deposited on the anodic (oxygen evolving) and cathodic (hydrogen evolving) sides of the layered structure. However, the cost of this cell is very high, and the use of such high-efficiency tandem cells is usually reserved for space applications. Photobiological production of hydrogen by photosynthetic blue-green algae has recently been achieved without the usual poisoning of the algae by the evolved oxygen. However the conversion efficiency is very low (< 1%).

For photoconversion to electricity, the conversion systems can be configured so that the separated electrons and holes produce a photocurrent and photovoltage, rather than drive chemical reactions. The best systems to date are based on photoelectrochemical cells (semiconductor-molecule interfaces), producing power conversion efficiencies that have been as high as 17% . A recently developed cell that looks potentially promising is based on the dye sensitization of nanocrystalline titanium dioxide (a nontoxic and cheap paint pigment) films by adsorbed dye molecules. This potentially very cheap cell shows conversion efficiencies in the laboratory of about 10%. Another potentially major advantage of photoelectrochemical cells for electric power is that they can be configured to store the photogenerated electricity by using part of the photogenerated power to charge a third electrode in the cell , which can discharge in the dark. Such a cell becomes a photochargable battery that can deliver power day and night.

The grand challenge for direct solar photoconversion is to discover and develop conversion systems that exhibit combinations of efficiency and capital cost per unit area that result in delivered electrical or stored chemical energy at very low cost , and furthermore are stable and robust under operating conditions for 10-15 years. To reduce the cost of installed photoconversion systems to $0.20/ peak watt of solar radiation, a cost level that would make them economically very attractive in today's energy market, would require that they have a capital cost of about $\$100/m^2$ together with a conversion efficiency of about 40% or a cost of $\$2/m^2$ and an efficiency of 15 %. The power produced by such systems would yield electrical power at a cost of about 1-2 cents/kWh or H_2 at about 2-4 cents/kWh free energy equivalent. Such combinations of cost and efficiency require truly disruptive technologies that do not exist at the present time. However, these goals do not violate any fundamental scientific principles and are not beyond the realm of possibility.

One important strategy to attain these goals is to identify approaches that produce ultrahigh conversion efficiency. Present photon conversion devices based on a single threshold absorber, including solid-state semiconductor photovoltaics, all operate within a regime wherein the ultimate thermodynamic conversion efficiency is limited to about 32% with unconcentrated sunlight. In this regime, the photogenerated electrons and holes are in thermal equilibrium with the phonons (quantized lattice vibrations) of the light-absorbing material. This means that the energy of photogenerated electrons and holes in excess of the threshold energy (i.e., the bandgap) is not utilized for useful work, but rather is converted into heat. Furthermore, in this regime photons less energetic than the threshold energy are not absorbed. Recent research has shown that the equilibration of electrons and phonons (also referred to as hot electron cooling) can be slowed by 1 to 2 orders of magnitude in semiconductor quantum dots, quantum wells, and related nanostructures. Other researchers have shown that conversion efficiencies above the 32% limit may be achieved by the formation of resonant impurity bands in photoelectrodes produced from quantum dot solid arrays that can absorb two sub-bandgap photons to create one electron-hole pair, photon up-conversion whereby a higher energy photon is produced from two lower energy photons, and photon down-conversion whereby two smaller energy photons are produced from one energetic photon. Another approach to achieving high conversion efficiency, also yielding a theoretical thermodynamic maximum of about 65%, is to use multiple bandgap absorbers in a cascaded tandem configuration. In the limit of threshold absorbers matched to the solar spectrum the limit is 65%, but two tandem bandgaps as estimated to yield about 40% conversion and 3 tandem bandgaps to yield about 50% conversion.

Another approach to meet these cost/watt goals is to find chemical methods (referred to as disruptive technologies in the Photovoltaic overview) to fool the inexpensive photoconversion materials (like polycrystalline, nanocrystalline, and organic materials) into performing as if they were expensive single crystals, without actually incurring the costs to grow the expensive crystals themselves. This approach involves chemically treating these inexpensive materials with “solar paint” so as to fool their grain boundaries or interfaces into thinking they are part of the periodic crystal that this material is trying to emulate (e.g., see Fig. 4-6). A related strategy is to produce so-called interpenetrating networks. Use of such networks relaxes the usual constraint in which the carriers that are excited must exist long enough in their excited states to traverse the entire distance of the cell. Instead, the materials consist of a network of interpenetrating regions. There are two examples of these approaches that are just emerging; neither of them are economically or technologically viable today, but they seem like good approaches in the long run to achieve the difficult cost goals of 1-2 cents or less per kWh. In the end, this approach will have to be as cheap as painting your house and mass-produced like sheets of plastic or photographic film.

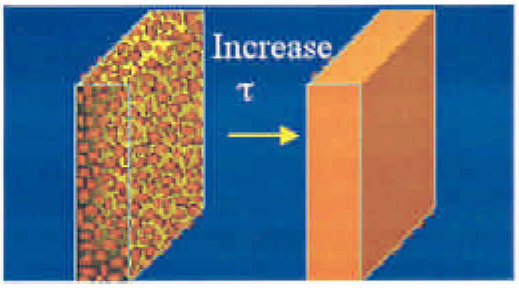


Figure 4-6. Solar paint passivates grain boundaries in inexpensive photovoltaics, causing them to perform like expensive single crystal materials.

Direct formation of fuels will also require development of inexpensive, robust, and efficient thermal and/or photochemical catalysts for the formation of such fuels from abundant, inexpensive, recyclable chemicals. Important targets include the direct photochemical splitting of water into H_2 and O_2, catalysts that individually reduce water to hydrogen and oxidize water to oxygen which could be used either in an integrated fashion with photoelectrochemical devices or in a modular fashion with PV systems, and catalysts that allow effect the reduction of CO_2 to organic fuels (such as methanol or methane) or which utilize H_2 with CO_2 to form hydrocarbon fuels.

All the various possible strategies for high efficiency, low cost, high stability and long lifetime solar photoconversion systems must be examined and compared to find the optimum system(s) to achieve the important goals described above for producing stored chemical free energy in fuels or electricity from renewable resources. This is particularly vital since photoconversion is a direct solar conversion process that utilizes the largest available renewable energy resource and has the potential to operate with ultrahigh conversion efficiencies and with very low cost materials.

Biomass

Biologically-based strategies for providing renewable energy can be grouped into two major categories:

- those which use features of biological systems to convert sunlight into useful forms (e.g. power, fuels) but do not involve whole living plants as we know of today, and
- those involving growth of plants and processing of plant components into fuels and/or power.

Given the current state of knowledge and uncertainty, it is far too soon to declare either of these "the winner" (or loser), and there are legitimate "homerun" possibilities in each category. It is recommended that both categories be pursued aggressively with roughly equal aggregate research effort considering the U.S. portfolio of energy-related research as a whole.

Among current and foreseeable plants and plant material, lignocellulosic biomass has the greatest potential for energy production and oil displacement in light of scale, cost, energy balance, and ecological considerations. Thus it is appropriate to focus consideration of research involving plant-based energy systems on cellulosic biomass. This should be done with an appreciation for the merit of well-justified research on plant types that are not foreseeable at this time, or to develop properties that circumvent the limitations of current non-lignocellulosic plants. It may be observed that the potential importance of biomass in meeting human needs currently met by non-sustainable resources depends on both technical and societal factors, a feature common to most renewable energy sources.

The domain of plant-based energy production can be categorized into work focused on plant production, and work focused on conversion of plant products. Both are very important and a roughly equal aggregated effort seems appropriate, considering the U.S. portfolio of energy-related research as a whole. Long-term improvements can be expected in the development of both biomass resources and the conversion technologies required to produce electrical power, fuels, chemical, materials, and other bio-based products. For example, the world's first biomass gasification system, in which wood chips were converted to gas to fire a boiler, was successfully operated. As molecular genetics matures over the next several decades, its application to biomass energy resources can be expected to significantly improve the economics of all forms of bio-energy. Improvements in economics, in turn, will likely lead to increased efforts to develop new technologies for the integrated production of ethanol, electricity, and chemical products from specialized biomass resources. Similarly, improvements in fuel cells can be expected to increase the value and demand for biogas. At the same time, near-term biomass markets in corn-ethanol and the co-firing of coal-fired power plants provide opportunities for learning-by-doing.

R&D challenges and opportunities can be classified into three broad areas. The first concerns terrestrial plants and algal systems in fresh and salt water. Productivity of plants in adverse environments (saline and degraded soils, high aridity ecozones) is very limited, yet to mitigate increasing human use of good soils and maintain ecosystem values such as biodiversity requires sustained long-term efforts. There may also be possibilities to increase the efficiency of photosynthesis and photosynthate storage. Recent work has started to elucidate not just the mechanism of photosynthesis but to also understand the molecular architecture of light harvesting and water splitting. Genomics first of Arabidopsis, and now underway for tree species (*Pinus* and *Populus*, already a candidate energy crop), and cereals (*Oryza* spp) will enable many aspects of the genome to be both understood and possibly manipulated to increase biomass production in total, of selected plant polymers and intermediates, and eventually to control both the composition and the macro-molecular architecture. Work on *Rubisco* the enzyme that transports almost 2/3 of all carbon dioxide in the atmosphere through the leaves of plants each year, may be one area that could pay off as well. With a more broad genetic understanding of plants both physiology and pathway work can benefit from technology transfer from societies large investment in biomedical technologies. In depth understanding of plant cell wall architecture, and of the mechanism and control of storage polymers in plants, detailed molecular mechanisms by which cellulose, other plant cell wall polysaccharides, and other key polymers are synthesized and deposited would facilitate novel materials, chemicals, and fuels from the biosphere.

The second area concerns post-harvest conversion of plant materials to fuels, chemicals, and materials. Currently the major biomass conversions use either thermochemical or bioconversion approaches. Gasification to molecules such as carbon monoxide and hydrogen, the components of synthesis gas, can generate desired fuels, chemicals and materials with suitable catalysts. Biological conversions require prior reduction of the plant cell wall polymers to simple molecules that are often monomers to the plant polymers such as glucose, xylose, and phenyl propane units from lignocelulosics, or complex and novel oligomers from starches or other storage compartments of plants.

Biotechnology offers a superb array of new and rapidly developing tools to advance our basic understanding of plants, enzymes and organisms. The advances during the past half-decade in the “omics” (genomics, proteomics, and metabolomics) also show great promise for continuing our understanding of the ways microbial cells live, multiply, and produce needed chemicals and materials. In addition, X-ray crystallography, neutron diffraction, molecular mechanics computer modeling, and electronic and atomic spectroscopies serve scientists to probe protein structure and elucidate chemical function. The “pull” from biomedical research needs will provide a steady stream of research innovations and tools available for use in other applications.

A third area of effort is in biomimetic construction of materials that today are unavailable naturally but could have preferred engineering properties at macroscales in textiles, the built environment, and many other areas. An opportunity is the development of new carbohydrate based nanoscale materials. Features unique to certain carbohydrate compounds induce them to self assemble into nanostructural materials that could have use as highly selective, structurally defined catalysts, and other applications. However, there is little known about how the structural features present in individual molecules translate into the ultimate shapes adopted by supramolecular structures. Once understood, carbohydrate based systems could develop with predictable properties as new nanomaterials for the future.

Looking back, a major issue is that our dependence on nonrenewable feedstocks for fuels, chemicals, and materials has been a direct function of our inability to manipulate complex polymeric molecules that compose plant resources to products other than food, feed, fuel, fiber and non-engineered wood polymers. Much about the current knowledge about plant cell wall structure, function, components, and physical and chemical properties has been derived as a way to obtain specific product performance targets – not necessarily to design at the molecular level the myriad of products that plant resources could provide if the science base were in place. Some chemical and materials technologies that are still in the market place are more than 100 years old. In plants, the interpenetrating networks of polymers and their complex biological synthesis suffer from great natural variability due to weather, geographic conditions, soil quality, water availability, and a host of other factors. Tools to unravel such complexity and provide the needed science base are now available and should be used to enable renewable resources for fuels, chemicals and materials to serve society’s needs for the future.

The "green revolution" increased remarkably the productivity of several grains thus decreasing concerns of the world's ability to feed a growing population. In fact, in 20 years, cumulative world agricultural production increased by 91% in developing countries and by 32% in the developed world. Significant increase in productivity was obtained through conventional genetics and a variety of inputs to fertilize the soil and control pests. This revolution includes environmental legacies of degraded and contaminated soils and water bodies.

The "green revolution for the next 50 years" needs to address productivity and selectivity of desired products to increase the efficiency of land and water use, while maintaining and improving soil, water, and air quality for future generations. This can only happen with a significant increase of the science base from which breakthroughs will emerge. It will require the integration of the body of knowledge from related areas such as genomes (sequencing and functional), developing and mining databases for information on properties and functions, and "omics", currently mostly developed for human life sciences, and applying these tools to plant science, enzymes, bacterial, fungal, and microbial consortia and photosystems, and other organisms at a much increased pace as well. Integrative, quantitative, experimental, and computational approaches will bring new knowledge, novel methods, and innovative technologies to engender a better understanding of complex biological systems and processes for renewable fuels, chemicals, and materials for the 21st century.

Promising research directions in the production of biofuels include low-cost production of enzymes, development of microorganisms for consolidated processes, improved performance of thermochemical processing, and advances in producing low-cost energy crops and controlling their composition. Many of these areas will benefit from advances in genetics and biochemistry. The yield of many field crops appears to be approaching upper limits. By contrast, it seems likely that the application of modern technology can lead to several-fold increases in the amount of biomass produced by woody species per unit area per unit time. Advances in this area are expected to come, in part, from advances in understanding the basis of plant growth and development. Improved understanding of the mechanisms that control the rate of cell divisions and expansion may provide novel opportunities to engineer plants that grow more rapidly (Figure 4.7). In addition, advances in characterizing the enzymes and processes responsible for the synthesis and deposition of cell wall polysaccharides may facilitate the development of genetically modified species with increased rates of cellulosic biomass production or the development of plants in which more of the cell wall biomass can be utilized for biofuel production. A major challenge in implementing research in this area is that the long lead-time between initiation of a genetic engineering experi-

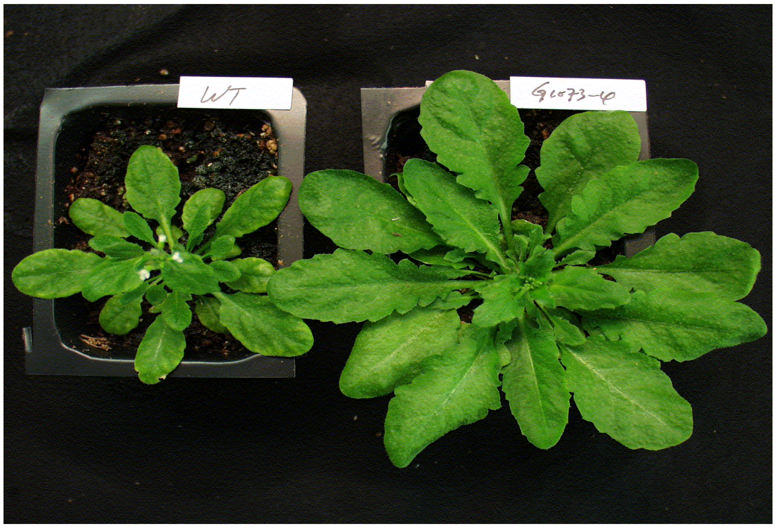


Figure 4.7. Increased expression of a single transcription factor has a major impact on biomass accumulation. Left: wild type. Right: transgenic.
Courtesy of Mendel Biotechnology.

ment in woody biomass production and the completion of the experiment is on the same time scale as a typical scientific career. Thus, novel career paths for scientists will need to be created before opportunities in this area will be evaluated. One of the most promising approaches today is the hydrolysis of fibrous biomass and subsequent microbial conversion of sugars to ethanol. The proliferation of microbial genome sequence information is a significant new resource in this area. A major opportunity is the development of technologies for conversion of non-cellulosic cell wall polysaccharides, such as pectins, to biofuels.

Hydropower

Advanced hydropower technology improves on available techniques for producing hydroelectricity by eliminating adverse environmental impacts and increasing generation and other operational efficiencies. Current technology often has adverse environmental effects, such as fish entrainment and the alteration of downstream water quality and quantity. The goal of advanced hydropower technology is to maximize the use of water for hydroelectric generation while eliminating these adverse effects.

R&D challenges include quantifying the biological response of fish affected by hydropower projects and modeling the forces inside turbines to predict stress levels on fish. Better computational fluid dynamics models may enable the design of “fish friendlier” turbines. The development and demonstration of retrofit technologies is also needed, so that the large number of hydropower plant licenses that are currently scheduled to expire after 2020 are able to take advantage of these advances during the relicensing process.

Summary

The contribution of renewable energy sources remained relatively small in the year 2000 and present data trends shown in Figures 4.1 and 4.2 are not encouraging. The U.S. Energy Information Administration projects a slight reduction in the fraction of energy supplied from renewable sources between the years 2000-2020. Although absolute usage of renewable energy sources is predicted to increase during this period, total energy consumption is expected to increase at a faster rate, with larger increases in natural gas and oil consumption. Substantial technical breakthroughs are required if the renewable energy technologies are to make a significant contribution to U.S. energy production, particularly for electricity, and the effort to reduce greenhouse gas emissions.

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FUSION ENERGY

A number of nuclear fusion reactions have been considered to provide a future source of energy, but the most feasible in the near term is the fusion of two hydrogen isotopes, deuterium and tritium (DT). The promise of DT fusion energy lies in its potential for an essentially unlimited fuel supply by extracting the required deuterium from terrestrial water supplies while breeding tritium in the reactor itself. The challenge of fusion lies in the need to build and operate one of the most complex engineering structures ever designed which must essentially contain a star in the laboratory. This entails understanding the physics of very high temperature gases (plasma physics) as well as developing the materials and engineering features needed to utilize this energy.

The technical issues that need to be resolved in order to make fusion power a practical reality fall into two broad classes: (1) the creation and maintenance of a burning plasma with an energy density high enough to permit net energy production, and (2) building and maintaining a structure that will permit this energy to be extracted and converted to electricity. There are two alternate schemes under investigation for containing a burning plasma: magnetic and inertial fusion energy (MFE and IFE). In the MFE concept, the plasma is confined and controlled by the interaction between the charged particles that comprise the plasma and powerful magnetic fields. IFE involves the use of either charged particle or laser beams to compress a small fuel pellet to a sufficiently high density for fusion to occur. Most of the pertinent issues related to fusion reactor technology are discussed in documents maintained by the Virtual Laboratory for (fusion) Technology (VLT), at the University of California, San Diego (website, http://vlt.ucsd.edu/).

MFE plasma science and technology has made significant progress in recent years as a series of experimental machines have been built and successfully operated. The larger of these machines include the Joint European Torus (JET) in the United Kingdom, the Tokamak Fusion Test Reactor (TFTR) (recently shutdown) and Doublet-IIID in the U.S., and the JT-60U in Japan. Based on the results obtained from operating these machines, including some experiments that involved burning tritium at JET and TFTR, there is increasing confidence in the plasma fusion community that a burning plasma experiment is feasible, and the international community is moving ahead with plans to build such a machine for this purpose. This machine, the International Thermonuclear Experimental Reactor (ITER), has been the subject of an international design activity since 1988 and a decision is expected this coming year on where to site the construction (see http://www/iter.org/). Candidate sites have been offered in Canada, by the European Union in France and Spain, and in Japan. The U.S. was initially an active partner in the ITER project, but stopped participating in 1999. However, the DOE under the current administration is discussing rejoining the project as the decision on construction approaches.

IFE science and technology has also made significant progress in recent years. Experiments on previous and existing facilities such as the Nova, Omega, and Nike lasers and other foreign facilities have given confidence that larger facilities will produce ignition and energy gain. The IFE program in the Office of Science benefits greatly from a larger inertial fusion program administered by the National Nuclear Security Administration (NNSA). In particular, NNSA is currently building a facility, the National Ignition Facility (NIF) to study burning IFE plasmas. A similar facility, the Laser Mega-Joule (LMJ), is under construction in France.

The issue of the next step experimental machine for investigating burning plasmas was the topic of a two-week meeting in Snowmass, CO in July 2002. This meeting involved more than 280 U.S. and foreign scientists in what was called the *2002 Fusion Summer Study.* Objectives of the *Fusion Summer Study* were:

- to review scientific issues in burning plasmas for MFE and IFE confinement,
- to provide a forum for critical discussion and review of proposed MFE burning plasma experiments and assess the scientific and technological research opportunities and prospective benefits of these approaches to the study of burning plasmas, and
- to provide a forum for the IFE community to present plans for prospective integrated research facilities, assess present status of the technical base for each, and identify a timetable and technical progress necessary for each to proceed.

The meeting summary (available at http://web.gat.com/snowmass/) strongly endorses building such an MFE burning plasma experiment, and identifies the issues and benefits associated with ITER and two alternate machines called FIRE (Fusion Ignition Research Experiment) and IGNITOR. As noted above, the burning plasma experiment for IFE conditions (http://www.llnl.gov/nif/) is currently under construction.

Although the successful control and maintenance of a burning plasma is not assured, increasing attention is now being placed on developing the materials and technology to use the DT fusion source to produce power. These latter issues are a focus of the material on the VLT website mentioned above. The high-energy neutrons created in the plasma will produce radiation damage problems in the structural materials that are similar to, but more severe than, those experienced by in-core components in fission reactors. In fact, materials development research in the fusion reactor program has in many cases paralleled that of advanced fission reactor programs. The major differences between the DT fusion and fission environments are the neutron energy spectrum. DT fusion neutrons are all born at 14.1 MeV while the fission source exhibits a spectrum with a peak near 2 MeV. The neutron spectra in both cases cover a wide range of energy as a consequence of scattering reactions. However, the presence of higher energy fusion neutrons has two major impacts: (a) higher energy primary atomic recoils and (b) high nuclear transmutation production since many such reactions have energy thresholds well above 2 MeV. In particular, the rate of helium and hydrogen generation by (n,α) and (n,p) reactions is on the order of 10 to 100 times higher in the DT fusion case. The required damage levels for components in the highest flux positions in DT fusion reactors are also greater than that in fission reactors.

The lack of an intense 14 MeV neutron source requires that the fusion program obtain radiation effects data primarily from irradiation experiments carried out in fission reactors. As a result, much of the previous experimental and modeling work in the fusion materials program has been aimed at determining the impact of the higher energy DT neutrons. Modern computational simulations support the view that the net effect of spectral differences between fission and fusion may be rather small. This conclusion is also supported by some experimental evaluations that indicates the use of a common correlation parameter (atomic displacements per atom, dpa) seems to account for spectral effects arising from differences in primary displacement damage production. However, the computational results provide information on the radiation damage source term only for times up to ~100 picoseconds, and do not account for the differences that may arise from transmutation products such as helium and hydrogen. Thus, additional research is required to confidently extrapolate the fission reactor data to DT fusion conditions. A good summary of the fusion materials research issues and opportunities is referenced below [Stoller et al. 1999].

Because of the system complexities, the need for materials research extends beyond radiation effects in structural materials. For example, plasma diagnostic systems require materials whose electrical performance may be degraded by irradiation, and the performance of optical materials used as windows and mirrors in both MFE and IFE systems may also be radiation sensitive. Superconducting materials are another example. Low cost, low degradation under irradiation and high temperature are desired properties. In addition, tritium must be bred by transmutation of lithium in a blanket region near the structural first wall. Both solid (ceramic) and liquid (liquid metals and molten salts) breeding materials have been investigated. Relevant research issues include the development and use of coatings to prevent the buildup of tritium in the blanket structure, corrosion issues, and the technology to extract tritium from the breeding medium.

If the technical issues with developing fusion energy are solved, further improvements may be required for this technology to be economically competitive. For example, a recent study [Delene et al. 2001] compared the projected cost (in the year 2050) of electricity from fusion with several other options, including coal, natural gas, nuclear fission, and wind. Two tokomak fusion designs included were ARIES-RS and ARIES-ST [Bathke 1997]. The other systems evaluated were generally advanced variants of current technologies: pulverized coal with flue gas desulfurization, pressurized fluidized-bed coal combustion, combined cycle coal-gasification, combined cycle natural-gas fired turbine, advanced light water fission reactor, advanced liquid metal fission reactor, and a wind turbine. The estimated baseline levelized cost of electricity from the fusion designs was 2.5 x 10^{-2} cents/MJ to 2.7 x 10^{-2} cents/MJ (91 and 97 mils/kWh) for the two fusion designs. This compares to a range of 8.3 x 10^{-3} cents/MJ to 1.9 x 10^{-2} cents/MJ (30 to 67 mils/kWh) for the other technologies. A range of assumptions was investigated in this study, but electricity from the tokomak fusion designs was consistently higher.

In summary, substantial levels of basic and applied research and development are required before the promise of fusion can be realized. The results of current plasma physics experiments increase confidence in the scientific feasibility of maintaining a burning plasma, and progress has been made in understanding the engineering issues associated with extracting and using the fusion energy produced. However, fundamental research related to materials performance, research on issues related to tritium breeding and extraction, and additional system design and integration studies are needed. Finally, technical feasibility does not ensure the economic viability of fusion. The perceived environmental advantages may offset some economic penalty, but history suggests that price will remain a strong selector in the energy marketplace.

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Other Resources

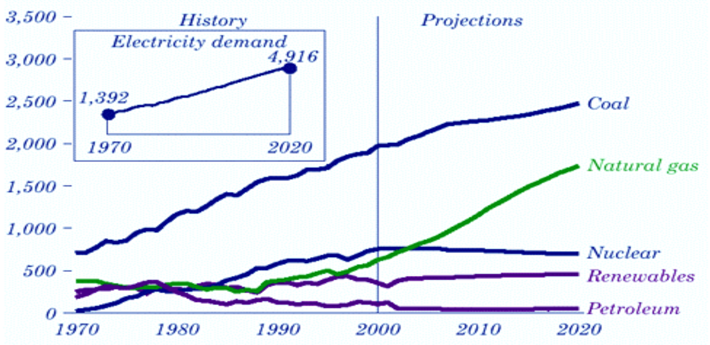
Inertial Fusion Energy Experiment. (http://www.llnl.gov/nif/)

ITER development. (http://www/iter.org/)

Virtual Laboratory for Technology (VLT), at the University of California, San Diego. (http://vlt.ucsd.edu/)

DISTRIBUTED ENERGY, FUEL CELLS, AND HYDROGEN

It is projected that by the year 2020 an estimated 6 trillion MJ (1.7 trillion kWh) of additional electric capacity, corresponding to about 200 generating plants with a 1 GW power capacity, will be required in the United States to meet new demand and replace lost capacity from retired power plants. (Figure 6-1.) This is almost twice the growth rate of the last 20 years. Estimates for the worldwide consumption of electricity show an increase from 12 billion MJ/s used in 1996 to possibly 22 billion MJ/s by 2020. Developing countries, where an estimated two billion people live in rural areas with no access to power grids, are projected to account for most of this increase. Distributed generation technologies are expected to capture a considerable part of this market with an estimated increased capacity of over 20,000 MJ/s (20 GW) per year over the next decade.



History: Energy Information Administration (EIA), Form EIA-860B, "Annual Electric Generator Report— Nonutility"; EIA, *Annual Energy Review 2000*, DOE/EIA- 0384(2000) (Washington, DC, August 2001); and Edison Electric Institute.

Figure 6-1. Electricity generation by fuel for the year 1970-2020 (billion kWh).

The term "distributed power generation" refers to placing small power generation units [typically less than 30 MJ/s (30 MW)] at or near customer sites to relieve burdens on existing transmission and distribution systems during peak use times or to provide standby power for customers that, either for health and safety or economic reasons (such as hospitals and some industries), cannot tolerate an interruption of service. Distributed power generation systems can be used in stand-alone situations, such as remote locations where no power grid exists or in industries where tight control of the quality and level of power is required. Heat generated by the power system can also be used in cogeneration applications, such as providing heating and cooling for buildings. Power sources for such applications need to be cost effective, dependable, efficient, relatively mobile, and have a minimal environmental impact. Gas turbines and reciprocating engines are already being used for distributed power generation and their efficiency may be improved further by continued materials and systems development. Emerging technologies, including microturbines and fuel cells, offer promise for providing additional options that could meet the efficiency and environmental criteria.

Critical issues in the envisioned technologies are the availability and nature of the fuel, its production, storage, transport, and efficient conversion into electrical energy. Fuel types may be divided broadly into carbon-free fuel (i.e., hydrogen) and carbon-containing fuels such as reformer gas or hydrocarbons.

Hydrogen as a fuel [adapted in part from IWG 2000]

It is recognized and accepted that once delivered to the energy conversion device, high purity hydrogen is the ideal fuel. Despite its abundance in nature, hydrogen is not a primary energy source, and must be produced from a primary energy source such as fossil hydrocarbons or coal, nuclear fission or fusion, hydroelectric, or renewable technologies. Depending on the source, its production may or may not involve CO_2 emissions. When hydrogen is produced from carbon-containing primary energy sources, e.g. by steam reforming of hydrocarbons, CO_2 appears as a by-product. Subsequent sequestration could result in low emissions of CO_2, compared to combustion, depending on the efficiency of the hydrogen production process. Nuclear power could be used to generate hydrogen, either through electrolysis of water or through thermochemical processes involving high temperature reactors. Hydroelectric power is well suited for the utilization of the off-peak plant capacity. Hydrogen from biomass or solid wastes could result in very low CO_2 emissions, depending on the amount of fossil fuel used for fertilization, cultivation, and transportation of the bioenergy feedstock. Zero-carbon dioxide hydrogen production concepts include:

- hydrogen by electrolysis of water, with electricity produced by nuclear, hydroelectric, solar or wind power plants;

- photoelectrochemical- and photobiological-based processes for producing hydrogen from water; and

- thermochemical conversion using advanced high-temperature nuclear or solar reactors, coupled to chemical reaction cycles.

It is important to consider the complete fuel cycle (i.e., the “well-to-wheel” efficiency [SNRA 2001, GM 2001], in the generation and use of hydrogen from fossil sources) when evaluating the overall environmental and fossil fuel savings for electrochemical energy conversion and when making comparisons with advanced combustion engines. The electricity consumed in the hydrogen generation by electrolysis could alternatively be directly delivered to the grid. Hydrogen as a fuel then retains merit in mobile or in remote applications, where a grid is not present, or where pollution reduction is an overriding concern. Furthermore, hydrogen has been proposed as a method of storing energy of intrinsically intermittent electrical power sources, such as wind and solar power.

Hydrogen is produced today in large quantities, primarily for use in the chemical and oil refining industries. Modest amounts of hydrogen are distributed by pipeline or truck to industrial users. Hydrogen production, storage and distribution methods are commercially available, but dramatic improvement, particularly of existing storage technologies for transportation, is needed if hydrogen is to become a major energy carrier in the future. Advanced storage concepts include complex hydrides, e.g., alanates [Zaluska et al. 2000], carbon adsorption and carbon nano-tube encapsulation. Many of the more promising concepts are still in the basic research stage, but are of questionable economic value, or are controversial [Ye et al. 2002, Züttel 2002]. Distribution systems would also have to be deployed that are capable of containing and pumping the low molecular weight fuel, utilizing materials that resist hydrogen embrittlement.

Key criteria for successful use of hydrogen in the transportation market is the energy density of the storage system, as compared to other fuels. Table 6-1 [Berry and Aceves 1998, Pettersson and Hjortsberg 1999]

Table 6.1. Estimated Storage Performance of Hydrocarbon in Tanks Designed for 640-km Range in a 34-km/l Gasoline Equivalent Car

Vessel type	Volume (l)	Weight (kg)	H_2 (kg)	E/V (MJ/l)	E/m (MJ/kg)	Reference
344 bar pressure H_2	237	37	5	2.5	22	Berry 1998
Liquid H_2	135	31	5	4.4	19	Berry 1998
344 bar cryogenic pressure H_2	126	66	5.17	4.9	9.4	Berry 1998
600 bar carbon/polymer H_2	--	--	--	3.5	7.5	Dillon 1997
"Metal hydride" H_2	66	184	5.7	10	3.7	Klos 1998
Methanol	62	46	--	11	15	Klos 1998
Gasoline	39	29	--	17	23	Klos 1998
Compressed natural gas	--	--	--	6-10	13-20	T-Raissi 1996

Source: Pettersson and Hjortsberg 1999

shows the projected volume and weight needed for a typical automobile using different hydrogen vessels and other fuels. Gasoline has the best performance in mobile applications. As yet, any of the known hydrogen storage methods do not compare, being either too heavy or to voluminous, or both.

In principle, the introduction of a hydrogen economy might proceed by a gradual transition from exclusive fossil fuel use to significant inclusion of non-carbon primary energy sources, reducing CO_2 and other emissions and full dependence on fossil fuels. At full market penetration, all conventional use of fossil fuels would be replaced by hydrogen derived from renewable, nuclear, or carbon-sequestered fossil-fuel sources.

Hydrogen as a fuel has been researched for nearly 25 years and is currently strongly promoted [Shell 2002] for mobile applications. Significant technical and economic uncertainties remain as obstacles to its broad deployment in the U.S. economy. At a minimum, before hydrogen can achieve a premiere status in the energy economy, dramatic advances will be required in hydrogen storage and carbon-free production technologies, while focused research programs aimed at innovation in this area should be formulated in realistic economic contexts.

Heat Engines

Heat engines, including various reciprocating types, gas turbines, and microturbines constitute a well-known and well-developed technology. They are presently the lowest-cost distributed generation technology. Since heat engines operate on Carnot cycle or other heat/pressure cycles, higher operating temperatures as well as heat recuperation can improve their overall efficiencies. The development of novel materials or coatings that can withstand combustion temperatures significantly above the present limits remains an area where basic materials research and development can produce significant benefit.

Heat engines are quite adaptable to alternative fuels such as landfill gas, propane, and gases derived from gasification of coal, biomass, and various types of waste. They can be used in a variety of applications because of their small size, low capital costs, easy start-up, reliable thermal output, good load-following characteristics, and heat recovery potential. In addition, developments over the past several years in exhaust catalysts and combustion design and control have resulted in significantly reduced pollutant emissions. They are suitable for many distributed power generation applications, and constitute a large portion of the combined heat and power (or cogeneration) market that currently accounts for about 7% of the electricity produced in the U.S. Typical installed costs are $250-450 per kJ/s and, in large size, can operate at a maximum efficiency of approximately 50% thermal.

Although heat engines have been characterized as being maintenance intensive, they have been produced for well over a hundred years, and therefore already have the support of a well-established base of sales and service outlets. Their ease of use and ready availability has, in fact, at times discouraged the search for alternative technology. The major drawbacks of combustion engines are their relatively limited lifetime (typically about 5000 hrs for reciprocating engines, e.g.), noise, and various pollutants, which need to be improved significantly for extended, continuous distributed service.

Fuel Cells

A fuel cell produces electric energy through an electrochemical reaction that combines a hydrogen or hydrocarbon fuel and air or oxygen to produce water, carbon dioxide (for hydrocarbon fuel or hydrogen derived from a carbon-containing primary fuel), and heat. Because they are not Carnot-cycle limited, fuel cells can be highly efficient, clean, quiet, and reliable. The fuel cell consists of an anode into which the hydrogen or hydrocarbon fuel is fed, a cathode through which the oxygen (or air) enters, and an electrolyte that separates the two electrodes. Polymeric electrolytes for the PEM fuel cells transport protons in association with several water molecules. Solid oxide electrolytes for the SOFC fuel cells exclusively transport oxygen ions. While the ions pass through the electrolyte, the electrons must take a separate path around the electrolyte, creating a current that can be utilized. The PEM fuel cells, operating around 100^{o}C are strictly hydrogen cells, where the hydrogen has to be supplied as such, or produced by reformers. They are presently intensely developed [Ballard 2002]. The solid oxide fuel cells, operating at temperatures up to 1000^{o}C can use not only hydrogen but also fossil fuels directly. This is a substantial advantage in a distributed generation scenario when a hydrogen infrastructure is not yet developed. In addition to water and heat, the fuel cell reactions produce carbon dioxide, not or minimally diluted by nitrogen – in contrast to combustion engines – that can be captured for recycling or sequestration.

There are five major types of fuel cells, each designated by the type of electrolyte used: alkaline (AFC), phosphoric acid (PAFC), polymer or proton-exchange membrane (PEMFC), molten carbonate (MCFC), and solid oxide (SOFC). Each of these are slightly different in the materials used for the different parts of the cell, the temperatures at which they will operate, and the source and type of fuel that they will accept. The dominant variants presently are the PEMFC and the SOFC, based on known cost and performance ceilings in the other fuel cell types. For the PEMFC a system that includes a “fuel reformer” can generate hydrogen from any hydrocarbon fuel, including natural gas, ethanol, methanol, and gasoline. Cells can be constructed to serve virtually any power requirement, from mJ/sec to MJ/sec, with little variation in efficiency.

Many potential applications for fuel cells are envisioned. More than 200 PAFCs have already been installed all over the world at stationary sites such as hospitals, nursing homes, hotels, office buildings, schools, airport terminals, etc., where they provide primary power or backup at a cost savings of 20-40% over conventional energy service. In addition, several are being used at landfills and wastewater treatment plants in this country where they use the methane gas produced at the site to generate power. Unfortunately, the PAFCs cost about \$3000 to \$5000/kW, and 10-15 years of manufacturing development have failed to impact this cost.

Since fuel cells produce little or no noise, have low emissions, and can operate directly or indirectly on propane, natural gas, or other fossil fuels, as well as locally derived hydrogen, they are ideally suited for distributed power generation applications. They can not only produce the needed electricity but also use heat from the fuel cell to provide hot water or space heating. The low-grade heat (~80^{o}C) from the current PEM fuel cell technology may also be used to provide air conditioning via a desiccant cooling cycle. The high temperature of the SOFCs also allows the exhaust gas to drive a turbine, in contrast to the PEMFC. Potential transportation applications include off-road utility vehicles, buses, trains, and even boats. As part of the national FreedomCAR Program, all the major automotive manufacturers (including Ford, General Motors, Honda, and Toyota) have a PEM fuel cell powered vehicle either in development or testing. SOFCs, under a strong development technology program through the National Energy Technology Laboratory (NETL) [NETL 2002], can offer higher overall efficiencies than PEM cells and, while mobile applications are also possible, they are envisioned chiefly for stationary distributed generation from a few kilowatts up to the megawatt range [NETL 2002].

In spite of the attractive system efficiencies, environmental benefits, and energy security that fuel cells in a distributed power generating economy could provide, they have yet to capture a significant portion of the energy market. A critical issue in this delay is the cost of the fuel cell systems. Presently, SOFCs and PEMFCs that have demonstrated extended performance (i.e., in excess of 10,000 hrs of continuous operation) are excessively costly. The current capital costs of such fuel cells (\$3000-10,000 per kJ/s) must be reduced considerably before they can become economically competitive with existing energy technologies. This situation is not a consequence of engineering or marketing inadequacy. Rather, the requirement of significant cost reduction has imposed the development of fuel cell systems that use inherently low-cost materials and processing techniques. The development has been hampered by an insufficient science base that can accurately predict materials properties and compatibilities in fuel cell environments.

Research Needs

There are many research opportunities in the development of novel fuel sources, efficient fuel cells, engines and turbines for distributed energy applications. Fundamental research is needed to improve the understanding of the chemical, physical, and mechanical properties of materials used in fuel cells, and in hydrogen generation, transportation, and storage. Advancements in these areas could lead to new designs and possibilities for using lower-cost and easier-to-manufacture materials. Significant advances are needed for stack materials, oxygen cathodes, and membranes, including metals, ceramics, and polymers. These could lead to the development of durable PEMFCs that operate at higher temperatures, and SOFCs that operate at lower temperatures.

Hydrogen direct combustion devices can benefit from continued fundamental research. Needed are engine and turbine materials that resist corrosion and operate efficiently and reliably at higher temperatures, more durable and lower cost sensors and instrumentation, and better performing hydrogen-natural gas fuel blends.

A breakthrough in hydrogen storage technologies would profoundly impact the feasibility of the hydrogen economy.

The areas where innovative basic materials research, sensitive to economic factors, can be formulated to lead most effectively to energy improved technology may be broadly listed as:

- materials physics and chemistry of functional surfaces and interfaces, including structural, electrochemical, catalytic, and corrosion protection functions;
- predictive theories of composition and structure of ceramic and polymeric materials for high oxygen ion or proton conduction, constrained by cost;
- materials physics and chemistry of mixed electron/ion conductors;
- materials physics and chemistry of ultrahigh capacity, lightweight hydrogen storage materials;
- materials physics and chemistry of novel hydrogen production technologies; and
- limits of strength of materials for hydrogen pressure vessels, both theoretical and after processing.

Summary

Distributed power generation is still in its infancy. For advanced distributed power generation systems to become a reality for general power production applications, significant manufacturing cost reductions and further improvements in materials performance are needed in all of the systems listed above. These improvements will depend principally on innovative development of high-performance and yet low-cost materials, as well as on identification of cost-effective manufacturing techniques. While the near term options for distributed generation applications include reciprocating engines and gas turbines, in a distributed power generation economy operating on hydrogen or carbon containing fuels, fuel cells in combination with microturbines can ultimately provide the needed environmental benefits, reduce the critical dependence on fossil fuel, and provide the necessary energy security.

The realization of these materials-limited advanced technologies depends critically on the information that basic materials sciences studies need to provide.

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TRANSPORTATION ENERGY CONSUMPTION

The U.S. transportation sector includes highway, air, rail, shipping, pipeline, and off-road transport, as well as other categories such as recreational boats and military fuel consumption. In the year 2000, the sector consumed about 28.8 EJ (27.3 Quads) of primary energy, which translates into 28% of total U.S. energy consumption. The sector is also the nation's primary oil consumer at 27 EJ (13.3 million barrels per day [mbd]) in the year 1999, or about 67% of total U.S. consumption. Transportation is almost exclusively dependent on petroleum; over 97% of all energy used in the sector comes from oil. Transportation is responsible for almost one-third of U.S. carbon emissions, substantial amounts of most air pollutants, and two-thirds of U.S. oil consumption (Table 7.1). In the same year, the sector emitted 502 million metric tons (MtC) of carbon, or 32% of the U.S. total carbon emissions. In the face of strong continuing demand for transportation services, slow turnover of fleets, gasoline's dominance of light-duty vehicle fueling infrastructure, and low energy prices that provide only modest incentives for improved efficiency, U.S. transportation energy consumption and greenhouse gas (GHG) emissions are expected to grow robustly over the next few decades.

Table 7.1. Contribution of the Transportation Sector to National Issues and Problems for the Year 1999

National Issue	Amount	% of U.S. Amount
Climate Change – Carbon Emissions	502.0 MtC	33
Air Pollution – CO	84.6 Mt	80
Air Pollution – NOx	11.6 Mt	54
Air Pollution – VOC	7.7 Mt	44
Air Pollution – PM-10	0.5 Mt	3
Air Pollution – PM-2.5	0.5 Mt	7
Air Pollution – SO_2	0.7 Mt	4
Oil Dependence – Oil Use	27.1 EJ (25.65 Quads)	67

Source: EIA 2001 (CO_2 and oil dependence), EPA 2002 (other air emissions)

Overview of the Sector

Highway travel dominates the U.S. transportation sector, consuming 75% of the total energy used by the sector. In the highway sector, light-duty passenger travel is dominant, accounting for 74% of highway energy consumption, and 56% of *total* transportation energy consumption. Figure 7.1 shows the modal breakout of energy consumption. The characteristics of the various fleets in the sector and recent trends in energy use provide important clues to likely future energy use in the sector and the potential for reducing GHG emissions. Some critical points about the transportation sector include:

- New light-duty passenger vehicles have been adopting fuel-efficient technologies over the past decade and a half, but consumer shifts to increasing vehicle size, weight and especially performance have nullified potential fuel economy gains from these technologies.

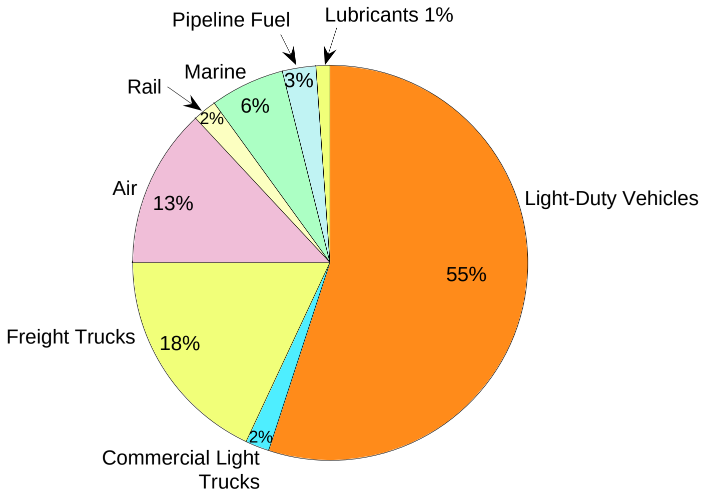

Figure 7.1. Year 2000 Transportation Energy Use by Mode (27.3 Quads/28.8 EJ)
Source: EIA 2001

- Important new technologies have entered the fleet, including port fuel injection, four- valves/cylinder engines, variable valve control, structural redesign for improved safety and reduced weight, growing use of high-strength steel and steel substitutes such as aluminum and plastics, and low-rolling resistance tires.

- Counteracting trends indicate the consumer shift to more inefficient vehicles, including the growing sales share of light-duty trucks (including Sport Utility Vehicles), which now comprise 46% of light-duty vehicle sales, up from 17% in the year 1980; horsepower to weight ratios 45% higher than in year 1980, an increase in weight over year 1980 vehicles [Heavenrich and Hellman 1999]; greater shares of four-wheel drive installed on 47% of year 1999 model light trucks, and other luxury features.

- As a result of a decade of low gasoline prices, consumer surveys show that today's auto purchasers generally are not interested in fuel economy.

- The "potential technology" portfolio for automobiles has been enhanced substantially by government/industry joint research and development programs [NRC 1999]. The impacts of this research are both direct and indirect, including stimulation of competitive developments in Europe and Japan.

- Freight transport now consumes about 30% of U.S. transportation energy, with freight energy use, but *not* gross ton-miles, dominated by heavy truck carriage (over 50% of energy use, about one-quarter of ton-miles) [Davis 1998, table 2.13], the most energy-intensive mode aside from air freight. Air freight and freight truck energy use are the most rapidly growing freight modes because of the U.S. economy's shift towards higher value (and more time-sensitive) goods. A countervailing trend is greater use of multi-modal shipments, advanced by the rationalization of U.S. freight railroads and the benefits of improved computerized information systems.

Examples of Promising Technologies

The transportation sector has a wide variety of available and emerging technologies that offer the potential to reduce significantly the energy use and GHG emissions associated with transportation services.

Cellulosic Ethanol. About one billion gallons of ethanol produced from corn are currently used annually in U.S. transportation markets as a blend stock for gasoline [Davis 1998]. Although the efficiencies and fuel choices used over the fuel cycle in producing ethanol vary widely (e.g., fuel choices for powering the distillery can be corn stover, natural gas, or coal), recent studies show that the use of ethanol provides a moderate GHG advantage of about 20% over gasoline. Processes to produce ethanol from cellulose – from woody biomass or municipal wastes – for use as a gasoline blending agent or neat fuel offer reduction of greenhouse gases by about 80% compared to gasoline [Wang et al. 1999]. Land requirements could ultimately limit cellulosic ethanol production. About 15 billion gallons of ethanol (1.2 EJ/1.3 Quads) could be produced annually by converting municipal and agricultural wastes with minimal land requirements [Lynd 1997]. If about 35 million of the roughly 60 million acres idled by Federal programs were used for energy crops, about 25-32 billion gallons, or about 2.8-3.8 EJ (3-4 Quads) of ethanol could be produced annually (assumptions: 8.4 dry tons/acre/year crop productivity, 107.7 gallons of ethanol/ton yield) [Lynd 1997]. If only 10 billion gallons of ethanol were produced annually, this would leave 200 million dry tons of biomass for other uses, such as biomass power.

Hybrid Electric Drive Trains. A hybrid electric drive train combines an internal combustion engine or other fueled power source with an electric drive train including an electric motor and battery (or other electrical power source, e.g., an ultra capacitor). Potential efficiency gains involve recapture of braking energy (with motor used as generator, captured electricity stored in the battery); potential to downsize the engine, using the motor/battery as power booster; potential to avoid idling losses by turning off the engine or storing unused power in the battery; and increasing average engine efficiency by using the storage and power capacity of the electric drive train to keep the engine operating away from low efficiency modes.

Lower Weight Structural Materials. The use of alternative materials to reduce weight has been historically constrained by cost considerations, manufacturing process technology barriers, and the difficulty of these materials in meeting automotive requirements for criteria such as surface finish quality, predictable behavior during crash tests, or repairability. The last few years have seen significant developments in overcoming such barriers through design changes such as a space frame-based structure; advanced new manufacturing technology for plastics, composites, ceramics, and aluminum; and improved modeling techniques for evaluating deformability and crash properties.

Direct Injection Gasoline and Diesel Engines. Direct-injection lean-burn gasoline engines have already been introduced in Japan and Europe, but have been restricted here by a combination of tight emission standards and high sulfur content in gasoline. Catalytic converters capable of reducing NO_x emissions from lean-burn engines are very sensitive to fuel sulfur content, and no simple remedy has been found. Direct-injection diesel engines have long been available for heavy trucks, but recently have become suitable for automobiles and light trucks, with reductions in noise and emission problems. These new engines are about 25-30% more fuel efficient, on a per gallon basis, than conventional gasoline engines (roughly half of the gain from higher engine energy efficiency and half from the higher energy density of diesel fuel). Diesel engines are about 15% more efficient on the basis of carbon emissions over the fuel cycle. Federal Tier 2 emission regulations require light-duty diesel vehicles to attain the same (low) NO_x levels as gasoline vehicles, as well as stringent particulate levels. These standards will require new active aftertreatment that may reduce the fuel economy benefit significantly. Federal emission standards for heavy-duty engines that become effective in the year 2007 are similarly challenging. These new federal standards present a challenge to diesel’s viability. Federal rules will require diesel fuel to be less than 15 ppm sulfur after the year 2006. Further improvements in diesel technology offer substantial promise in heavy-duty applications, especially for heavy trucks but also include marine and rail applications.

Fuel Cells. Fuel cells have been called the "Holy Grail" of clean powertrain technology, with promise of zero or near-zero criteria pollutant emissions and very high efficiency. The recent optimism has been driven by strong advances in technology performance, including rapid increases in specific power that now allow a fuel cell powertrain to fit into the same space as a conventional engine without sacrificing performance [Griffiths 1999]. However, fuel cells remain extremely expensive, and long-term costs are by no means clear. Further, important technical roadblocks remain, such as operation in extreme weather conditions. Another central issue is fuel choice. Fuel cells need hydrogen, either carried on board or produced by reforming methanol or gasoline. Carrying hydrogen may yield the cheapest and most fuel-efficient vehicle, but no hydrogen distribution and refueling infrastructure exists. A gasoline vehicle overcomes the infrastructure problem but is the most expensive and least efficient vehicle. Developing an adequate gasoline processor remains a critical task, with significant improvements required in processor weight and size, cost, response time, efficiency, and output of carbon monoxide, which can poison the fuel cell stack [NRC 1999]. While methanol could be an alternative, it is water soluble and toxic to humans with invisible flame that also requires a substantially improved fuel processor and, as yet, has no real infrastructure for distribution. Additionally, hydrogen and liquid fuel versions are likely to be more expensive initially than an equivalent conventional automobile. Hydrogen is an energy "carrier", not an energy feedstock, and must be produced from other energy resources. Hydrogen production from fossil feedstocks would require carbon sequestration to avoid net GHG emissions. Further, the cost of producing hydrogen must be weighed against any improvement in efficiency.

Aircraft Technology. Several major technologies offer the opportunity to improve the energy efficiency of commercial aircraft by 40% or more. The Aeronautics and Space Engineering Board of the NRC [NRC 1992] concluded that it was feasible to reduce fuel burn per seat mile for new commercial aircraft by 40% by about the year 2020. Of the 40% reduction, 25% was expected to come from improved engine performance, and 15% from improved aerodynamics and weight. A reasonable preliminary goal for reductions in NO_x emissions was estimated to be 20-30%.

Potential Research Directions

In the long term, additional advances hold the promise of large reductions in energy use, GHG emissions, and air pollution from the transportation sector. Opportunities lie in new, revolutionary propulsion systems and alternative fuels and in the application of information technologies to manage and integrate intermodal transport systems in innovative and more efficient ways. Advances in information technology may create new opportunities to increase system-wide efficiency and substitute communication for transportation to enhance economic well being and the overall quality of life. Promising areas for continuing research include:

Hybrid, Electric, and Fuel Cell Vehicles. Developing commercially viable, mass-market electric-drive vehicles (EVs) would free the automobile from dependence on carbon-based liquid fuels while simultaneously reducing vehicular emissions. Hybrid electric vehicles (HEVs) combine an internal combustion engine (ICE) with an electrical power source (battery and electric motor). Fuel-cell-powered electric vehicles (FCEVs) have been demonstrated with and without batteries for onboard storage of electrical energy. If fuel cell technology could be sufficiently advanced and the infrastructure for supplying hydrogen fuel developed, a potentially pollution-free propulsion system would be available (depending upon how the hydrogen is produced). On-board hydrogen and biofuels offer the options for zero net GHG emissions from personal transportation, should that be required for stabilization of atmospheric carbon. While HEVs are already on the market, their incremental costs are too high to enable large-scale market penetration.

HEVs, EVs, and FCEVs all face formidable technical hurdles, many of which they share. Developing low-cost, rapidly rechargeable batteries is a critical factor in the success of HEVs and EVs. FCEVs will also require cost reductions (by nearly an order of magnitude) as well as improvements in hydrogen storage and reliability. Carbon savings from EVs depend directly on the primary energy sources used to generate the electricity that charges the batteries. Potential advances in electricity generation technology could make EVs very-low-carbon vehicles. However, the choice of fuels used by electrical utilities and how they are produced will determine the extent of CO_2 reductions over those of conventional vehicles.

Freight Vehicles. Freight vehicles—heavy trucks, railroad locomotives, and ships—are the second largest energy consumers in the transport sector after light-duty vehicles. Heavy trucks and locomotives are almost universally powered by highly efficient (40-45%) diesel power plants. The efficiency of diesel engines could be improved further to 55% by use of technologies such as advanced thermal barrier coatings; high-pressure fuel injection; turbocharging; and reduced-friction and lightweight, high-strength materials. Fuel cells are an especially promising technology for locomotives, where problems of size, fuel storage and reforming are greatly reduced. Emissions of NO_x and particulates remain the greatest barriers to ultrahigh-efficiency diesels, while for fuel cells, cost and the state of development of mobile fuel cell systems present the biggest challenges. Because freight vehicles and their power plants have useful lives measured in decades, the transition to low-carbon technologies would require decades.

Alternative Fuel Vehicles. Alternative transportation fuels are those that require substantial changes in conventional infrastructure, whether in fuel production, distribution, and retailing or in vehicles. Most alternative fuels currently under consideration are being explored for their ability to reduce pollutant emissions or displace petroleum and would have modest GHG reduction potential. Fuels such as compressed natural gas and propane can reduce carbon emissions by 10-20%, on a full fuel-cycle basis, over conventional gasoline or diesel fuel. Far more promising in reducing GHG are biofuels, such as biodiesel produced from soy or rapeseed oils or ethanol or methanol produced from cellulosic feedstocks. Vehicle technology for using ethanol and biodiesel is at a relatively advanced stage of development. The chief barriers to widespread use of these fuels are cost and limitations on feedstock production.

Air and High-speed Ground Transport. Commercial air travel is the fastest growing energy-using mode of transport. It is also the mode that has achieved the greatest improvements in energy efficiency during the past three decades. Yet commercial air transport is also the most petroleum dependent. Opportunities to replace kerosene jet fuel appear to be many decades away. In the meantime, petroleum displacement in high-speed intercity transport may be achievable by integrating high-speed rail systems with the commercial air network. Operating at 180 to 300 mph, magnetically levitated or steel wheel rail cars could substitute electricity for kerosene in short-distance (<500 miles) intercity travel, at the same time relieving both air traffic and highway congestion. Such benefits will depend, crucially, on the level of train ridership. Although air transport has already more than doubled its energy efficiency over the past quarter century, opportunities remain for at least another 50% improvement during the next 25 years. Propfan technology, improved thermodynamic efficiency of turbine engines, hybrid laminar flow control and other aerodynamic improvements, and greater use of lightweight materials could accomplish this 50% improvement. These approaches are currently under development by NASA and aircraft and engine manufacturers. A potentially important issue for civil aviation is the possible advent of a new generation of far more energy-intensive supersonic high-speed civil transports. The unique requirements of supersonic and hypersonic aircraft could eventually drive the development of alternative fuels for commercial transport.

Having the best and most efficient commercial aircraft technology will reduce carbon emissions and petroleum use, which is critical to retaining competitiveness in the U.S. aircraft industry. The principal impediment to continued efficiency improvement and lower carbon emissions is likely to be the relatively low cost of jet fuel, providing an inadequate incentive to adopt new, more complex, and possibly more costly aircraft technology. Land use and infrastructure investment options offer powerful strategies for reducing the energy- and carbon-intensity of today's transportation sector. Advances in information technology and a variety of policy levers offer the potential to develop urban spatial structures that decrease the demand for travel while maintaining accessibility. The exploding growth of e-commerce and the internet economy could fundamentally reshape the nation's demand for energy services. Vehicle technology for using ethanol and biodiesel is at a relatively advanced stage of development. The chief barriers to widespread use of these fuels are cost and limitations on feedstock production.

Summary

Energy use and carbon emissions from transportation have grown steadily and appear likely to continue to grow without new policies or sharp changes in fuel prices and availability. The direct physical causes of this growth have been:

- Travel demand has continued to grow strongly as incomes and population have risen; for example, personal vehicle miles traveled (vmt) grew by 2.8% per year during the years 1974-1995.
- Light-duty fuel economy has stagnated over the past decade.
- Vehicle technology has changed over time, but much of the technology has been used for purposes other than higher efficiency.

Several factors will strongly influence future levels of transportation energy use and GHG emissions. On the favorable side, a variety of technology options currently are available to reduce energy use and emissions, and a substantial portfolio of advanced technologies is under development. Obtaining large emissions reductions will require counteracting a number of factors, including:

- inexpensive fuel and consequent disinterest in fuel economy among light-duty vehicle purchasers;
- fuel efficiency trade-offs with vehicle characteristics that *are* of interest to vehicle purchasers such as acceleration performance, vehicle size, and consumer features such as four-wheel drive, etc.;
- time required for redesign, retooling, and fleet turnover because the full benefits of new technologies take years to develop;
- high costs and/or important technological and market risks associated with some of the most promising fuel economy technologies; and
- uncompetitive features of alternative modes of personal transport (travel time, security, comfort, etc.)

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RESIDENTIAL, COMMERCIAL, AND INDUSTRIAL ENERGY CONSUMPTION

In addressing the issues regarding the residential, commercial and industrial energy consumption, the research focus should be established with an eye on the future energy landscape and requirements, and not be limited by the current prevailing technologies and demand patterns. In looking forward, Society will be confronted with significant new challenges in the next 50 years. The availability of a rich, high quality, scientific research base carried to the pre-competitive level will be the best strategy for coping with future energy requirements. A new way of thinking by policy makers and scientific program managers will be needed to establish a viable long-range research agenda. The activities supported will not only have to deal with their own intrinsic dimensions but with the impact of extrinsic advances of science and technology more generally in an increasingly integrated manner than in the past. The development of applications and hand off to industry will require feasibility and cost-effectiveness demonstrations, following the basic research phase.

The objective of the workshop is to come up with several aggressive and imaginative research directions that will have the potential for a significant impact on reducing residential, commercial and industrial energy consumption with commentary on the methodology used in the identification of these research directions. Several tentative suggestions are listed in this background paper for consideration as possible new research directions. The focus of the workshop is to seriously develop bold, new research directions through briefings, discussions and brainstorming.

For ease of analysis, the energy consumption of the residential, commercial and industrial sector has been divided into two subgroups. The first subgroup combines the commercial and residential energy use in the buildings sector, while the second subgroup summarizes the energy use for the diverse industrial sector. Much of this information was taken from the report, *Scenarios for a Clean Energy Futures* [Interlaboratory Working Group 2000].

Buildings (Commercial and Residential) Sector

Overview of Sector: Energy is used in buildings to provide a variety of services such as space heating, space cooling, water heating, lighting, refrigeration, and electricity for electronics and other equipment. In the U.S., building energy consumption accounts for a little more than one-third of total primary energy consumption and related greenhouse gas emissions. The cost of delivering all energy services in buildings (such as cold food, lighted offices, and warm houses) was about $234 billion in the year 2000 [U.S. DOE 2002]. About 69% of building sector energy use is electricity, and this sector uses about 68% of all electricity generated nationally. Natural gas accounts for 23% of total energy in this sector, and electricity and natural gas account together for about 92% of building sector primary energy use. Oil consumption is only 2% of the total, although it is a significant heating fuel in the Northeast.

Buildings Sector Primary Energy Use in Year 2000: Figure 8-1 and Figure 8-2 show the percentage breakdown of primary energy use by end-use in residential and commercial buildings, respectively. The breakdown of carbon emissions by end-use tracks the primary energy breakdown closely. Space heating is by far the largest identified end-use in the residential sector, accounting for just about one third of the primary energy. Water heating is next, followed by space cooling, refrigerator/freezers and lighting. The adjustment (9%) is for miscellaneous uses not identified and to reconcile totals to the EIA (Energy Infor-

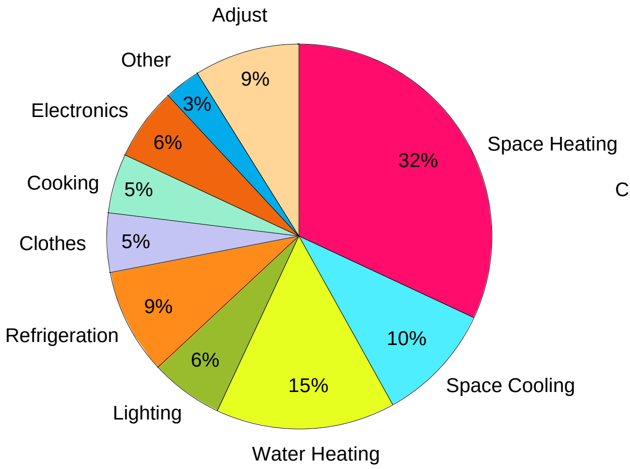

Figure 8-1. Primary energy consumption in residential buildings by end use for year 2000. Total primary energy use = 21.0 EJ (19.9 Quads). *Source: U.S. DOE 2002*

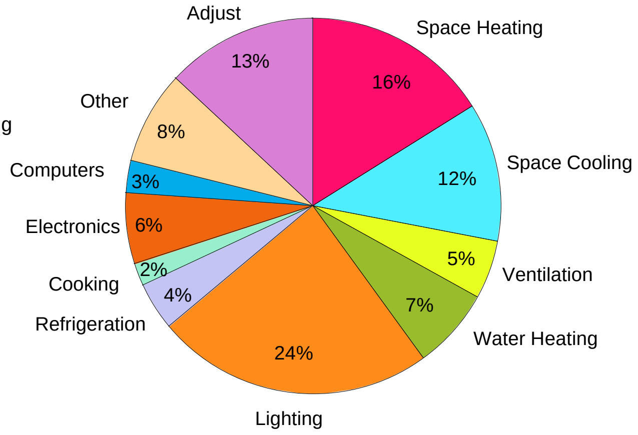

Figure 8-2. Primary energy consumption in commercial buildings by end use for year 2000. Total primary energy use = 17.4 EJ (16.5 Quads). *Source: U.S. DOE 2002*

mation Agency) *State Energy Data Report*. In the commercial sector, lighting accounts for about one quarter of total primary energy use, and is far and away the largest identified end-use in this sector. Space heating is next, followed by office equipment, cooling, and water heating. The "miscellaneous uses" category contains cooking, transformers, traffic lights, exit signs, district services, automated teller machines, telecommunications equipment, medical equipment, and other unidentified end-uses. It also includes an adjustment term to ensure that the total commercial sector energy use adds up to the totals reported in EIA's *State Energy Data Report*.

This energy portrait in year 2000 will of course not remain static in the next two decades, and that has important implications for energy policy design. EIA projects in its *Annual Energy Outlook 2002 Reference Case Forecast* [EIA 2001], for example, that energy demand for personal computing and office equipment services in the commercial sector will increase over 4% per year. By contrast, EIA also projects sharp *decreases* in home energy use for refrigeration and freezers, due to implementation of standards and technological improvements. These projected shifts mean that by year 2020 energy demand for refrigeration will have fallen to 5% of total use (versus 9% now), while energy use for commercial office equipment will increase its share from 9 to 14% of that sector.

Classification of Research Directions: Major transformations are possible in the energy features of buildings as the result of applied technology R&D and in the underlying basic sciences. In as much as most of these are best applied to new construction, their market penetration will probably occur after the year 2020.

Equipment and Appliances: By definition, the energy used in buildings is consumed by equipment that transforms fuel or electricity into end-uses, such as delivered heat or cooling, light, fresh air, vertical transport, cleaning of clothes or dishes, information management, or entertainment. The overall efficiency of this transformation depends largely on the efficiency of the equipment itself.

Numerous opportunities exist to develop equipment that is much more efficient than that currently available.

- It may be possible to virtually eliminate space heating in many climates by means of building shells with very high resistance to heat loss or gain involving high insulation walls, ceilings, and floors and triple pane windows with transparent heat-reflecting films; wide use of passive designs; and mass-produced components (walls, ceilings) with very low infiltration rates.

- Microtechnology could greatly increase heat and mass transfer rates, with highly efficient applications to chemical and thermal systems. One potential buildings application, microheat pumps, could be distributed throughout the building as part of the walls or window. This distributed approach would allow selected rooms or even parts of rooms to be heated or cooled as needed.

- Multifunctional equipment and integrated systems offer the opportunity for a significant increase in efficiency improvement. For example, an integrated water heating/space cooling system that uses heat pumping to meet space heating, air conditioning, and water heating needs could be 70% more efficient than the combined efficiencies of systems in use today.

- Dramatic declines in the energy consumed by supermarket refrigeration systems could be achieved with distributed system designs. Such systems of the future would locate compressors close to display cabinets thereby avoiding the loss of refrigerant charge. Use of the waste heat by heat pumps for space conditioning would lead to further efficiency gains.

- As energy conversion technologies evolve, many buildings could become net producers of energy as roofs incorporate photovoltaic panels and fuel cells and microturbines generate more power than is required on site. In addition, fuel cells and microturbines produce waste heat that can be employed to serve building thermal loads. These power technologies could transform the entire demand and supply chain in terms of energy generation, distribution, and end-use.

- Building control systems of the future will likely incorporate smart technology to closely match energy and water supply and ambient conditions with the needs of building occupants. Building loads and central plants supplying the loads will be more integrated and optimized to enhance the efficient use the energy streams into and out of the building.

The Building Envelope: The building envelope provides fundamental thermal load control for a building. Walls, roofs, and floors block or delay the flow of heat between a building's interior and exterior. Windows can also block heat flow, provide daylight, transmit solar energy, and provide a view of the outside. High-capacitance internal walls, ceilings, and floors can provide thermal storage that reduces energy use by storing solar energy and reduces peak loads by balancing energy use over a 24-hour period. Improvements in the energy performance of these building elements reduce energy use in buildings and thereby reduce Green House Gas (GHG) emissions.

Decreasing the building thermal load reduces the need for heating and cooling energy. The following emerging building envelope technologies will significantly reduce building energy use:

- super insulation, based on vacuum principles
- new-formula high-efficiency foam insulation that uses no chlorofluorocarbons (CFCs) or hydrochlorofluorocarbons
- advanced gas-filled, multiple-glazing, low-emittance windows and electrochromic glazing
- roof systems that promote self drying, thereby preventing moisture from degrading its insulation
- passive solar components
- durable high-reflectance coatings
- advanced thermal storage materials

Intelligent Building Systems: The process of designing, constructing, starting up, controlling, and maintaining building systems is very complex. If it is done properly, the final product delivers comfort, safety, and a healthy environment and operates efficiently at reasonable cost. If any part of this process breaks down, the product fails to deliver these benefits. The lost health and productivity in office environments alone costs U.S. businesses hundreds of billions of dollars each year. In addition, operating these "broken" systems is estimated to cost at least 30% of commercial building energy use (more than $45 billion). The key to designing and operating buildings efficiently is the ability to manage information, deliver it in a timely manner to the proper audience, and use it effectively for building design and operation. More intelligently designed and operated buildings use energy more efficiently and thus reduce GHG emissions.

Sensors and Controls: To best optimize the energy efficiency, air quality, and personal comfort of an entire building, monitoring of the interior space is critical. An essential requirement for effective monitoring will be the development of low-cost, low-power sensors. Poor office environments cost U.S. businesses more than $400 billion a year in productivity losses and increased health care costs. To achieve maximum energy efficiency, a whole-building perspective is needed that integrates sensors, controls, and communications to anticipate changes in the environment and respond dynamically while maintaining comfort and air quality. First-order estimates indicate that such an approach will reduce annual energy consumption by 2.1 EJ (2 quads), reducing energy costs by $55 billion and carbon emissions by 35 MtC [Christian 2002].

Industrial Sector

Overview of Sector: The industrial sector is extremely diverse and includes agriculture, mining, and manufacturing industries. In year 2000, the industrial sector (manufacturing industries only) consumed about 37 EJ of primary energy, accounting for close to one-third of the primary energy consumed in the U.S. that year. As shown in Figure8-3, the most energy-intensive subsectors include chemicals, petroleum refining, forest products (pulp and paper), steel, mining, aluminum, metal casting, and glass. The large electricity component represents the energy lost in conversion to electricity by the electric industry in serving the other industries.

Among sources of energy, the industrial sector heavily favors natural gas and electricity, as shown in Figure 8-4. Losses in energy generation, distribution, and conversion, are substantial; less than half of the total energy input to industry for heat and power is actually delivered to the process.

Figure 8-5 provides a breakdown of the share of CO_2 emissions by industrial subsector. Carbon dioxide emissions from industrial energy use as well as process emissions from cement manufacture were 478 MtC, accounting for 31% of total U.S. CO_2 emissions [EIA 2001].

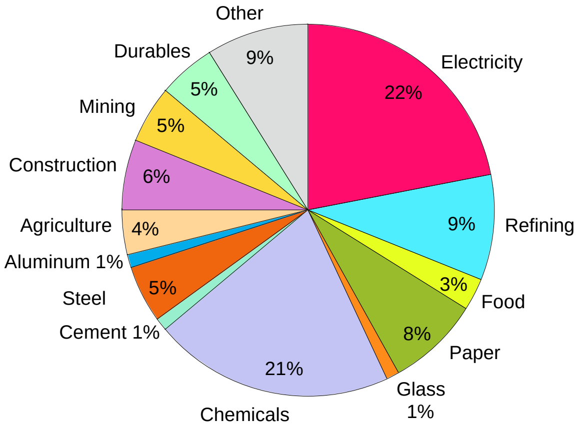

Figure 8-3. Primary energy use by industrial subsectors for the year 2000. Total primary energy use = 37.5 EJ (35.5 Quads). *Source: EIA 2001*

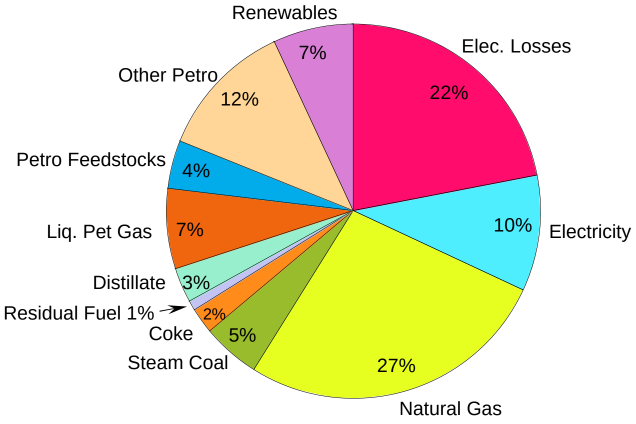

Figure 8-4. Industrial energy use by source for the year 2000 = 37.5 EJ (35.5 Quads). *Source: EIA 2001*

Classification of Research Directions: Overarching Themes

Industrial equipment offers significant opportunities for improving energy efficiency. In the longer term, however, the most substantial gains in energy efficiency will come from changes in systems rather than changes in individual devices. Four major technological pathways for improving industrial energy efficiency have been identified (Figure 8-6). Following a brief discussion of these pathways, opportunities for basic science research in specific industrial subsectors are identified.

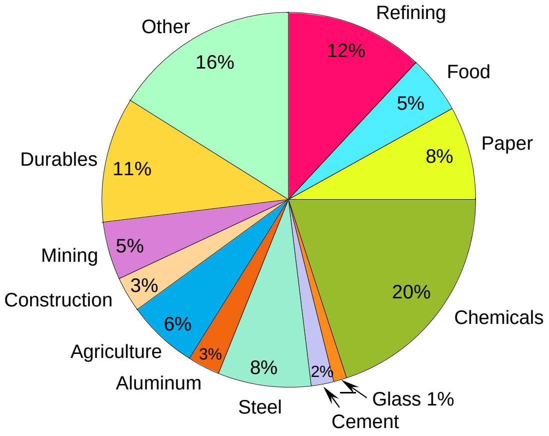

Figure 8-5. Carbon emissions by industrial subsector for the year 2000 (478 MtC). *Source: EIA 2001*

Energy Conversion and Utilization. Industrial energy efficiency could be improved by incorporating the best technologies in a systems approach (e.g., advanced turbine systems, improved combustion technologies, and optimal use of thermal energy in a systems approach to plant design). In the longer term, further gains may come from the use of fuel cells and gasification of biomass and in-plant residues.

Industrial Process Efficiency. Revolutionary new processes could greatly reduce the energy intensity of producing primary metals, chemicals, and other products. Numerous technical hurdles involving fundamental science must be overcome for the successful development of such processes. Incremental improvements to existing technology (both industry-specific and crosscutting) yield substantial cumulative energy savings.

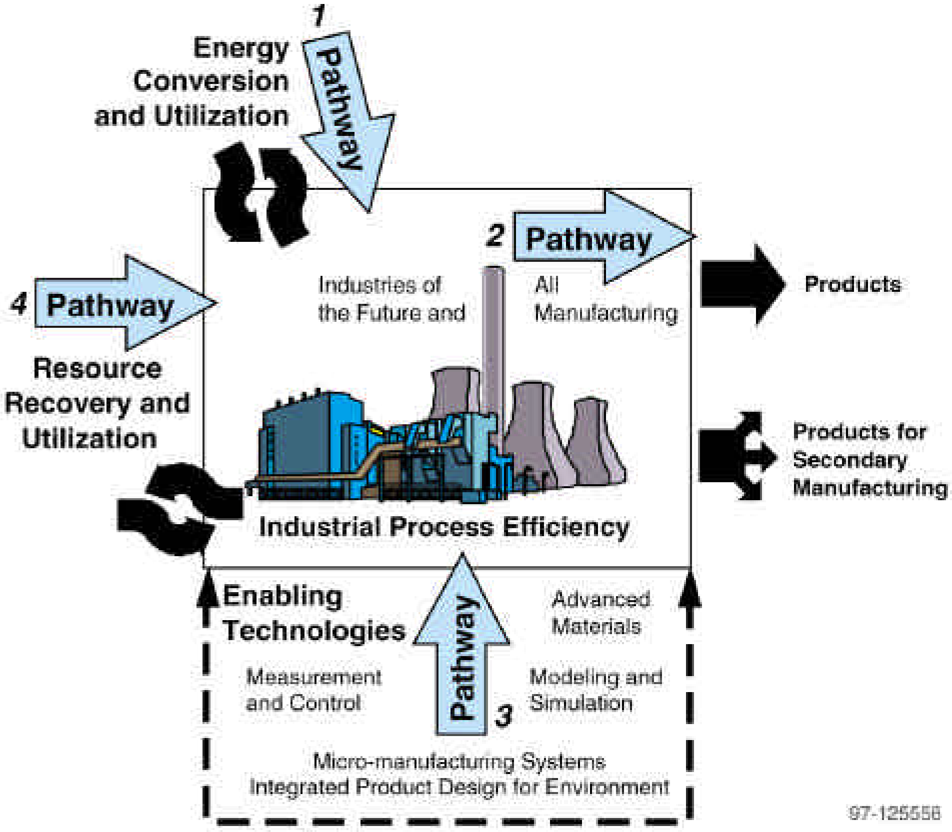

Figure 8-6. Technology Pathways for Industrial Energy Efficiency

Enabling Technologies. Advances in information processing and control, materials science, and combustion technologies could significantly improve existing processes *and* could lead to fundamental breakthroughs in the development of revolutionary processes. The greatest opportunities for energy savings include novel information processing techniques, intelligent control systems, and advanced modeling and simulation. The development of better fundamental physical and chemical data on combustion phenomena and other industrial reactions and processes will be required for advanced models and control schemes. In addition, industry needs more efficient combustion technologies and long-life industrial materials capable of withstanding high-temperature and corrosive environments.

Resource Recovery and Utilization. Through technological advances, manufacturers could select raw materials that will eliminate waste discharge or undesirable by-products. Substantial energy savings and greenhouse gas reductions are possible through fundamental changes in the way raw materials are obtained, the properties they exhibit, and the way they are used in the design process.

Classification of Research Directions: Industry-Specific

Significant reductions in industrial energy intensity (and greenhouse gas emissions) could be achieved through R&D in the underlying basic science of major industrial processes and crosscutting areas. The importance of each industrial subsector to the total energy consumption is presented in Figure 8-3.

Aluminum. The production of primary aluminum using conventional electrolytic cell technology is energy intensive, with an average electricity requirement of 15 kWh per kilogram of output. Although scrap-based aluminum production uses only 5% of the energy used in primary production, there is a continuing need for primary aluminum production. The development of advanced cell concepts such as nonconsumable anodes and wettable cathodes, as well as novel alternatives to electrolysis (e.g., carbothermic reduction), is underway and could result in large energy savings (>25%) and dramatic greenhouse gas reductions. The basic science needed to further these developments include fundamental knowledge on high- and low-temperature salt chemistry, solubilities and conductivities in salt melts, and high-temperature vapor kinetics and gas diffusion characteristics. Downstream processes (including casting, forming, finishing) could be improved through research on alloy development, improved measurement and prediction of physical and mechanical properties, and the development of thermal-physical data for solidification modeling.

Chemicals and Petroleum Refining. The overall U.S. chemical industry consumed about 7.6 EJ of primary energy in year 2000; the most energy-intensive segment is organic chemicals, followed by plastics. Nearly 50% of the energy used within the industry is transformed into chemical products. Petroleum refining, the most energy-intensive manufacturing industry in the U.S., accounted for another 3.2 EJ of primary energy consumption in 2000.

The development of new, energy-efficient processes for performing the separations and reactions in these industries depend on developments in basic science, including:

- *Separations.* High-priority research applications include separations from dilute solutions, bioprocesses, and gaseous mixtures. Distillation R&D needs include predictive methods of mass transfer under various conditions and understanding basic physical kinetics of mass transfer between phases and hydrodynamics of fluids within the column. The greatest improvements in separation technologies are expected to come from new materials (such as resins, membranes, and selective adsorbents) and in the design of new hybrid systems (such as complexation filtration, magnetic filtration, field-enhanced filtration and distillation, reactive extraction and distillation, and membrane reactors).

- *Reaction Engineering.* New process chemistries based on new feedstocks and reaction media will require new equipment and reactor designs (e.g., sonic, micro, photochemical, short-contact). Other needs include experimental methods to observe heterogeneous catalytic transformations and new cells and chemistries for chlor-alkali.

- *Alternative Feedstocks.* New chemistries are required to efficiently convert biomass, unused by-products, and abundant materials such as one-carbon compounds into useful raw materials for chemical processes.

- *New Reaction Media.* Fundamental studies are needed to advance the development of chemistry in alternative reaction media.

- *Catalysis.* New catalysts are needed for reaction pathways focused on ultrahigh selectivity, higher molecularity, longer life, self-reparability, and higher regio- and stereospecificity. Oxidation catalysts for carbon/carbon and carbon/hydrogen bond activation are also needed.

- *Interfacial Science.* A fundamental understanding of the chemistry at interfaces of multiphase systems is needed to develop new chemistries, reactions, and separations processes.

Forest Products. In the year 1998, the U.S. pulp and paper industry consumed 3.0 EJ of primary energy. Most of the opportunities for basic science research are in the area of sustainable forestry. The goal of work in this area is to develop trees with reduced lignin and increased cellulose content, which would save energy and chemicals by reducing pulping and bleaching requirements. Specific needs include better characterization of cellulose to improve recovery of cellulose and polysaccharides, sequencing of active genome of model plant species (Arabidopsis), identification of genes controlling quantitative and qualitative traits in tree species, and understanding of critical limitations to accelerating plant growth. In addition, better understanding of the corrosion mechanics in heat recovery environments could lead to significant energy savings through improved heat recovery in pulp mills.

Glass. Glass production in the U.S. consumed nearly 0.2 EJ in year 2000. The majority of energy is used in relatively inefficient, fuel-fired furnaces to melt glass. Basic R&D needs include the development of high-temperature, corrosion-resistant, long-lasting materials for processing equipment; new methods of heat recovery; and chemistry and tools for identifying gases and properties in order to improve environmental control of the furnace.

Metal Casting. Domestic foundries consumed about 0.4 quad of energy in 2000. Advancements in materials technologies could help the industry optimize its processes while producing superior castings with highly controlled properties. R&D needs include the development of better chemical and physical data on the properties of metals in the liquid and semisolid states, knowledge of alloy-microstructure-chemistry-property relationships, and clean metals technologies. Techniques are also needed to more accurately predict product properties as a function of the casting process used.

Mining. Opportunities for energy savings exist in the areas of exploration and resource characterization, as well as in mining processes themselves. R&D needs include resource characterization technologies, better understanding of the time resolution barrier in geophysics (to improve the accuracy of deep sensing of rocks, minerals, elements, and structures more than 1,000 feet beneath the surface), and better understanding of hydrodynamics of mineral/water suspension and mineral and solution properties and behavior of fine particles in solution.

Steel. The U.S. steel industry consumed 1.7 EJ of primary energy in 2000. Integrated (ore-based) steelmaking is more than twice as energy-intensive as secondary (electric arc furnace) steelmaking. As with aluminum, the limited availability of suitable supplies of scrap dictate a continuing need for ore-based steelmaking. The average energy intensity for the industry overall is currently about 17.5 million Btu/ton. The industry is seeking revolutionary iron and steelmaking processes that will reduce energy intensity by eliminating cokemaking and blast furnace ironmaking. Such processes will require advances in fundamental knowledge and control of the physical and chemical phenomena. In concert with many other industries, the steel industry also needs better data on the thermophysical and thermochemical properties of materials, enabling the development of predictive models and simulations. Similarly, process models for improved control systems could lead to higher energy efficiency in all industrial processes.

Crosscutting. Technologies used throughout industry, such as combustion, materials, and sensors/controls/automation, require enabling technological advances that can improve existing processes and can also spur development of totally new industrial processes and technologies. The high temperatures and corrosive environments of many industrial processes (e.g., ironmaking) have limited the extension of many recent technological advances into these industries, and advanced materials with superior properties are needed. Wireless sensor systems and novel information processing techniques could have widespread benefits, as could improved burner designs and heat recovery techniques.

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APPENDIX C

CHARGE AND ORGANIZATIONAL DETAILS

Introduction

The Basic Energy Sciences Advisory Committee appointed this subpanel to help identify the basic research needed to resolve key issues in the development of a secure energy future for the United States. The charge letter to the subpanel is included in this appendix. The focus of the discussions of the subpanel was "the future." Generally, for the solution of critical issues that require first-class basic research and the transition of the identified solutions to practice, experience has shown that an extended time scale is required, of the order of several years. The issue of a "Secure Energy Future" is even more demanding, and the time scale considered in the discussions was several decades.

Early in the discussions about the subpanel's activities, it was determined that it was important that the discussions to identify the research directions should involve as large a group of stakeholders as possible, whose members were knowledgeable in the appropriate areas of DOE's research. At the same time, it was recognized that meaningful discussions could not be accomplished in extremely large groups.

To focus the discussions, eight major energy areas, or topical areas, were identified:

- Fossil Energy;
- Nuclear Fission Energy;
- Renewable and Solar Energy;
- Fusion Energy;
- Distributed Energy, Fuel Cells, and Hydrogen;
- Transportation Energy Consumption;
- Residential, Commercial and Industrial Energy Consumption;
- Cross-Cutting Research and Education; and
- Energy Biosciences Research.

For each of these topical areas (with the exception of Energy Biosciences), chairpersons were selected. Their initial task was to identify a small group (4-6) to help them identify some needed basic research directions. The chairs were:

- Marvin Singer (DOE Office of Fossil Energy), Fossil Energy;
- John Ahearne (Sigma Xi), Nuclear Fission Energy;
- George Crabtree (Argonne National Laboratory), Renewable and Solar Energy;
- Charles Baker (University of California San Diego), Fusion Energy;
- Lutgard C. DeJonghe (University of California Berkeley), Distributed Energy, Fuel Cells, and Hydrogen;
- Jan Herbst (General Motors R&D Center), Transportation Energy Consumption;
- Mildred Dresselhaus (Massachusetts Institute of Technology), Residential, Commercial, and Industrial Energy Consumption; and
- Rick Smalley (Rice University), Cross-Cutting Research and Education.

The Workshop

The second phase of the subpanel's work was the workshop held in Gaithersburg October 21–25, 2002. Prior to the workshop, additional members were identified to expand the small groups into Topical Teams of 10 to 12 members. The Teams were selected to be representative of the stakeholders: they included members from academia, the National Laboratories, industry, and the applied mission Offices of DOE. In addition, members of the Office of Basic Energy Sciences were present, primarily to act as a resource for the Teams.

The Team members are listed at the end of this appendix. From this, it can be seen that over 100 people were involved as active members of the Teams at the workshop. Of these, 27% were from academia, 39% from the National Laboratories, 16% from industry, and 18% from DOE and other government agencies. Staff members from the Office of Basic Energy Sciences were also involved; these were evenly divided between the Materials Science and Engineering (MS) Division and the Chemical Sciences, Geosciences, and Biosciences (CS) Division.

After introductory presentations(found in Appendix D), the major focus of the 4-day workshop was interactive discussions among the members of the Teams. The details of the workshop program are included in this appendix. On Thursday morning, the Topical Team Chairs presented the conclusions of their deliberations. The slides from these presentations are included as Appendix E. On Thursday afternoon, Professor Smalley presented the results of his Team, who had been reviewing the progress of the other Teams; and also introduced three new topics.

On Friday morning, a discussion involving the subpanel and Team chairs identified a limited number of Research Directions on the basis of the proposals made by the Teams. There were approximately 34 proposed research directions (PRDs) from the week's deliberations (The full text of all of these are included in Appendix A). Rather than identify a shorter list of research directions, the group elected to identify the common threads from the full list. The next section of this report describes these.

In addition, during the Friday discussions, the group suggested that an additional workshop be held to provide additional insights on possible research directions related to energy biosciences. This area was incorporated in several of the PRDs, but the experts needed to support these topics were not at the October workshop. The second workshop was accomplished on January 13-14, 2003; the equivalent membership and attendance data and the PRDs for that workshop are included in the Appendices.

Products of the Workshop

The products of the workshop were the PRDs and the summary recommendations. The Teams prepared the support documents for the PRDs in a roughly consistent format. The format consists of two parts: an Executive Summary, readable by a lay audience, of about one page and a more extended technical description of the PRD of approximately three pages. In general, no references were used in these documents; appropriate references were included in the Factual Documents (Appendix B). The Teams were asked to identify the DOE applied mission to which each proposed research best related, and an estimate of the time required to achieve the stated goals. However, no discussion of the funding requirements was included in the text.

June 18, 2001

Professor Geraldine L. Richmond
Department of Chemistry
210 Willamette Hall
University of Oregon
Eugene, OR 97403-1253

Dear Professor Richmond:

I very much appreciate your willingness to serve an additional term as Chair of the Basic Energy Sciences Advisory Committee (BESAC). I believe that the continuity in leadership you provide is critical as BES hosts its first Committee of Visitors and as BESAC embarks on new challenges, which are detailed below. Under your leadership during the past few years, BESAC activities have produced extraordinary results that already have – and will continue to have – broad impacts in the Basic Energy Sciences program. I want to thank you for your leadership of BESAC, and I also want to express my sincere appreciation for the superb job that you did during your testimony on May 17th at the Hearing on *Department of Energy Office of Science – Issues and Opportunities* before the U.S. House of Representatives Committee on Science. I have heard from many that your testimony was articulate, focused, and had an enormous impact.

During the coming year, I would like BESAC to take on two new challenges relating to the research programs of the BES program. I expect that each will require one or more workshops. I have provided an overview of each activity below. The first activity is an extension of work that was done in the areas of nanoscale science and complex systems. I know that BESAC has been engaged in activities relating to nanoscale science, including the formation of Nanoscale Science Research Centers, and has clearly articulated that scientific understanding at the nanoscale is required for the development of larger functional systems that use nanoscale building blocks. *The report of the workshop on Complex Systems outlined an exciting science agenda that integrates the disciplines of physics, chemistry, materials science, and biology to build on the foundations that now have been put in place by the National Nanotechnology Initiative. I would like you to help refine that research agenda.* In the world "beyond nano," it will be necessary to use atoms, molecules, and nanoscale materials as the building blocks for larger supramolecules and hierarchical assemblies. As was described in *Complex Systems – Science for the 21st Century*, the promise is nanometer-scale (and larger) chemical factories, molecular pumps, and sensors. This has the potential to provide new routes to high-performance materials such as adhesives and composites, highly specific membrane and filtration systems, low-friction bearings, wear-resistant materials, high-strength lightweight materials, photosynthetic materials with built-in energy storage devices, and much more. The magnitude of the challenge is perhaps more daunting than any faced before by these disciplines. I would greatly appreciate BESAC's help in defining these challenges.

The second activity might build on some of the ideas discussed above to answer the question: *What are the 21st century fundamental scientific challenges that BES must consider in addressing the DOE missions in energy efficiency, renewable energy resources, improved use of fossil fuels, safe and publicly acceptable nuclear energy, future energy sources, science-based stockpile stewardship, and reduced environmental impacts of energy production and use?* Over the years, the BES research portfolio has evolved to address these issues and more. There have been many successes.

The *National Energy Policy* noted that the U.S. economy grew by 126 percent since 1973, but energy use increased by only 30 percent. Approximately one-half to two-thirds of the savings resulted from technological improvements in products and services that allow consumers to enjoy more energy services without commensurate increases in energy demand. At the heart of these improvements is fundamental research. During this 30-year period, the basic research supported by the BES program has touched virtually every aspect of energy resources, production, conversion, efficiency, and waste mitigation. The basic knowledge derived from fundamental research has resulted in a vast array of advances, including • high-energy and high-power lithium and lithium ion batteries and thin-film rechargeable microbatteries; • thermoacoustic refrigeration devices that cool without moving parts and without the use of freons; • compound semiconductors, leading to the world's highest efficiency photovoltaic solar cells; • strong, ductile alloys for use in high-temperature applications; • new steels, improved aluminum alloys, and high-performance magnet materials; • polymer materials for rechargeable batteries, car bumpers, food wrappings, flat-panel displays, wear-resistant plastic parts, and polymer-coated particles in lubricating oils; • new commercial processes for ethanol production, pulp and paper manufacturing, and *in planta* production of oils; and • new catalysts for the production of polymers and for a host of other products and energy-efficient processes; and • a host of new instruments, such as superconducting quantum interference devices (SQUIDs) that can sense minute magnetic fields for use in applications ranging from resource exploration to monitoring the human brain and heart. *These advances came by exploiting the results of basic research that sought answers to fundamental questions. The challenge is to continue the tradition of discovery. To that end, I would like BESAC to oversee a small number of workshops (perhaps 2 or 3) that articulate 21st century discovery potential in DOE mission areas. Defining the role and challenges of basic research is particularly timely given the recent release of the President's National Energy Policy.*

I would hope that by the time of the February 2002 BESAC meeting, the "Beyond Nano" workshop will have taken place and at least one workshop in the second category is scheduled. Again, thank you for your continued expert leadership of our largest Office of Science program.

With best regards,

signed June 18, 2001

James F. Decker
Acting Director
Office of Science

cc:
P. Dehmer, SC-10
I. Thomas, SC-13
S. Long, SC-10

Basic Research Needs to Assure a Secure Energy Future: Organization, Workshop, and Follow-up Activities

Dr. John Stringer, EPRI, Workshop Chair

Dr. Linda Horton, ORNL, Co-Chair

Fossil Energy

Marvin Singer, Chair
Director, Advanced Research
Office of Fossil Energy, DOE

Tim Armstrong, ORNL
Tof Carim, DOE-BES
Cindy Dogan, Albany Res Lab
David Keith, CMU
Tina Nenoff, SNL
Eric Suuberg, Brown U
Anbo Wang, VPI
John Wimer, NETL

Mike Bockelie, Reaction Eng.
Bob Carling, SNL
Brian Gleeson, Ames/U of Iowa
Larry Myer, LBNL
Doug Ray, PNNL
Roger Turpening, DOE- BES
Nick Woodward, DOE-BES

Distributed Energy, Fuel Cells, and Hydrogen

Lutgard DeJonghe, Chair
Professor of Ceramics
Materials Science and Engineering
University of California, Berkeley

Meilin Liu, Georgia Institute of Technology
Joan Ogden, Princeton University
Vitalij Pecharsky, Iowa State University
Philip N. Ross, LBNL
Subhash Singhal, PNNL
John Turner, NREL
Douglas Wheeler, UTC Fuel Cells
Mark Williams, NETL
Dick Kelley and Frank Tully, DOE-BES

Nuclear Fission Energy

John Ahearne, Chair
Executive Director
Sigma Xi
Scientific Research Society

Allen Croff, ORNL
(acting chair for workshop)
Ralph Bennett, INEEL*
Bob Gottschall, DOE-BES
Andy Klein, Oregon State
Frank Goldner, DOE-NE
John Taylor, EPRI*
Neil Todreas, MIT*
Todd Allen, ANL-W

Jim Beitz, ANL
Bill Millman, DOE-BES
Jack Richards, Cal Tech
Rob Versluis, DOE/NE
Brian Wirth, LLNL
Bill Weber, PNNL
Mike Kassner, Oregon State

*Did not attend workshop

Residential, Commercial, and Industrial Energy Consumption

Millie Dresselhaus, Chair
Institute Professor,MIT
Physics and Electrical Engineering

Sam Baldwin , DOE-EE
Hylan Lyon, Marlow Industries
Gerald Mahan, Penn State U.
Anne Mayes, MIT
Steve Selkowitz, LBNL
Jerry Simmons, SNL
Harriet Kung, DOE-BES
Aravinda Kini, DOE-BES

Speakers:
Anil Duggal, GE
Jerry Simmons, SNL
Woods Haley, UMN
Ron Judkoff, NREL
Ertugrul Berkcan, GE
Dickson Ozokwelu, DOE-EE
Vitalij Pecharsky, Ames/Iowa State

Panel Members with Phase I Task:
Paul Alivisatos, LBNL
Sam Bader, ANL
Terry Michalske, SNL

Transportation Energy Consumption

Jan Herbst, Chair
Materials and Processes Laboratory
GM R&D Center

Channing Ahn, Cal Tech.
Tarasankar DebRoy, Penn. State U.
Jim Eberhardt, DOE-EE
Ed Grostic, ORNL
Oren Hadaller, The Boeing Company
Kenneth Hass, Ford Motor Company
Joseph Heremans, Delphi Res. Labs
Chris Sloane, General Motors

Iver Anderson, AMES
Suresh Baskaran, PNNL
Bill Kirchhoff, DOE-BES
Paul Lessing, INEEL
Paul Miles, SNL
Kevin Ott, LANL
Matesh Varma, DOE- BES

Renewable and Solar Energy

George Crabtree, Chair
Senior Scientist and Director
Materials Science Division
Argonne National Laboratory

Sam Baldwin, DOE-EE	Tom Baker, LANL
John Cooke, ORNL	Dan Ginosar, INEEL
Jerry Hunt, ANL	Mack Kennedy, LBNL
Lonnie Ingram, U. of Florida	Nate Lewis, Cal. Tech.
Larry Kazmerski, NREL	Joe Paladino, NETL
Jeff Mazer, DOE-EE	Sharlene Weatherwax, DOE-BES
Arthur Nozik, NREL	Jane Zhu, DOE-BES
Jay Spivack, GE	

Fusion Energy

Charles Baker, Chair
Virtual Laboratory for Technology
University of California, San Diego

Mohamed Abdou, UCLA	Sam Berk, DOE-Fusion
Roger Bangerter, LBNL	Russ Jones, PNNL
Jill Dahlburg, General Atomics	John Lindl, LLNL
Phil Efthimion, Princeton	Eric Rohlfing, DOE-BES
Neil Morley, UCLA	Kurt Schoenberg, LANL
Steve Zinkle, ORNL	Scott Willms, LANL

Cross-Cutting Research

Rick Smalley, Chair
Professor of Chemistry
Rice University

Ivan Bekey, Bekey Designs
Kwan Kwok, DARPA
Gerry Lavin, DuPont
John Mankins, NASA
Yoram Shoham, Shell
Jeff Tester, MIT
Nate Lewis, CalTech
Art Green, ExxonMobil

All Topical Team Chairs
John Stringer, EPRI
Linda Horton, ORNL

Schedule

Monday, October 21st
Presentations from
DOE's SC, EE, FE, and NE

Overview of the Office of Science, James Decker, Deputy Director

Overview of the Office of Basic Energy Sciences, Patricia Dehmer, Director

Overview DOE's Office of Fossil Energy Programs, Rita A. Bajura, Director, NETL

Basic Research Needs in Support of Advanced Nuclear Reactor and Fuel Cycle Technologies, R. Shane Johnson, Associate Director for Advanced Nuclear Research, Office of Nuclear Energy, Science and Technology

Science Issues in the Office of Energy Efficiency and Renewable Energy, Sam Baldwin Chief Technology Officer and Member, Board of Directors Office of Energy Efficiency and Renewable Energy

Schedule

Tuesday and Wednesday
October 22nd and 23rd
Breakout Sessions

1. Fossil Energy
2. Distributed Generation
3. Nuclear Energy
4. Industrial, Residential, Commercial
5. Transportation
6. Renewable Energy
7. Fusion Energy

Schedule

Thursday, October 24th
Morning
Closing Topical Area Summaries

	Thursday, October 24, 2002		
8:30am - 11:30am	Closing Plenary Session -- Team Reports (15 minutes)	All Invited	Salons E, F&G
	1. Fossil Energy	1. Marvin Singer	
	2. Distributed Generation	2. Lutgard DeJonghe	
	3. Nuclear Energy	3. TBD	
	4. Industrial, Residential, Commercial	4. Millie Dresselhaus	
	5. Transportation	5. Jan Herbst	
	6. Renewable Energy	6. George Crabtree	
	7. Fusion Energy	7. Charles Baker	
11:30am - 12:00pm	Open Discussion	John Stringer	

Thursday morning concluded the workshop for most attendees.

Schedule

Thursday, October 24th
Afternoon

Topical Chairs and Crosscutting Team assembled for Crosscutting Research Topical Area

Thursday, October 24, 2002			
1:00pm - 4:00pm	Meeting of the Cross-Cutting Research Team	Rick Smalley, Rice University Representatives from Topical Groups Cross-Cutting Research Group Members	Salon D
4:00pm - 4:30pm	Close of Cross-Cutting Research Team	All Invited	Salons E, F&G
4:30pm - 5:00pm	Closing Remarks and Expectations for Friday	John Stringer	Salons E, F&G
7:00pm	Dinner		TBD

Schedule

Friday, October 25th
The beginning of Phase III

Stringer, Horton, Topical Team Chairs, BES Planning Staff

- Summarize proposed research directions and identify overlapping topics
- Discuss logistics for coordination/assembly of results
- Identify needs for expansion of information
- Define schedule and template for documentation

Follow up Workshop: Energy Biosciences

- Held January 12-14, 2003 in Palo Alto, CA
- Introductory Presentations on:

The Need for a Research Plan for a Secure Energy Future
John Stringer
Summary of the October 21st – 25th Workshop Results
Linda Horton
Current Status of Biochemical and Biotechnology Research in the Office of Basic Energy Science
Walter Stevens

- Balance of time spent on discussions of research directions related to Energy Biosciences

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Energy Biosciences Research

Mark Alper, LBNL
Heinz Frei, LBNL
Evan Hughes, EPRI
Laurie Mets, Univ. Chicago
John Shanklin, BNL
Chris Somerville, Stanford Univ.
Walt Stevens, BES
Lut De Jonghe, UCB

Other Attendees:
John Stringer, EPRI
Linda Horton, ORNL

APPENDIX D

INTRODUCTORY PRESENTATIONS -- OCTOBER WORKSHOP

U.S. Department of Energy's

Office of Science

Overview of the Office of Science

for the BESAC Workshop on
Basic Research Needs
to Assure a Secure Energy Future

Dr. James F. Decker, Deputy Director
October 21, 2002

DOE's Office of Science (SC)

- Supports basic research that underpins DOE missions.
  - Provides over 40% of federal support to the physical sciences (including more than 90% of high energy and nuclear physics)
  - Provides sole support to select sub-fields (e.g. nuclear medicine, heavy element chemistry, magnetic fusion, etc.)
  - Supports the research of 15,000 PhDs and graduate students
- Constructs and operates large scientific facilities for the U.S. scientific community.
  - Accelerators, synchrotron light sources, neutron sources, etc.
  - Used by about 18,000 researchers every year
- Provides infrastructure support for the ten SC laboratories.

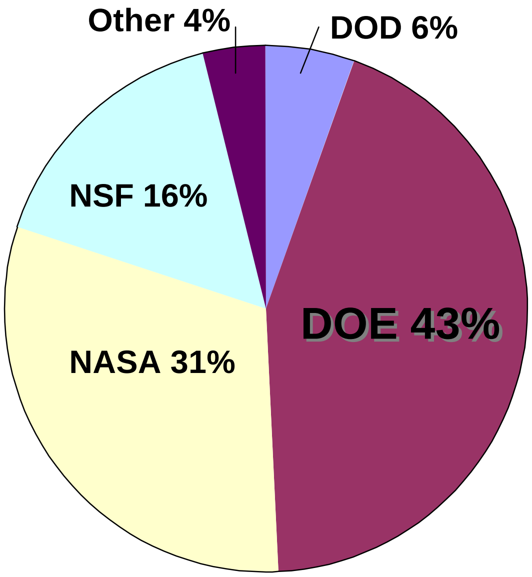
The Department of Energy is a Science Agency

Top Five Government Research Organizations for*:

Physical Sciences	Mathematics & Computing	Life Sciences	Environmental Sciences
1. Energy (1,938)	**1. Energy (862)**	1. HHS (18,216)	1. NASA (1,113)
2. NASA (1,152)	2. DOD (861)	2. USDA (1,342)	2. NSF (515)
3. HHS (794)	3. NSF (515)	3. DOD (616)	3. Interior (353)
4. NSF (593)	4. HHS (181)	4. NSF (500)	4. DOD (301)
5. DOD (364)	5. Commerce (78)	**5. Energy (267)**	**5. Energy (298)**

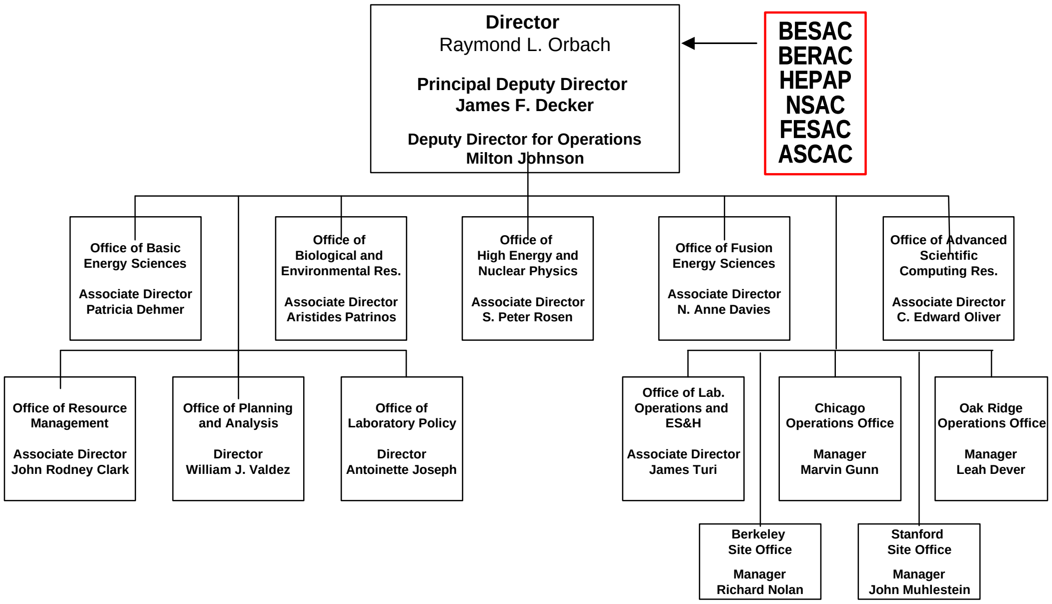
* *Numbers are FY 2002 dollars in millions - Source: NSF -- Preliminary Federal obligations for research, by agency and field of science and engineering: fiscal year 2002*

DOE Provides 43% of Federal Support to the Physical Sciences



Source: NSF - Division of Statistical Research Services

Office of Science Organization



Director
Raymond L. Orbach

Principal Deputy Director
James F. Decker

Deputy Director for Operations
Milton Johnson

BESAC
BERAC
HEPAP
NSAC
FESAC
ASCAC

Office of Basic Energy Sciences
Associate Director
Patricia Dehmer

Office of Biological and Environmental Res.
Associate Director
Aristides Patrinos

Office of High Energy and Nuclear Physics
Associate Director
S. Peter Rosen

Office of Fusion Energy Sciences
Associate Director
N. Anne Davies

Office of Advanced Scientific Computing Res.
Associate Director
C. Edward Oliver

Office of Resource Management
Associate Director
John Rodney Clark

Office of Planning and Analysis
Director
William J. Valdez

Office of Laboratory Policy
Director
Antoinette Joseph

Office of Lab. Operations and ES&H
Associate Director
James Turi

Chicago Operations Office
Manager
Marvin Gunn

Oak Ridge Operations Office
Manager
Leah Dever

Berkeley Site Office
Manager
Richard Nolan

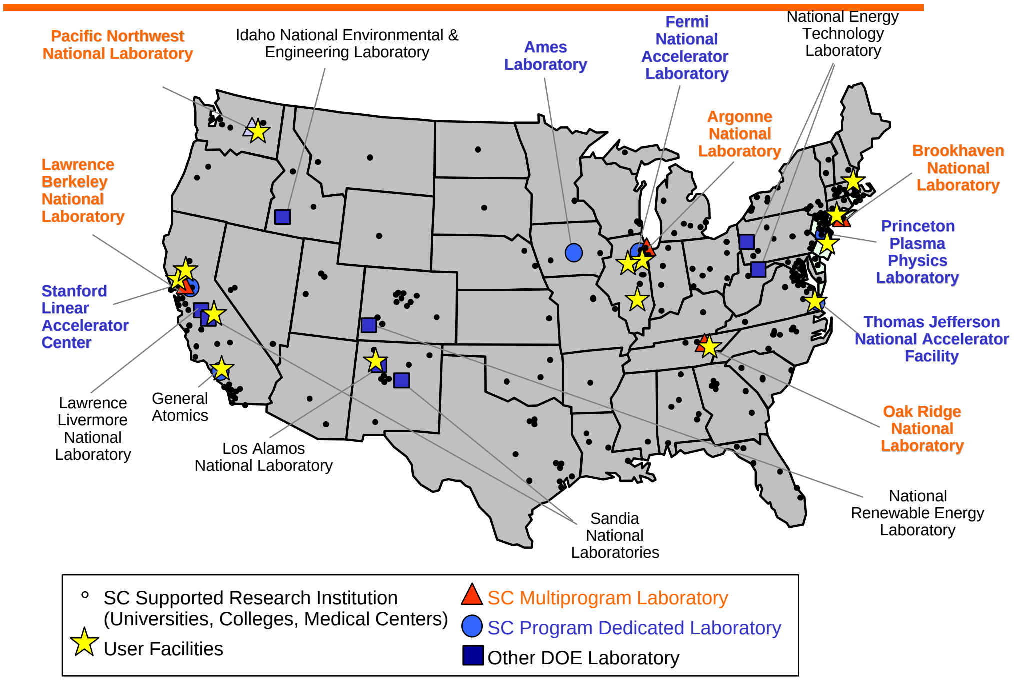
Stanford Site Office
Manager
John Muhlestein

FY2003 Budget Request

OFFICE OF SCIENCE
FY 2003 PRESIDENT'S BUDGET REQUEST
(B/A in thousands)

	FY 2001 Comparable Approp.	FY 2002 Comparable Approp.	FY 2003 President's Request
SCIENCE			
Basic Energy Sciences	973,768	999,605	1,019,600
Advanced Scientific Computing Research	161,296	157,400	169,625
Biological and Environmental Research	514,064	570,300	504,215
High Energy Physics	695,927	713,170	724,990
Nuclear Physics	351,794	359,035	382,370
Fusion Energy Sciences	241,957	247,480	257,310
Energy Research Analyses	950	995	1,020
Science Laboratories Infrastructure	26,887	37,130	42,735
Science Program Direction	139,861	152,475	139,479
Small Business Inn. Research and Technology Transfer	93,069	-	-
Subtotal	3,199,573	3,237,590	3,241,344
Safeguards and Security	39,081	47,609	48,127
Reimbursable Work	(4,648)	(4,460)	(4,383)
Total Safeguards and Security	34,433	43,149	43,744
Total Science	3,234,006	3,280,739	3,285,088

SC Laboratories, User Facilities, and the Institutions that Use Them



Basic Energy Sciences

Research

Science at the nanoscale: increased research in condensed matter physics and materials synthesis and processing.

- X-ray and neutron scattering: research and new instrumentation at the major user facilities.
- Other core research programs: heavy-element chemistry, separations and analysis, materials chemistry, photochemistry, combustion, and catalysis.

- **Facilities**
  - New and upgraded instrumentation.
  - Continued high level of service at major user facilities.
- **Construction, Engineering & Design**
  - Construction of the Spallation Neutron Source is fully funded.
  - Nanoscale Science Research Centers (NSRC): continue engineering & design at ORNL, LBNL, SNL/LANL.
  - Begin construction of the NSRC at ORNL.
  - The Linac Coherent Light Source at SLAC begins project engineering and design.

Biological and Environmental Research

- Genomes to Life will enable revolutionary advances in energy supply, greenhouse gas mitigation, and environmental cleanup.
    - Bioterrorism detection/defeat.
- The Human Genome Program will provide high quality complete sequence of Chromosomes 5, 16, and 19.
- Climate Change Research underpins the President's initiative. Research and observations will improve climate models and understanding of the global carbon cycle.
- Climate Change Research Initiative.
- The Environmental Management Science Program is transferred from the Office of Environmental Management.
- Boron Neutron Capture Therapy.

Genomes to Life

Genomes to Life builds on advances in sequencing, molecular science and computing to understand and eventually harness microbes and microbial communities to address DOE's energy, environmental and national security missions. In FY 2003 we will:

- Continue joint research that combines capabilities of DOE's advanced biological and computational sciences programs.
- Support DNA sequencing of microbes closely related to potential bio-threat agents.
- Determine the composite DNA sequence and functional capability of microbes in a complex microbial community to address DOE energy, environmental, and national security needs.
- Begin the complex task of characterizing all of the multi-protein molecular machines and their associated regulatory networks in microbes of importance to DOE's energy, environmental, and national security missions.
- $15M increase enables full funding for up to 4 multidisciplinary, multi institutional research teams at universities and national labs needed to address the 4 goals of Genomes to Life.

Fusion Energy Sciences

- **Science and Enabling R&D**
  - Innovation in fusion energy, plasma science and related technologies are part of the Administration's National Energy Policy.
  - Explore innovative approaches to confining, heating, and fueling plasmas.
- **Facilities**
  - Significantly increase operating time on three national fusion facilities to resolve issues in energy transport and plasma stability, using a variety of heating techniques.
- **Fabrication, Engineering & Design**
  - Expand concept innovation with fabrication of a new stellarator, the National Compact Stellarator Experiment (NCSX), at the Princeton Plasma Physics Laboratory

High Energy & Nuclear Physics

Nuclear Physics

Increased facility operating time to:

- Create and study a quark-gluon plasma at the Relativistic Heavy Ion Collider
- Explore how quarks bind together to form protons and neutrons at the Continuous Electron Beam Accelerator Facility

High Energy Physics

Exploit the opportunity to answer two key questions about matter and energy:

- Explore the origin of mass in the search for the Higgs boson at the Tevatron
- Understand the absence of antimatter in the Universe by studying Charge-Parity Violation at the B-Factory

Advanced Scientific Computing Research

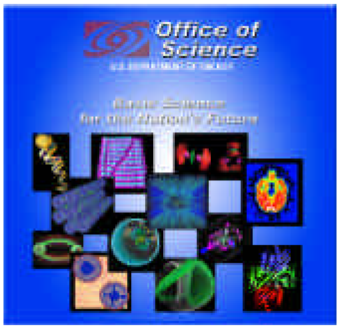
- **Mathematical, Information, & Computational Sciences**
  - **Supports operation of supercomputer and network facilities available to researchers 24-7-365:**
    - National Energy Research Scientific Computing Center (NERSC),
    - Advanced Computing Research Testbeds, and
    - Energy Sciences Network (ESNet).
  - **Scientific Computing Research Investments:**
    - Applied Mathematics,
    - Computer Science, and
    - Advanced Computing Software Tools.
  - **High Performance Networking, Middleware and Collaboratory Research Investments:**
    - Networking,
    - Collaboratory Tools, and
    - National Collaboratory Pilot Projects.
- **Laboratory Technology Research**

Scientific Discovery through Advanced Computation

- SciDAC brings the power of tera-scale computing and information technologies to several scientific areas -- breakthroughs through simulation.
- SciDAC is building community simulation models through collaborations among application scientists, mathematicians and computer scientists -- research tools for plasma physics, climate prediction, combustion, etc.
- State-of-the-art electronic collaboration tools will facilitate the access of these tools to the broader scientific community to bring simulation to a level of parity with theory & observation in the scientific enterprise.
- Topical Computing (TC)
  - FY03 increases will reconfigure some resources at existing facilities around TC concept.
  - These facilities will support applications communities to develop the operational model.
  - Full-scale TC facilities will be proposed in FY-04.

The Future

- Reasserting U.S. Leadership in Scientific Computation
- The Beauty of Nanoscale Science
- Building a 21st Century Workforce
- Dark Energy—the Mystery that Dominates the Universe
- Fusion: Bringing a Star to Earth
- Scientific Foundations for Countering Terrorism
- Using Nature’s Own Tool Kit to Clean Up the Environment
- Biotechnology for Energy Security



Occasional Papers
Spring 2002

BASIC ENERGY SCIENCES -- Serving the Present, Shaping the Future

Basic Research Needs to Assure a Secure Energy Future

A BESAC Workshop

Patricia M. Dehmer

Director, Office of Basic Energy Sciences
21 October 2002

http://www.sc.doe.gov/production/bes/bes.html

Remarks by Secretary Abraham

Brookhaven National Laboratory – June 14, 2002

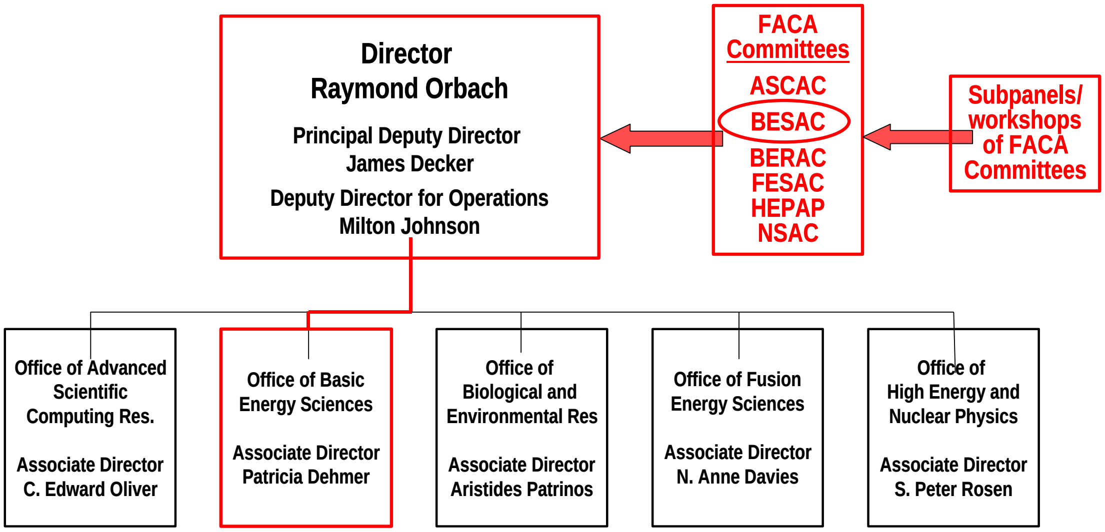
DOE and American Leadership in Science

The Department of Energy could well have been called the Department of Science and Energy given our contribution to American science. And the reason we are so deeply involved in science is simple. Our mission here at DOE ... as I have stressed since becoming Secretary ... is national security.

And in my view, a serious commitment to national security demands a serious commitment to science, including basic research. This commitment strengthens our energy security, international competitiveness, economic growth, and intellectual leadership. Moreover, if we ever hope to leapfrog today's energy challenges we must look to basic research.

I think it's clear. A nation that embraces basic research embraces a brighter future.

What Does “A BESAC Workshop” Mean?



Director
Raymond Orbach

Principal Deputy Director
James Decker

Deputy Director for Operations
Milton Johnson

FACA Committees
ASCAC
BESAC
BERAC
FESAC
HEPAP
NSAC

Subpanels/ workshops of FACA Committees

Office of Advanced Scientific Computing Res.
Associate Director
C. Edward Oliver

Office of Basic Energy Sciences
Associate Director
Patricia Dehmer

Office of Biological and Environmental Res
Associate Director
Aristides Patrinos

Office of Fusion Energy Sciences
Associate Director
N. Anne Davies

Office of High Energy and Nuclear Physics
Associate Director
S. Peter Rosen

Conversations with BESAC on the Workshop

“The basic research community has focused on many of the known problems in energy technologies for many years – the workshop should not rehash these areas.”

“Rather, the workshop should focus on new, revolutionary basic research opportunities.”

The Basic Energy Sciences Program Mission

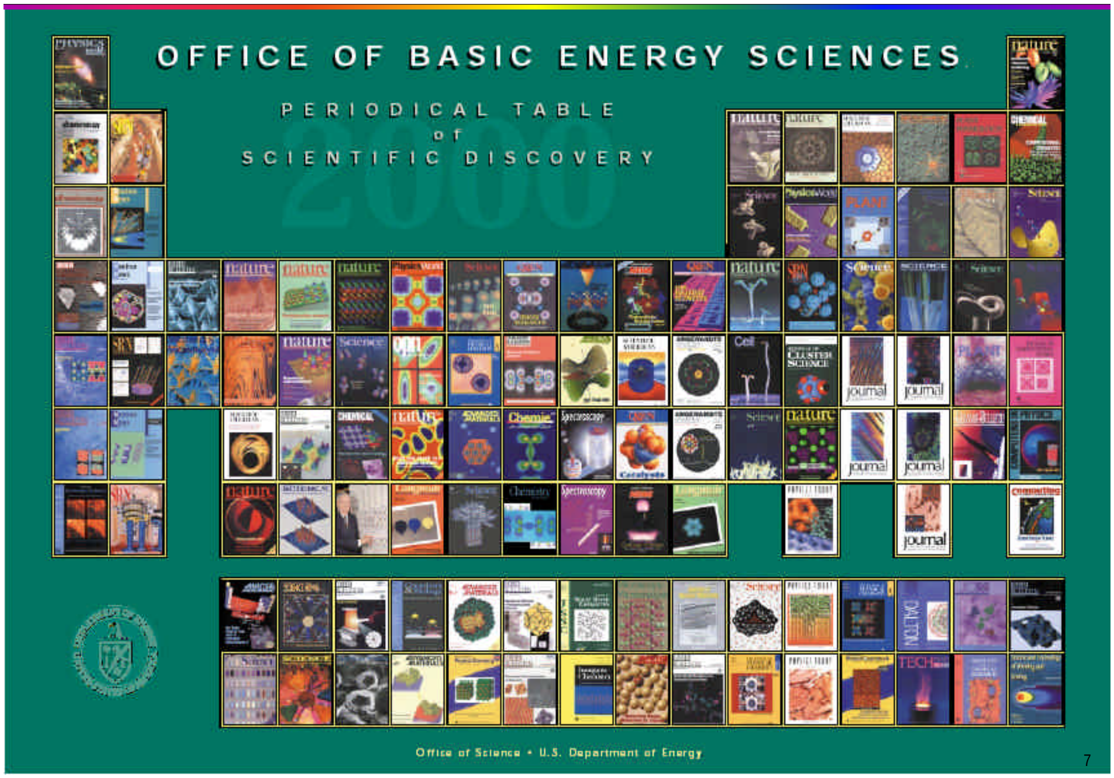
"... to foster and support fundamental research to expand the scientific foundations for new and improved, environmentally conscientious energy technologies"

"... to plan, construct, and operate major scientific user facilities for the Nation"

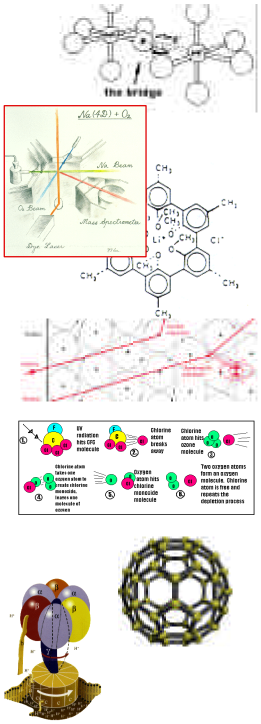
The Basic Energy Sciences Program ...

- ☑ ... is one of the Nation's largest sponsors of basic research.
- ☑ ... supports research in more than 150 academic institutions and 13 DOE laboratories.
- ☑ ... supports world-class scientific user facilities, providing outstanding capabilities for characterizing materials of all kinds.
- ☑ ... is uniquely responsible in the Federal government for supporting research in materials sciences, chemistry, geosciences, and aspects of biosciences related to energy resources, production, conversion, efficiency, and use – all in an environmentally conscientious manner.

Past Accomplishments

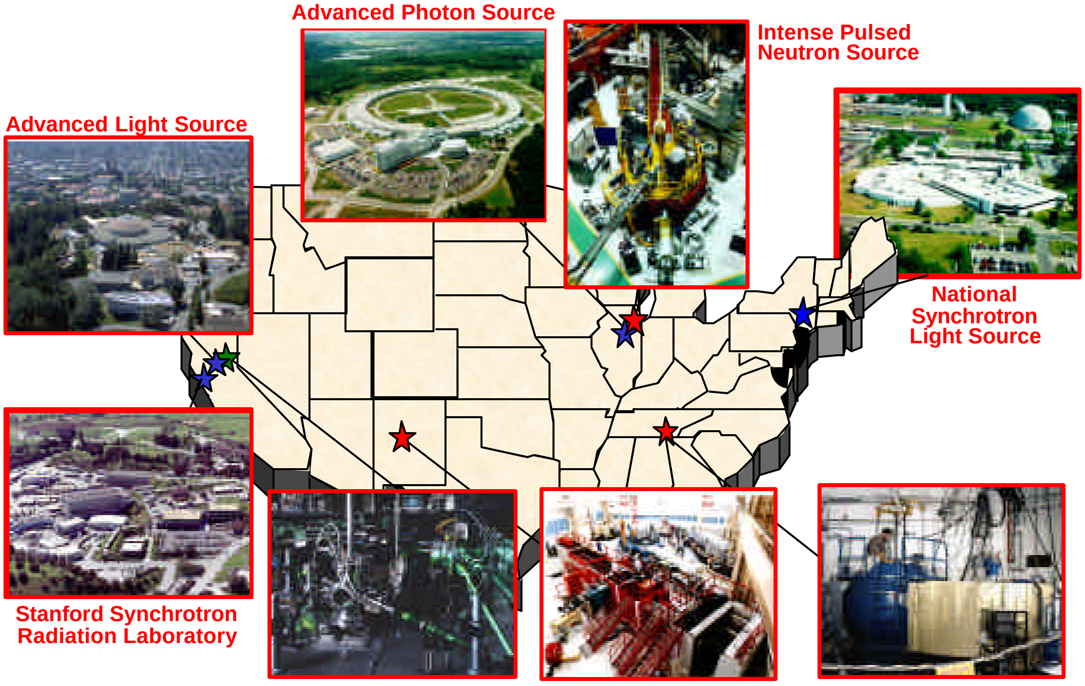


Nobel Prize Research Supported During the 1980s and 1990s



1983 Chemistry	**Henry Taube, Stanford University, for "his work on the mechanisms of electron transfer reactions, especially in metal complexes”**
1986 Chemistry	**Yuan Tseh Lee, UC Berkeley, for "dynamics of chemical elementary processes”**
1987 Chemistry	**Donald J. Cram, UC Los Angeles, for "development of molecules with structurally specific interaction of high specificity"**
1994 Physics	**Clifford G. Shull (MIT) for “pioneering contributions to the development of neutron scattering techniques for studies of condensed matter”**
1995 Chemistry	**Frank Sherwood Rowland (UC, Irvine) for “work in atmospheric chemistry, particularly concerning the formation and decomposition of ozone”**
1996 Chemistry	**Richard E. Smalley and Robert Curl (Rice U) for “collaborative discovery that carbon could occur in a uniquely beautiful and satisfying structure that engendered an entirely new branch of chemistry”**
1997 Chemistry	**Paul D. Boyer (UC, Los Angeles) for “elucidation of the enzymatic mechanism underlying the synthesis of adenosine triphosophate (ATP)”**

The BES Major Scientific User Facilities


Advanced Photon Source

Intense Pulsed Neutron Source

Advanced Light Source

National Synchrotron Light Source

Stanford Synchrotron Radiation Laboratory

Combustion Research Facility

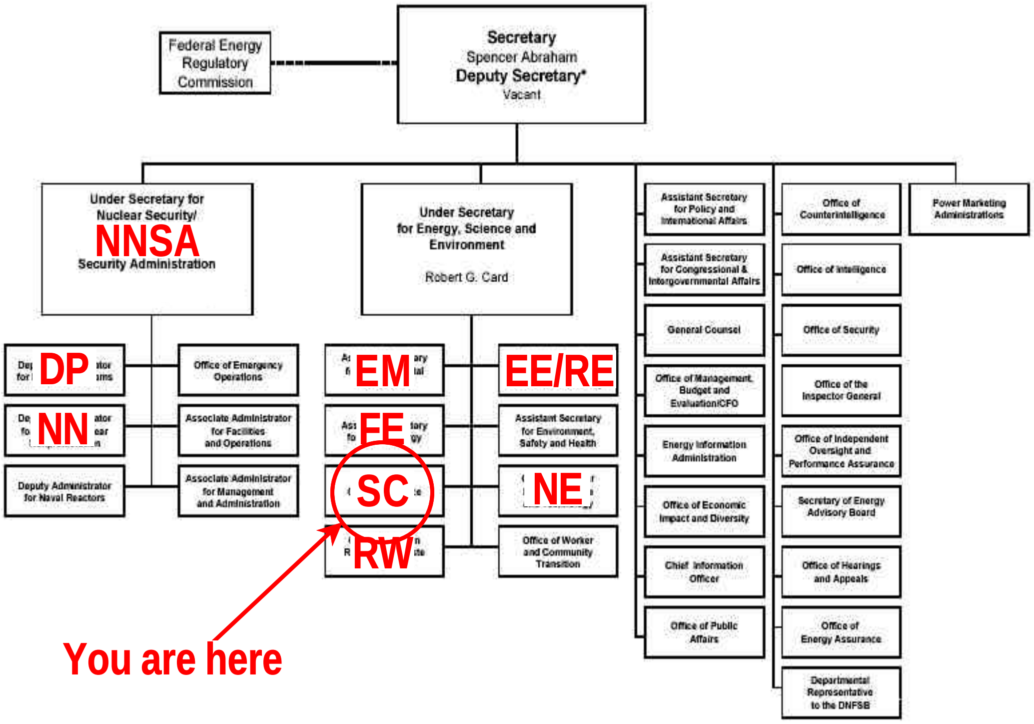
Manuel Lujan Jr. Neutron Scattering Center

High-Flux Isotope Reactor

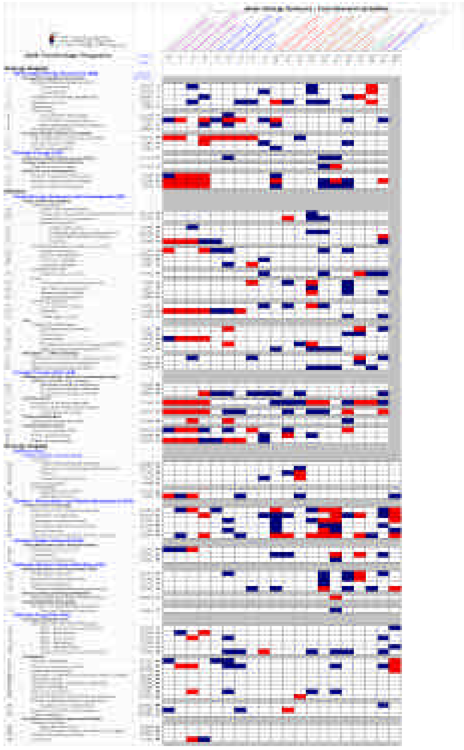
The Spallation Neutron Source

The Spallation Neutron Source (SNS) will be the world's most powerful accelerator-based, pulsed neutron source. It will be used for neutron scattering research in condensed matter physics, materials sciences, magnetic materials, polymers and complex fluids, chemistry, and biology. The SNS project cost is $1.4B; completion will be in 2006.

DEPARTMENT OF ENERGY



BES Research for National and Energy Security



Renewable Energy Resources (RE)

Nuclear Energy (NE)

Fossil Energy (FE)

Energy Conservation (EE)

Fusion Energy Sciences (SC)

Environmental Management (EM)

Nuclear Waste Disposal (RW)

Defense Nuclear Nonproliferation (NN)

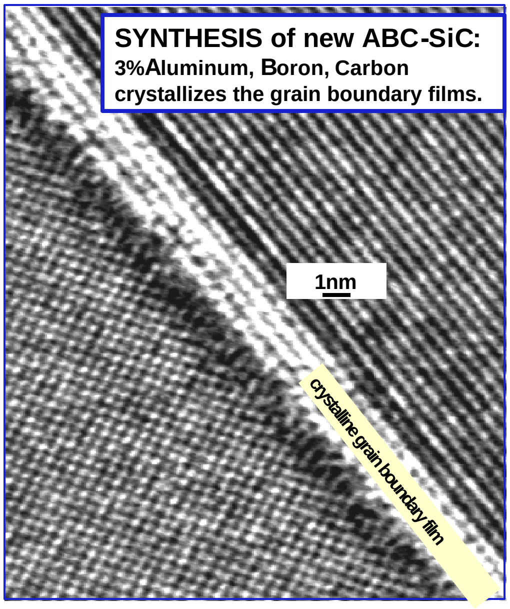
Defense Programs (DP)

Strong, Tough, and Creep-Resistant Ceramics

ceramic turbine (Honeywell)
silicon nitride or silicon carbide

Grain boundary films, as thin as 1 nm, affect mechanical properties of ceramics

- **Doubled fracture resistance**
- **Resistant to high-temp deformation**
- **High strength**

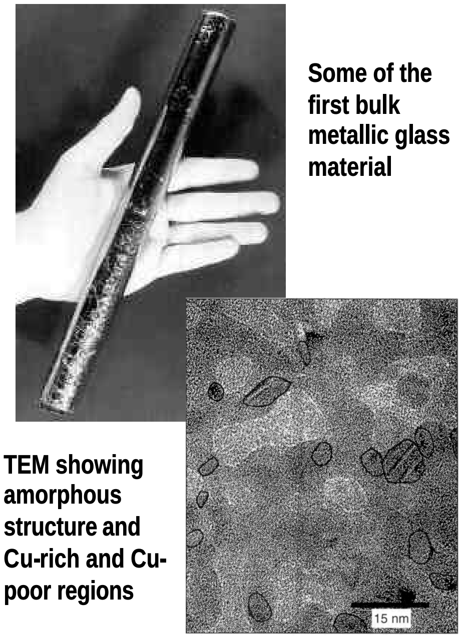


SYNTHESIS of new ABC-SiC:
3%Aluminum, Boron, Carbon crystallizes the grain boundary films.

Lutgard De Jonghe, Robert O. Ritchie
Materials Sciences Division
LBNL

Bulk Metallic Glasses

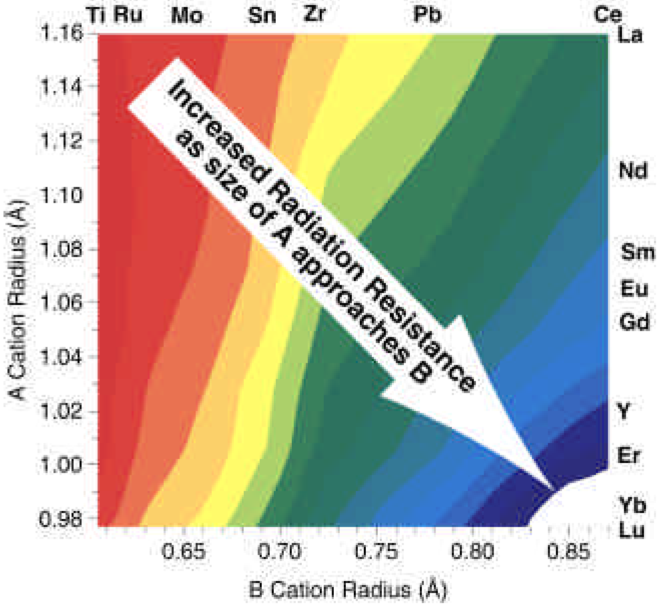
New alloys that form bulk metallic glasses at low cooling rates have led to significant advances in the study of undercooled liquid metals and the glass transition in metallic systems. These materials do not have crystalline structure, but rather the atoms are randomly positioned like in a liquid. This structure leads to improved toughness and large plastic strain to failure because of the lack of grain boundaries which in crystalline materials are points of weakness.



Some of the first bulk metallic glass material

TEM showing amorphous structure and Cu-rich and Cu-poor regions

Nuclear-Friendly Materials

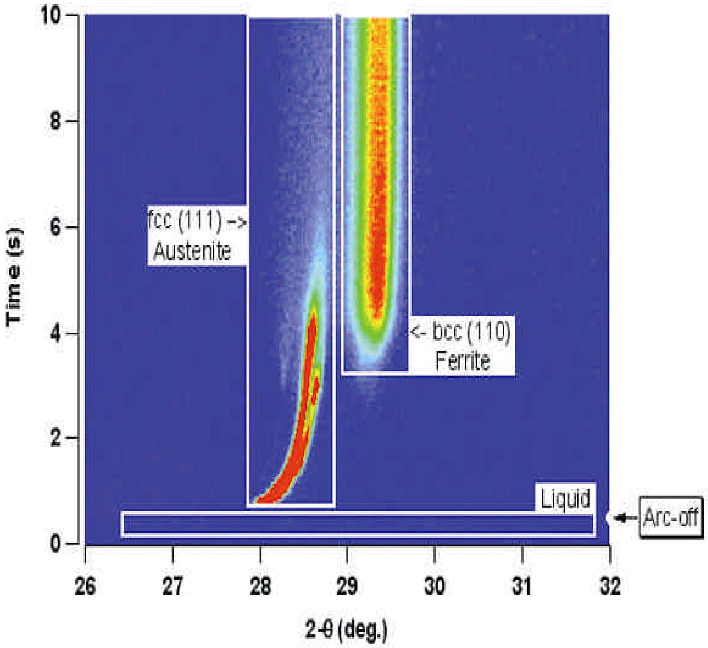


Changing the constituent A and B elements in $A_2B_2O_7$ compounds profoundly affects radiation performance.

Dramatic improvements in radiation tolerance were found as the metallic elements A and B become more similar in size.

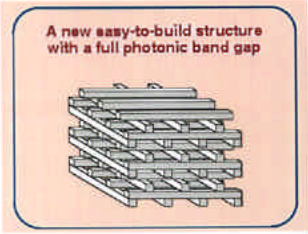
X-rays Diffraction to Understand Welds

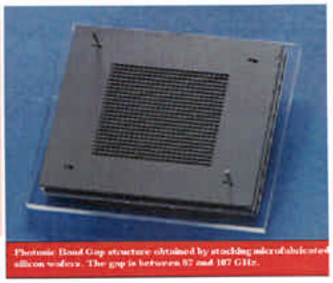
In-situ synchrotron investigations of welding, combined with computer modeling and microstructural characterization, help understand the solidification process and the resultant materials properties.

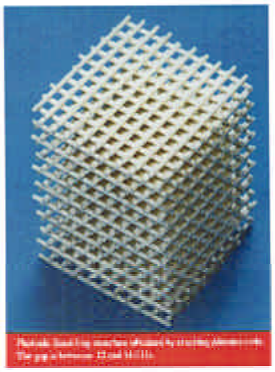


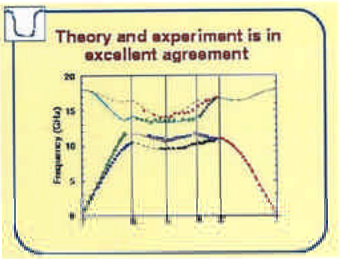
Time resolved X-ray diffraction shows non-equilibrium weld solidification

Photonic Band Gap Structures



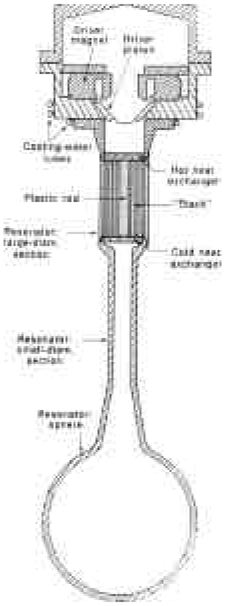






By designing materials where certain wavelengths do not propagate, one can build very high Q cavities, highly directional antennas, and enhanced low loss propagation.

Thermoacoustic Refrigeration



Oscillating temperature and heat flux accompany the oscillating pressure in sound waves. Combining oscillating temperature, pressure, heat, and motion, we create “thermoacoustic” heat engines, refrigerators, and mixture separators, with efficiency now close to that of mature technologies.

Los Alamos National Laboratory, G. Swift, et al.

Organometallic Catalysts

CHEMICAL & ENGINEERING NEWS

C&EN

Catalysts

Metallocene compounds launch new era in polyolefins Page 15

The study of weakly bound ligands in organometallic compounds led to industrial polymerization catalysis.

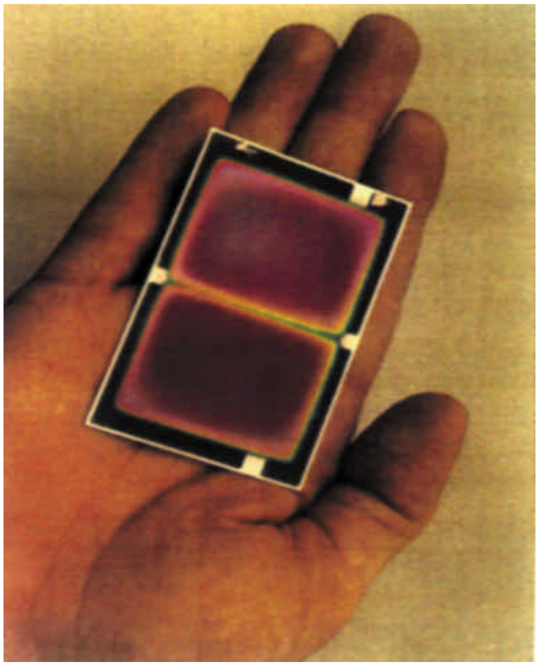
alkene

Catalyst

polymer

Rechargeable Thin-Film Lithium Batteries

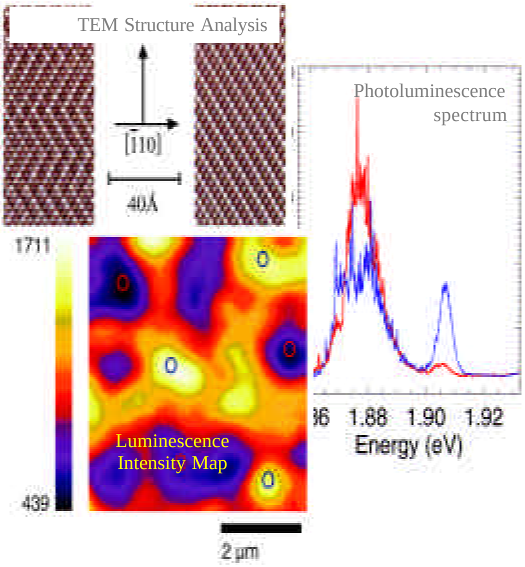
- Revolutionary solid electrolyte
  - (lithium phosphorus oxynitride)
  - stable in contact with lithium metal
  - enables highest energy density
- Rechargeable battery
  - 1/2 the thickness of plastic wrap
  - can be fabricated on silicon
  - resulted in 4 CRADAs and 1 license
  - used in medical and consumer devices, smart credit cards, miniature hazardous materials monitors, memory backup power reservoir



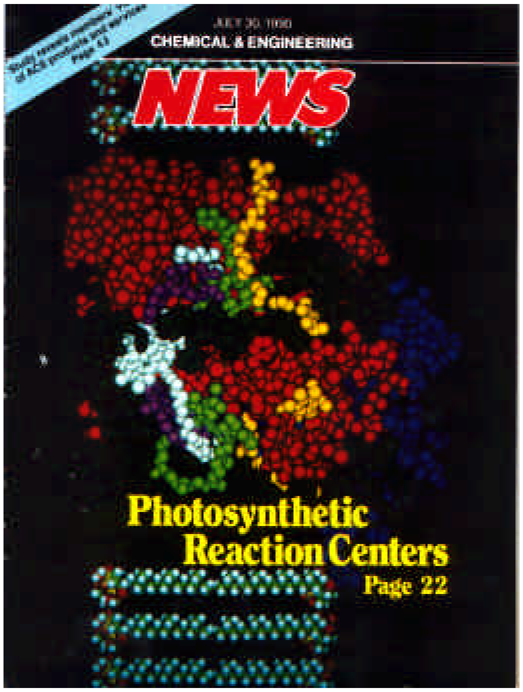
Semiconductor Alloys Lead to Record Solar Cell

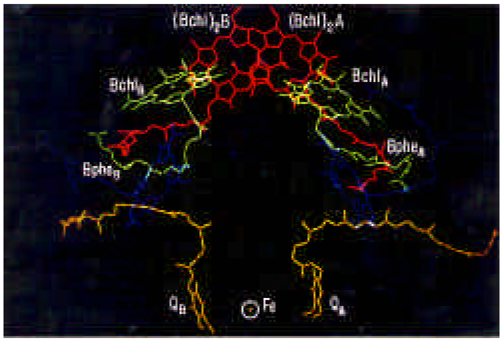
Studies relate spontaneous ordering in a semiconductor alloy to optoelectronic properties

- Superstructure ordering modifies energy band structure.
- Allows tailoring optical properties to optimize solar cell performance.
- Resulted in a record-performance “triple junction” photovoltaic device (32.4% efficiency!)
- These devices are being applied in space-based applications and terrestrial light concentrator devices.



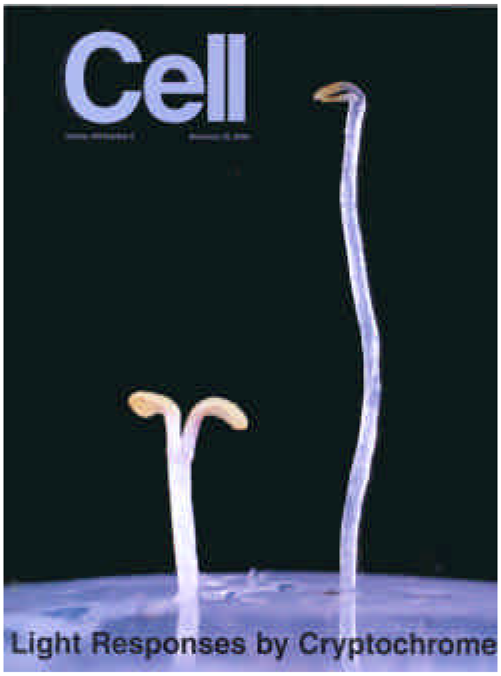
Photosynthetic Reaction Center





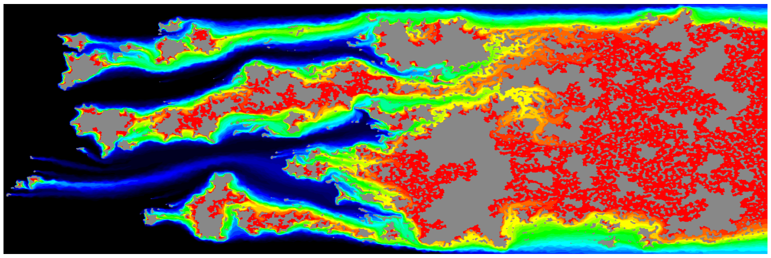
The fundamental process by which plants and bacteria convert and store solar energy as chemical free energy occurs in the photosynthetic reaction center. One electron is pumped by the action of light from the primary donor, bacteriochlorophyll dimer $(BChl)_2A$, to a quinone acceptor, Q_A. The charge separation process is studied as the prototype for simpler model systems.

Plant Response to Blue Light

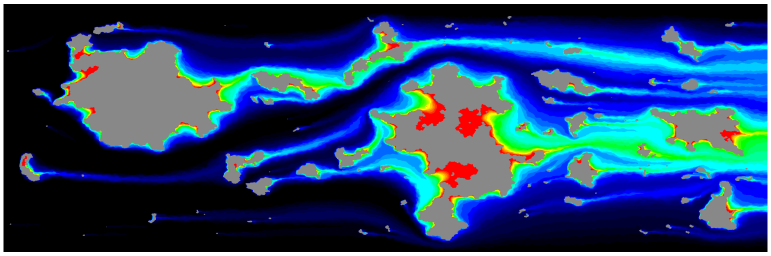


Plants use different photoreceptors to sense the quality and quantity of light in the surrounding environment; this information is conveyed by molecular-level signaling mechanisms to allow plants to adjust their growth and development accordingly. Potential developmental responses to cryptochrome action include seed germination, stem elongation, and flowering.

Patterns and Predictions of Subsurface Flow



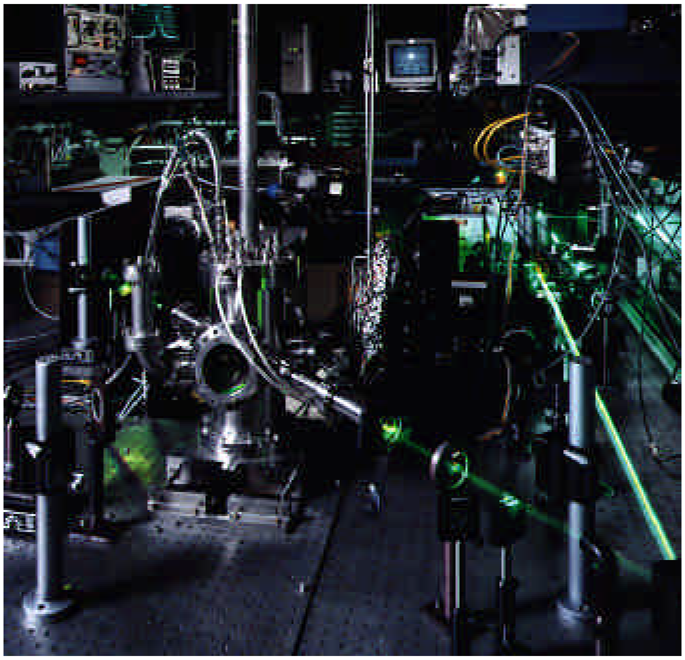
C=0.2



C=0.4

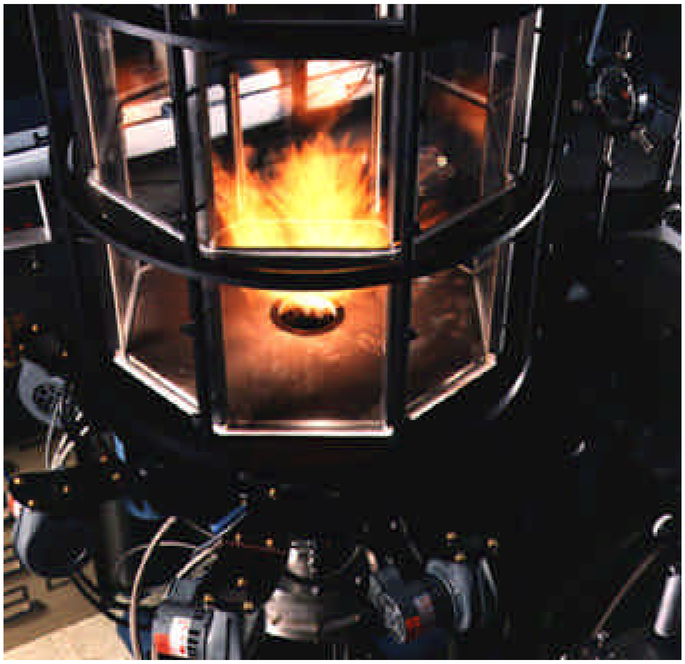
Recovery of subsurface fluids, whether oil and gas or contaminants, requires understanding the ways fluids flow within porous and fractured rocks and soil.

The Combustion Research Facility



- Research addresses
  - Energy sciences
  - Energy efficiency
  - Environmental impact
  - Fuel flexibility
- Core programs provide
  - Basic to applied research
  - Unique laser facilities
  - Partnerships with academia and industry

Basic Research and Applied Programs at the CRF



- Basic
  - Combustion chemistry
  - Optical diagnostics
  - Reacting fluid flows
- Applied
  - Engine combustion and emissions
  - Industrial furnaces and boilers
  - Manufacturing processes
  - Alternative fuels
  - Field measurements
  - Remote sensing

"Generic" Scientific Opportunities

- ***Realizing the nanoscale revolution***

  Tailoring materials one atom at a time for desired properties and functions

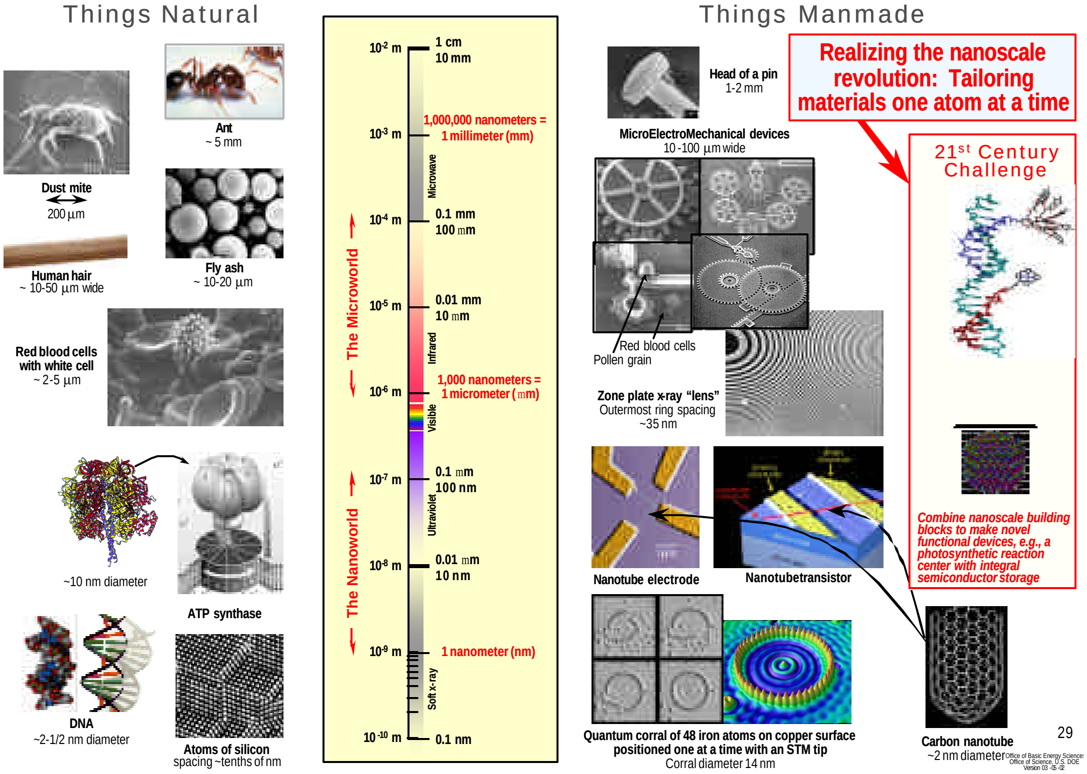
- ***Complex systems***

  Understanding collective, cooperative, and adaptive phenomena and emergent behavior

- ***Harnessing the power of advanced computing***

  Investigating condensed matter and materials physics, chemistry, and biosciences

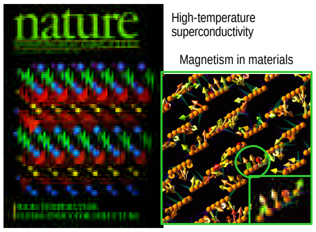
The Scale of Things -- Nanometers and More



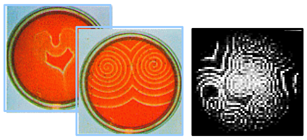
Office of Basic Energy Sciences
Office of Science, U.S. DOE
Version 03-05-02

Complex systems:

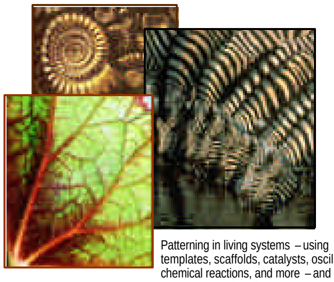
Understanding collective, cooperative, and adaptive phenomena and emergent behavior



Collective effects and emergent behavior in inorganic systems



Oscillatory chemical reactions



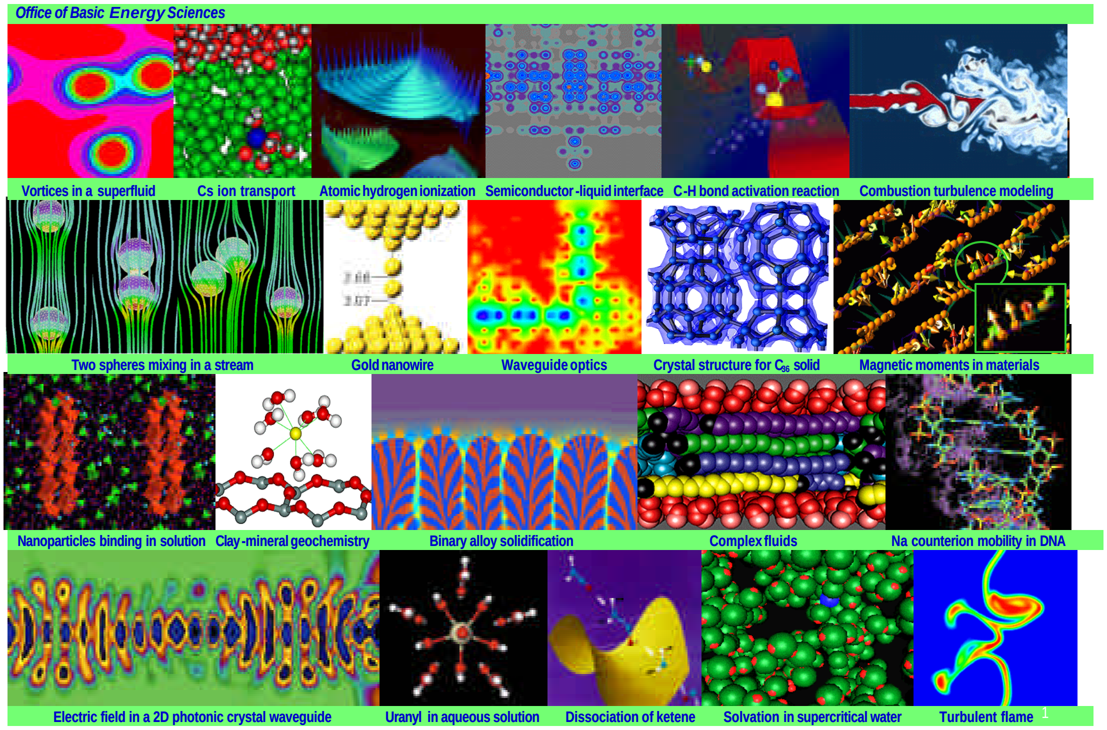
Patterning in living systems – using templates, scaffolds, catalysts, oscillatory chemical reactions, and more – and emergent functionality

Interactions among individual components can lead to coherent behavior that can be described only at higher levels than those of the individual units. This can produce remarkably complex and yet organized behavior.

- **Electrons interacting with each other and the host lattice in solids give rise to magnetism and superconductivity.**
- **Chemical constituents interacting in solution give rise to complex pattern formation and growth.**
- **Living systems self assemble their own components, self repair them as necessary, and reproduce; they sense and respond to even subtle changes in their environments.**

Harnessing the Power of Advanced Computing for Condensed Matter and Materials Physics, Chemistry, and Biosciences

Office of Basic Energy Sciences



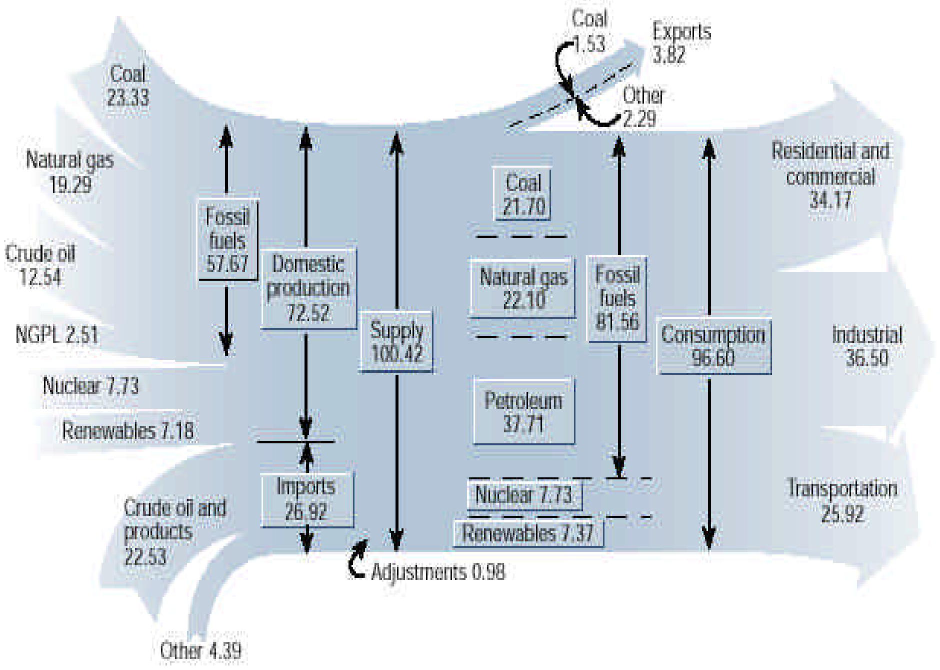
Vortices in a superfluid | Cs ion transport | Atomic hydrogen ionization | Semiconductor-liquid interface | C-H bond activation reaction | Combustion turbulence modeling

Two spheres mixing in a stream | Gold nanowire | Waveguide optics | Crystal structure for C_{36} solid | Magnetic moments in materials

Nanoparticles binding in solution | Clay-mineral geochemistry | Binary alloy solidification | Complex fluids | Na counterion mobility in DNA

Electric field in a 2D photonic crystal waveguide | Uranyl in aqueous solution | Dissociation of ketene | Solvation in supercritical water | Turbulent flame

Fundamental Research for Energy Security



Conversations with BESAC

"The basic research community has focused on many of the known problems in energy technologies for many years – the workshop should not rehash these areas."

"Rather, the workshop should focus on new revolutionary basic research opportunities."

Overview
DOE’s Office of Fossil Energy Programs

Basic Energy Sciences
Advisory Committee-
Sponsored Workshop

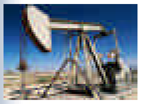
October 21, 2002
Rita A. Bajura
Director
NETL

FE Responsible for RD&D Program in Fossil Energy Supply, Delivery, and Use Technologies

Electric Power Using Coal

Environmental Control

V21 Next Generation

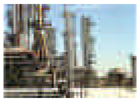


Carbon Sequestration

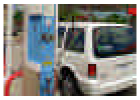
Clean Liquid Fuels

Exploration & Production

Refining & Delivery



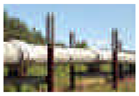
Alternative Fuels



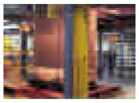
Future Fuels

Natural Gas

Exploration & Production



Pipelines & Storage



Fuel Cells

Combustion Turbines

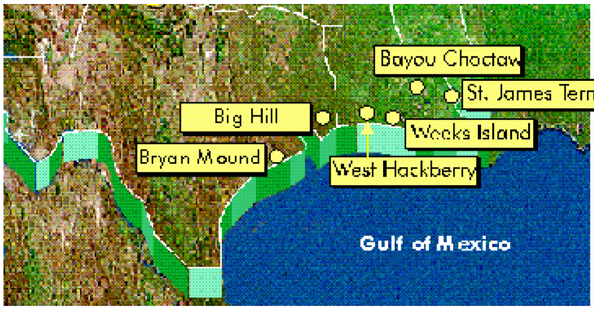
Photo of hydrogen fueled car: Warren Gretz, NREL

FE Responsible for the Strategic Petroleum Reserve

Maintain readiness of nation's emergency:

- Crude oil stockpile
- Northeast heating oil reserve

West Hackberry Louisiana

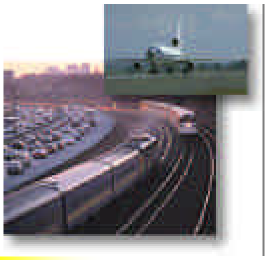


Energy Profoundly Impacts Our Quality of Life

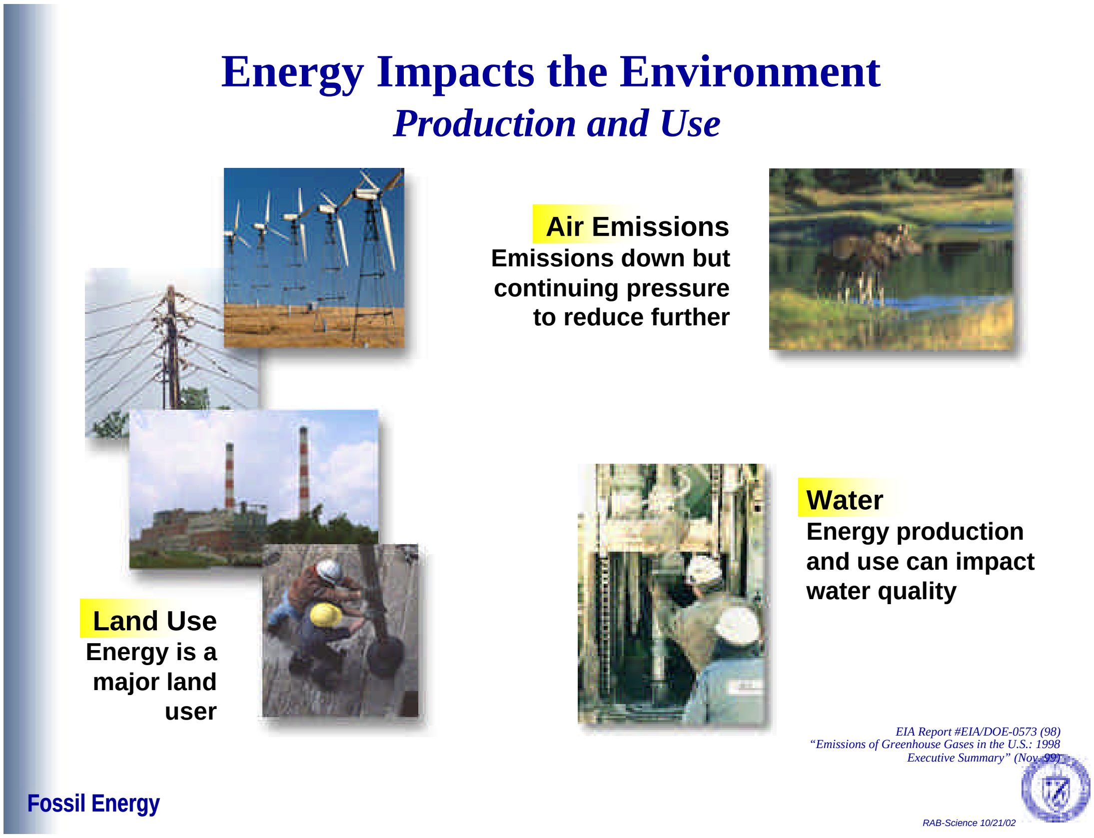
Comfort
Fuel warms our homes and provides electricity to wash our clothes and power our televisions

Food
Energy needed to produce food and to deliver clean water to our homes

Reliability
Reliable power for air traffic control, banking, and telecommunications



Mobility
Fuel provides mobility



Energy Impacts the Environment

Production and Use

Air Emissions
Emissions down but continuing pressure to reduce further

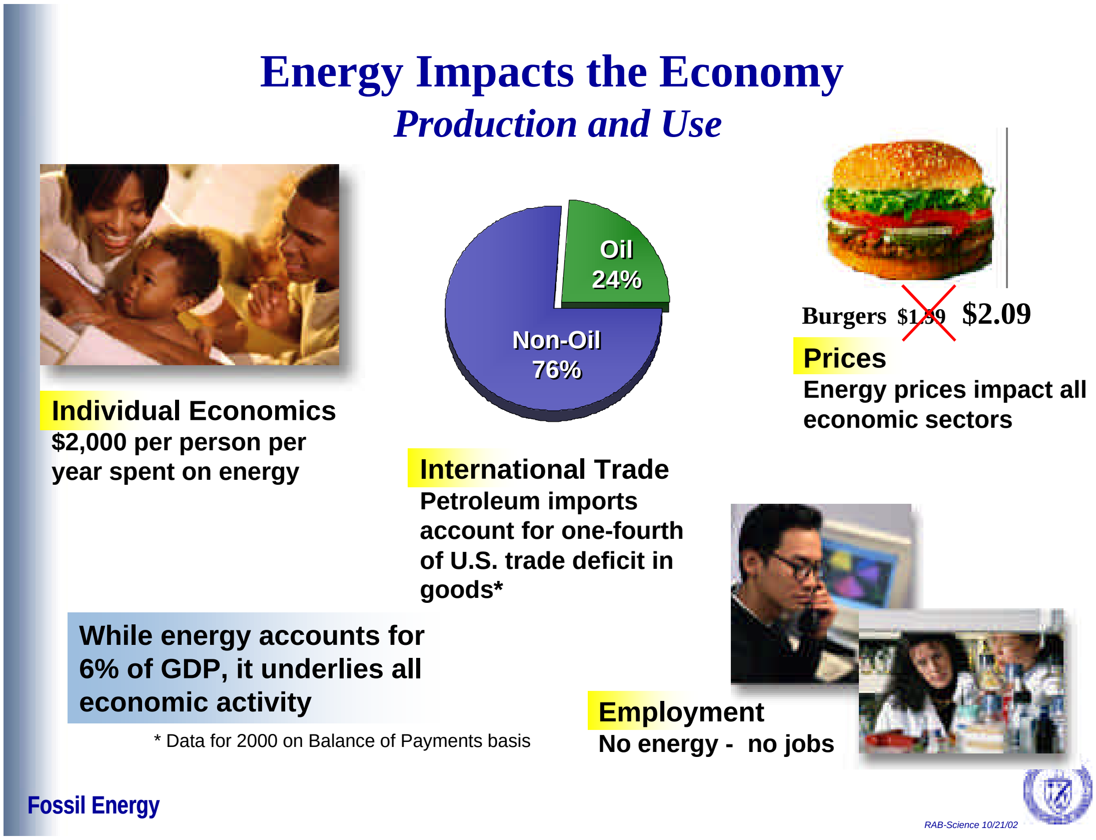
Water
Energy production and use can impact water quality

Land Use
Energy is a major land user

EIA Report #EIA/DOE-0573 (98)
“Emissions of Greenhouse Gases in the U.S.: 1998
Executive Summary” (Nov. 99)

Fossil Energy

RAB-Science 10/21/02



Energy Impacts the Economy

Production and Use

Individual Economics
$2,000 per person per year spent on energy

Oil 24%
Non-Oil 76%

International Trade
Petroleum imports account for one-fourth of U.S. trade deficit in goods*

Burgers ~~$1.99~~ $2.09

Prices
Energy prices impact all economic sectors

While energy accounts for 6% of GDP, it underlies all economic activity

* Data for 2000 on Balance of Payments basis

Employment
No energy - no jobs

Fossil Energy

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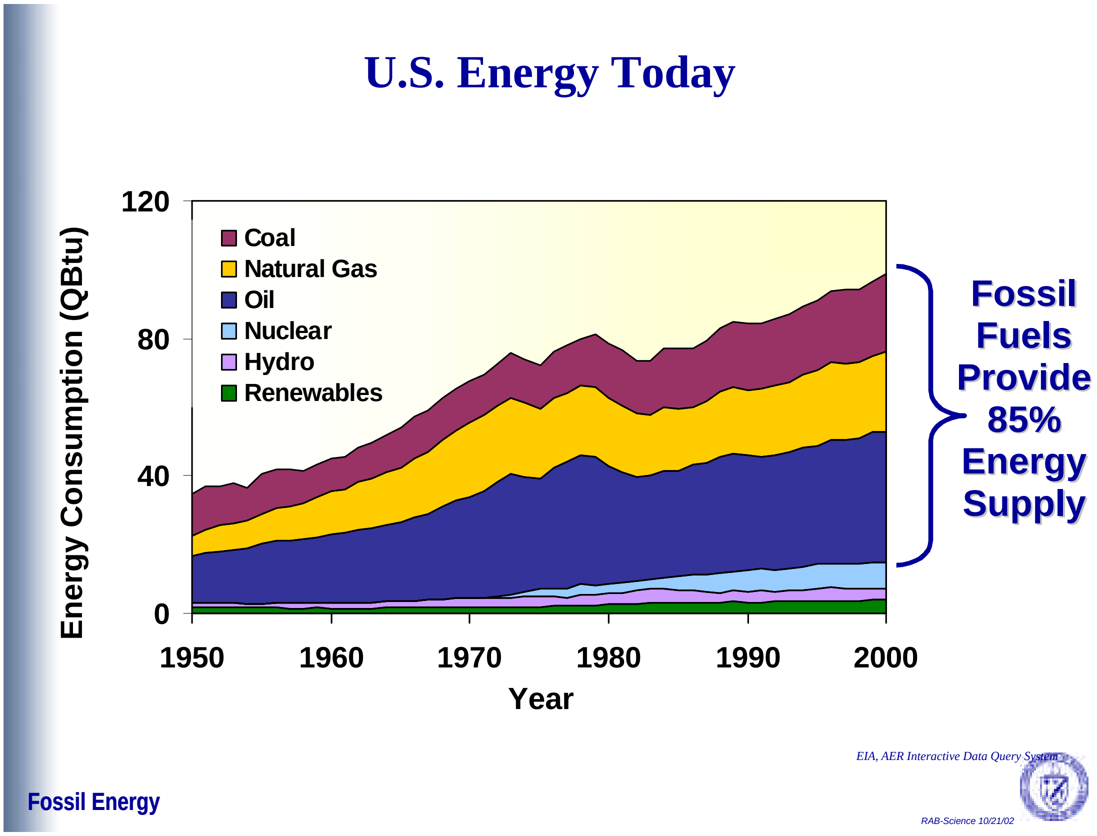

U.S. Energy Today

Fossil Fuels Provide 85% Energy Supply

EIA, AER Interactive Data Query System

Fossil Energy

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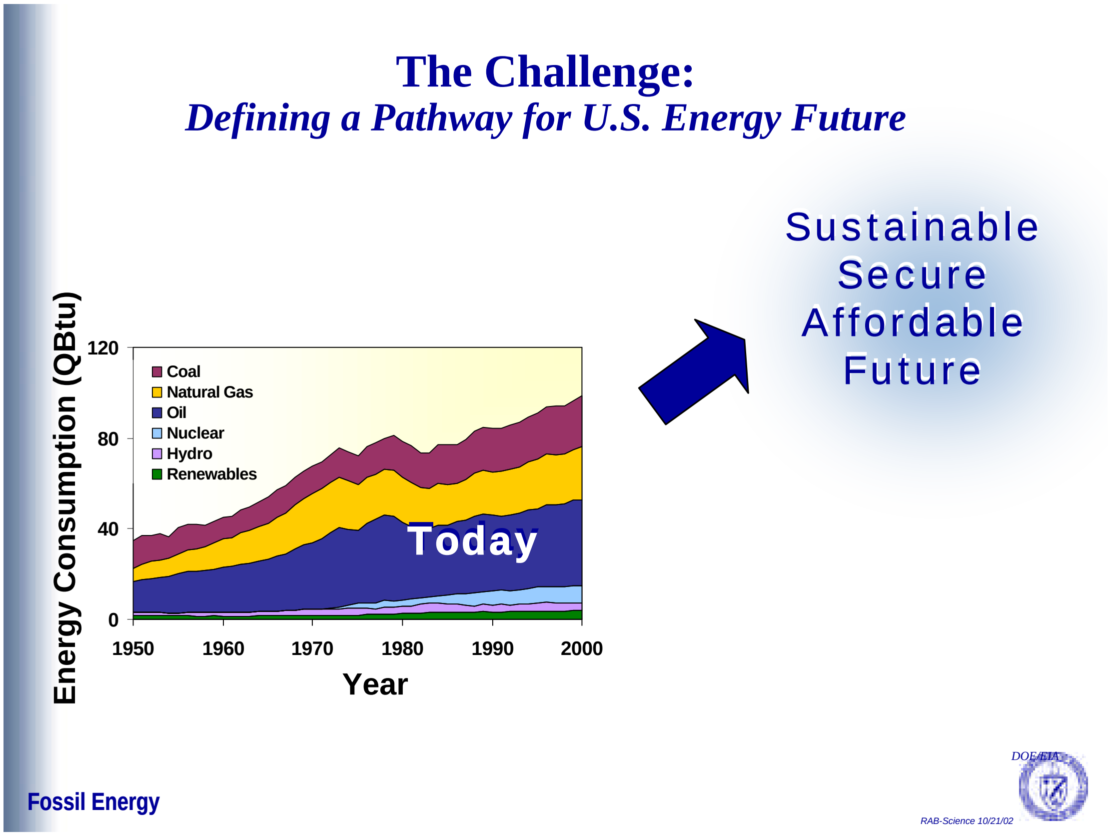

The Challenge:
Defining a Pathway for U.S. Energy Future

Sustainable
Secure
Affordable
Future

DOE/EIA

Fossil Energy

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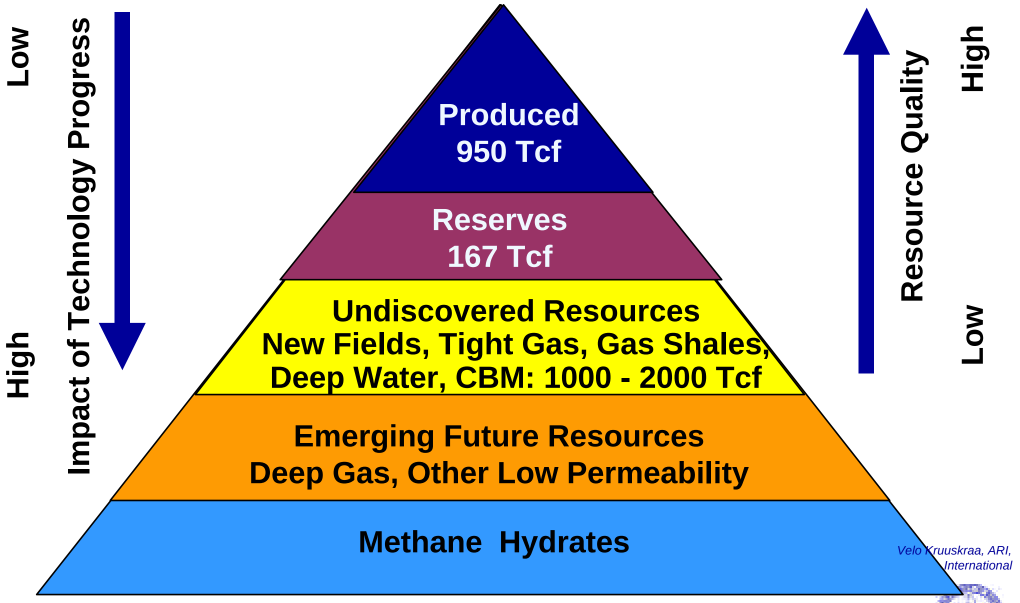
Issues Facing Energy

- **Local/regional environmental**
- Energy security
- Global supply/environmental

Resource Base Depends on Economics of Production

Natural Gas Resource Pyramid As of Year 2000



Low

Impact of Technology Progress

High

Produced
950 Tcf

Reserves
167 Tcf

Undiscovered Resources
New Fields, Tight Gas, Gas Shales, Deep Water, CBM: 1000 - 2000 Tcf

Emerging Future Resources
Deep Gas, Other Low Permeability

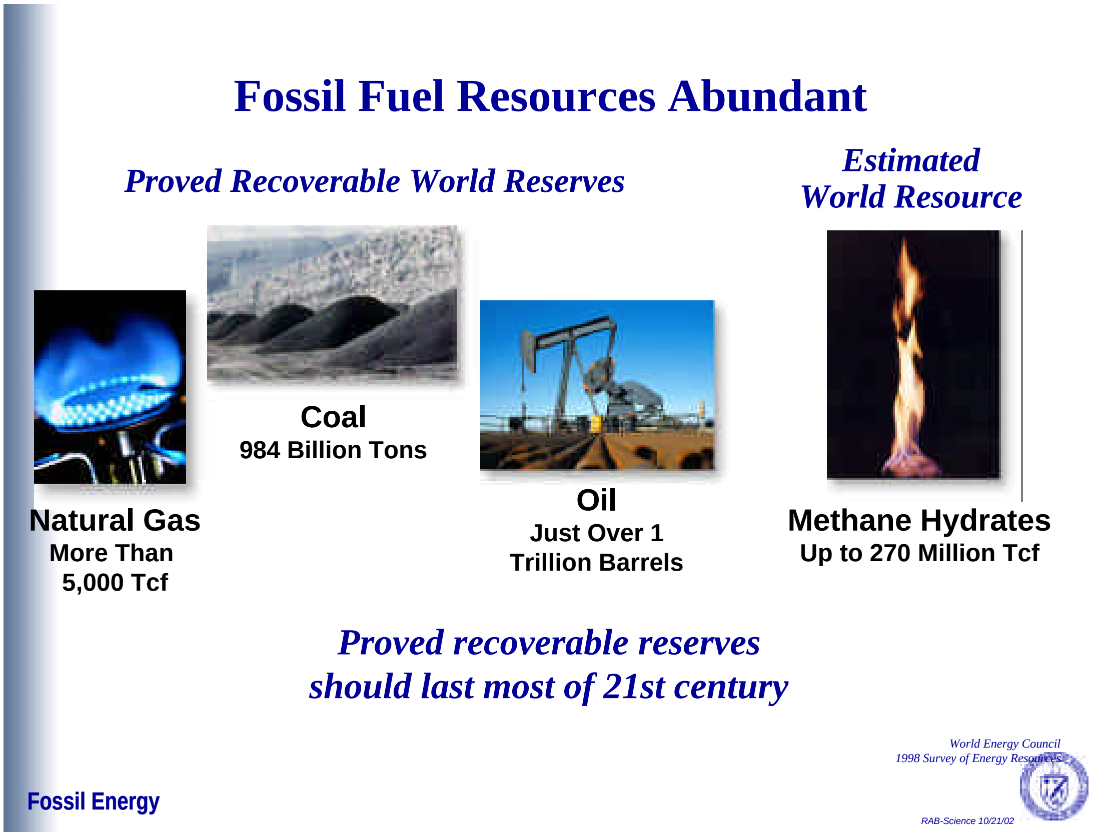
Methane Hydrates

High

Resource Quality

Low

Velo Kruuskraa, ARI, International



Fossil Fuel Resources Abundant

Proved Recoverable World Reserves

Estimated World Resource

Natural Gas
More Than
5,000 Tcf

Coal
984 Billion Tons

Oil
Just Over 1
Trillion Barrels

Methane Hydrates
Up to 270 Million Tcf

Proved recoverable reserves should last most of 21st century

World Energy Council
1998 Survey of Energy Resources

Fossil Energy

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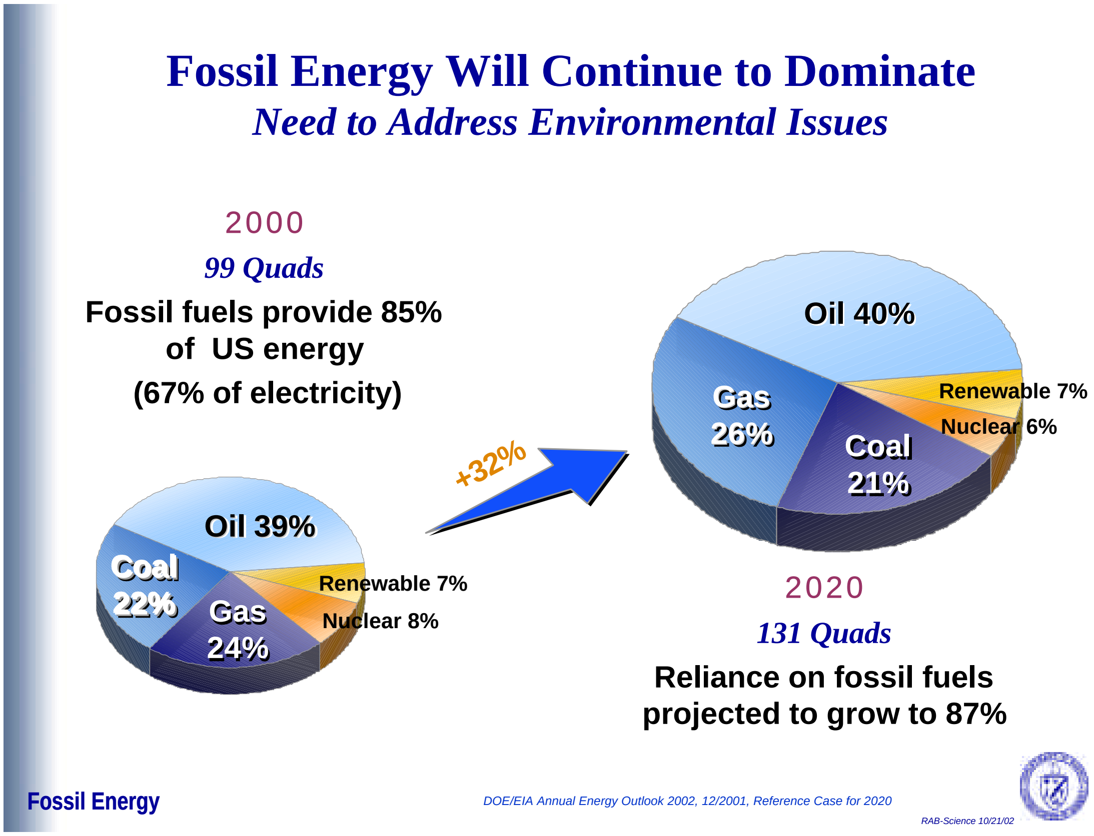


Fossil Energy Will Continue to Dominate

Need to Address Environmental Issues

2000

99 Quads

Fossil fuels provide 85%
of US energy
(67% of electricity)

Oil 39%
Coal 22%
Gas 24%
Renewable 7%
Nuclear 8%

+32%

Oil 40%
Gas 26%
Coal 21%
Renewable 7%
Nuclear 6%

2020

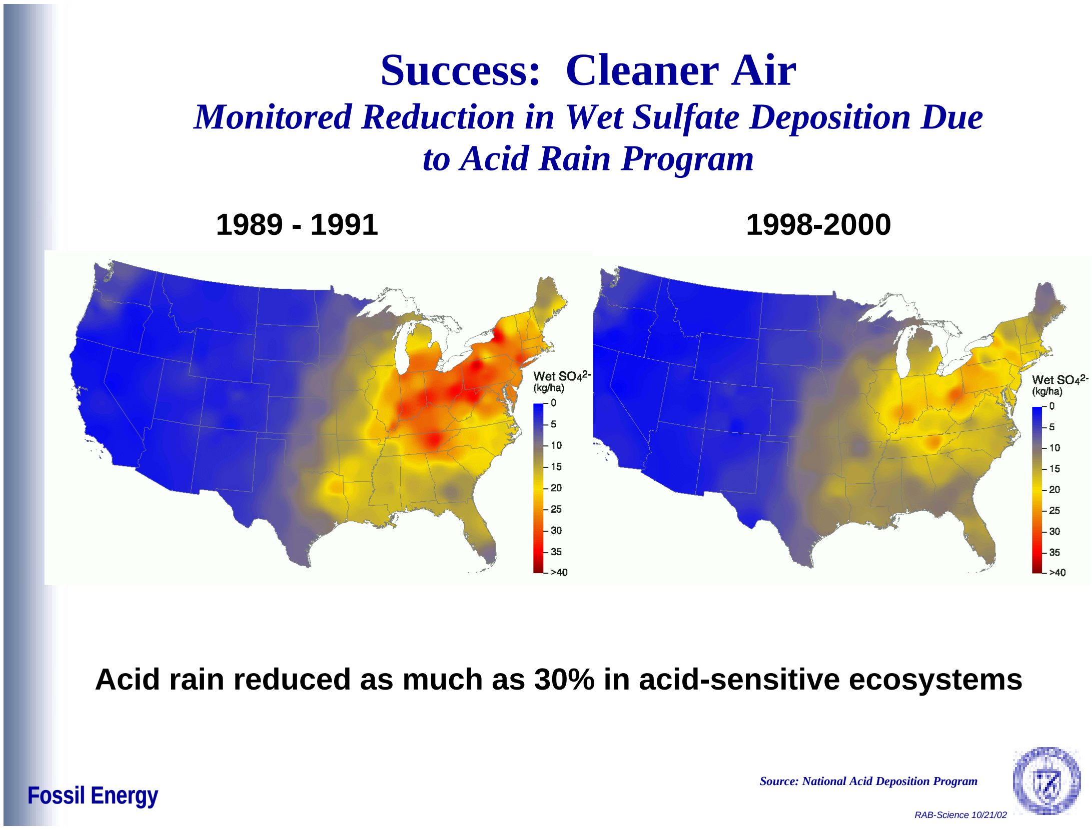
131 Quads

Reliance on fossil fuels
projected to grow to 87%

Fossil Energy

DOE/EIA Annual Energy Outlook 2002, 12/2001, Reference Case for 2020

RAB-Science 10/21/02

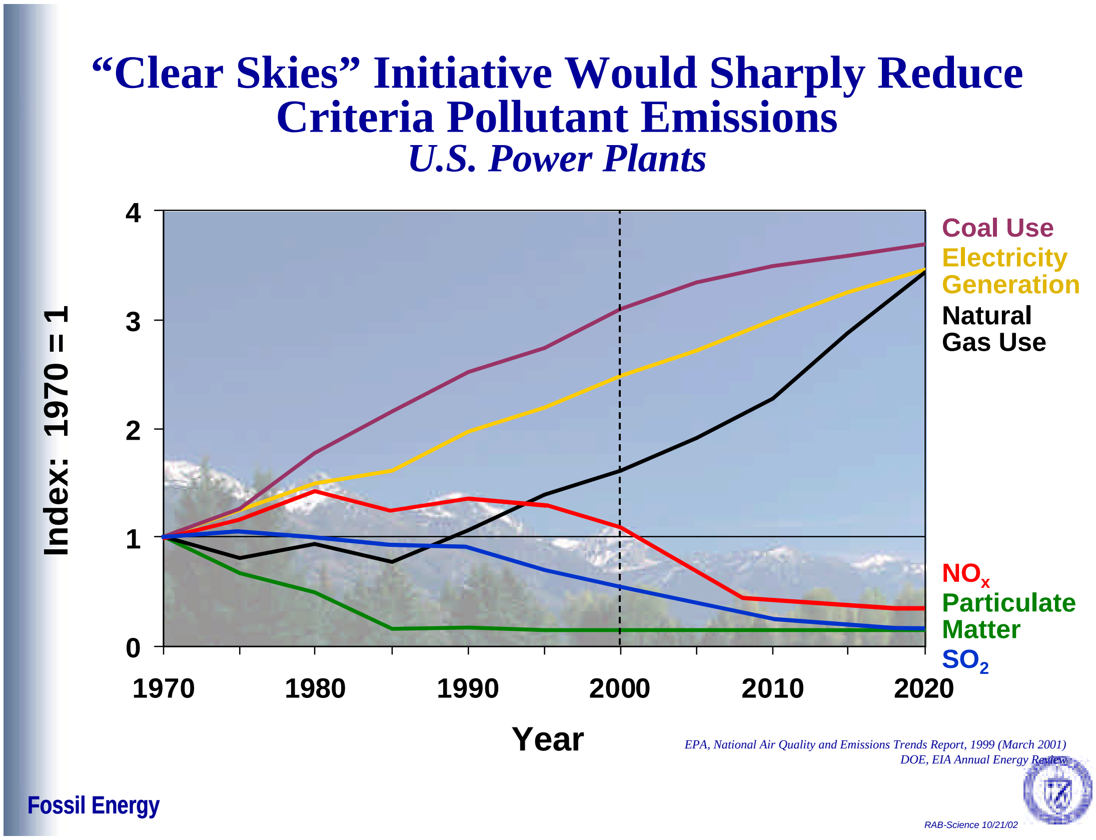


Success: Cleaner Air

Monitored Reduction in Wet Sulfate Deposition Due to Acid Rain Program

Acid rain reduced as much as 30% in acid-sensitive ecosystems

Source: National Acid Deposition Program

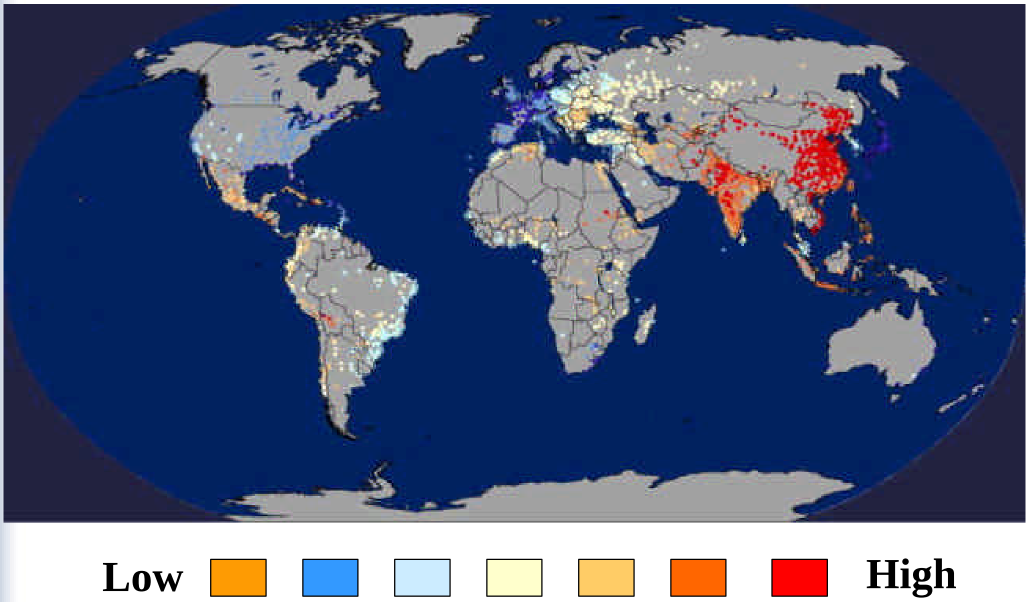


"Clear Skies" Initiative Would Sharply Reduce Criteria Pollutant Emissions

U.S. Power Plants

EPA, National Air Quality and Emissions Trends Report, 1999 (March 2001)
DOE, EIA Annual Energy Review

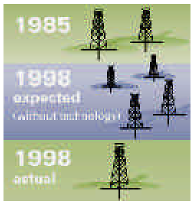
Concentration of Particulate Matter in Urban Areas



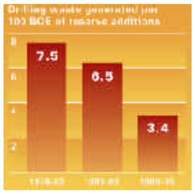
World Bank Atlas - 2001, Technology: Stationary Sources and Demand-Side Management, Terry Surles, California Energy Commission , May 1, 2002

Natural Gas & Oil Exploration & Production

Technology Reducing Environmental Impact



Fewer wells to add same level of reserves



Lower drilling waste volume

Lower produced water volumes

Smaller footprints

Greater protection of unique and sensitive environments

Mining is Critical to Quality of Life

Every American Born Will Need...

- 11.7 Tons Clays
- 1,925 lbs. Copper
- 1.8 Troy oz. Gold
- 295 Tons Coal
- 13.9 Tons Phosphate
- 3 Tons Aluminum
- 1,078 lbs. Lead
- 21.3 Tons Iron Ore
- 15.2 Tons Salt
- 1,001 lbs. Zinc
- 850 Tons Stone, Sand, Gravel
- 83,890 Gallons Petroleum
- 34.4 Tons Cement
- 34.5 Tons Other Minerals and Metals
- 6 million cu. ft. of Natural Gas

1,875 tons of minerals, metals, and fuels in a lifetime

2000 Mineral Information Institute, Golden, Colorado

Fossil Energy

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Coal Mining
Technology Reducing Environmental Impact

Made progress through improved

- Planning
- Permitting
- Groundwater management
- Utilization of coal mine methane
- Reclamation

Legacy programs exist

Reclaimed Surface Mine in Western PA

Contaminated Mine Drainage

Fossil Energy

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Issues Facing Energy

- Local/regional environmental
- Energy security
- Global supply/environmental

Fossil Energy

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Threats to Energy Security

- Increased
  - Terrorist threats
  - Oil and gas imports
  - Interdependencies
- Aging infrastructure
- Less reserve capacity

Fossil Energy

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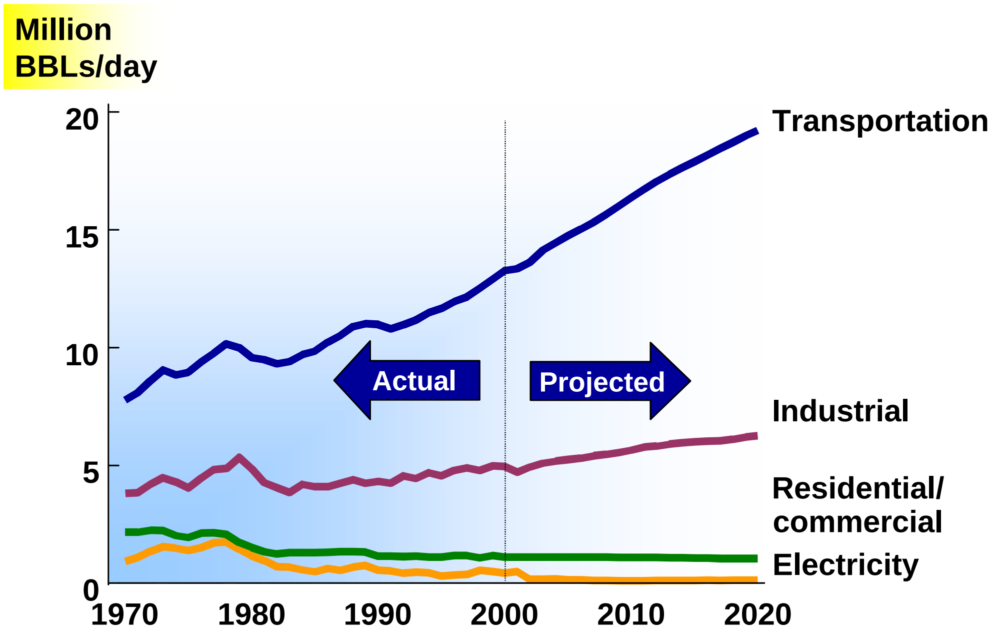
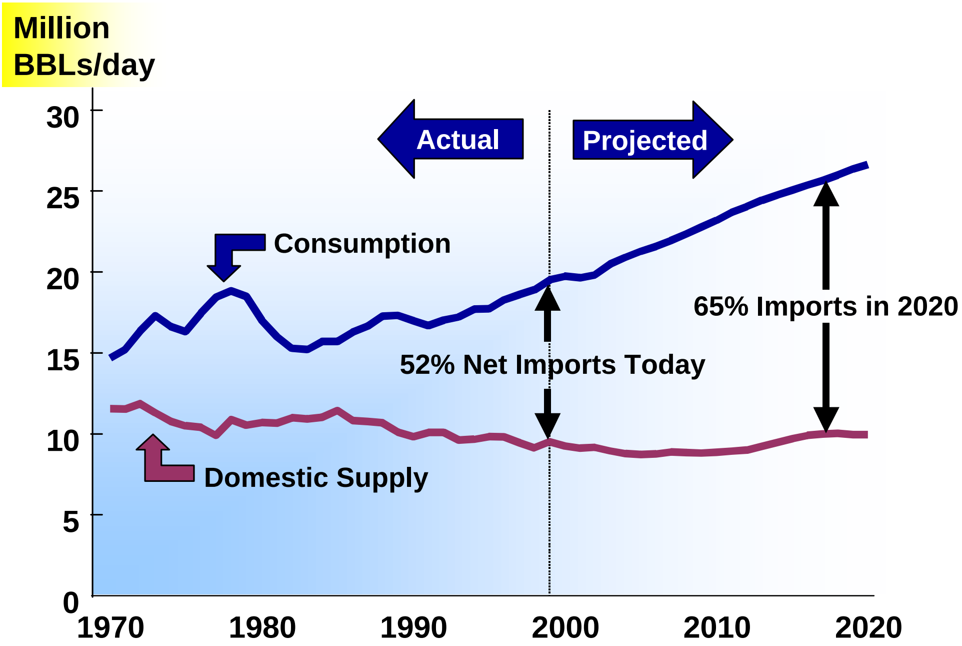
Transportation Consumes 2/3 U.S. Oil



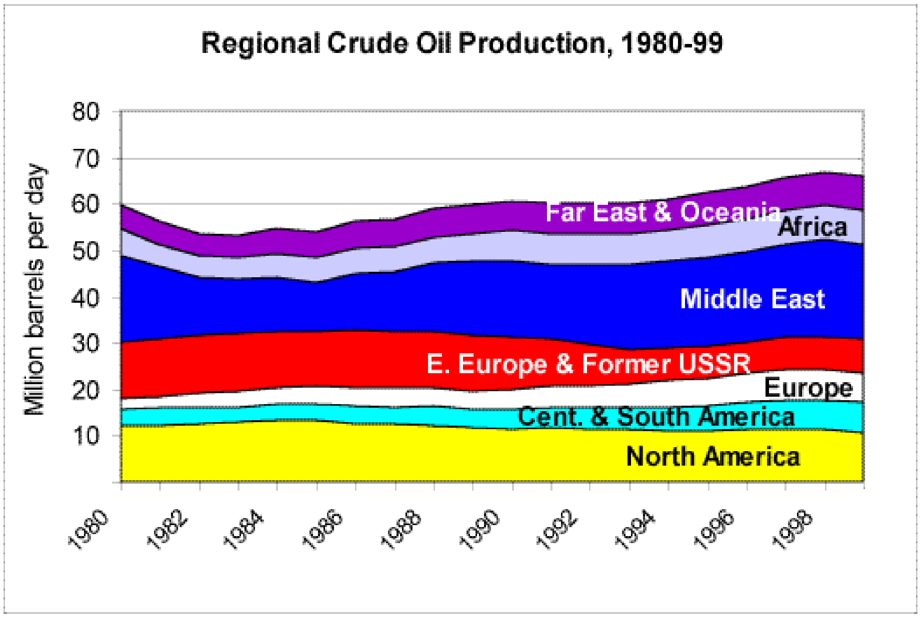
Annual Energy Outlook 2002

U.S. Oil Imports Rising

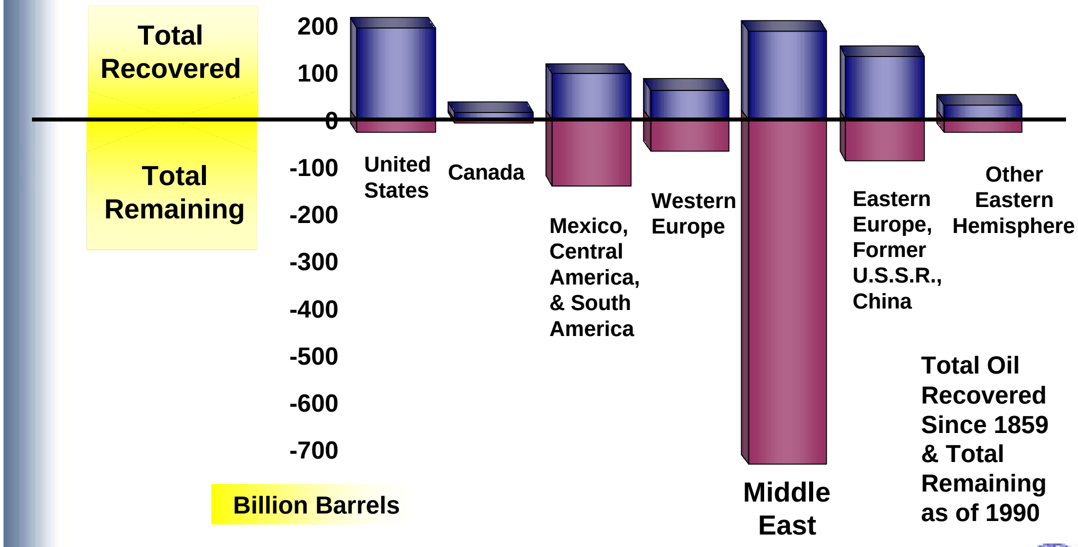


Annual Energy Outlook 2002

Much of World's Oil Comes from Unstable Regions



Bulk of World's Reserves in Middle East



Total Oil Recovered Since 1859 & Total Remaining as of 1990

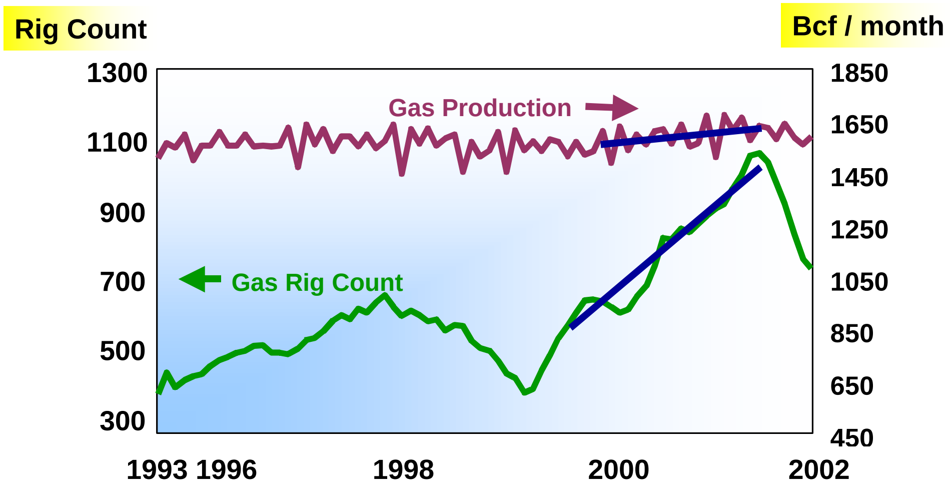
Demographics of Middle East

- Population is young, growing rapidly, poor
- Nations are young
- Rich/poor gap
- Rising internal energy use

Based on Matt Simmons

Production Lag Suggests Shrinking U.S. Gas Surplus

U.S. Drilling Rig Count vs. Gas Production

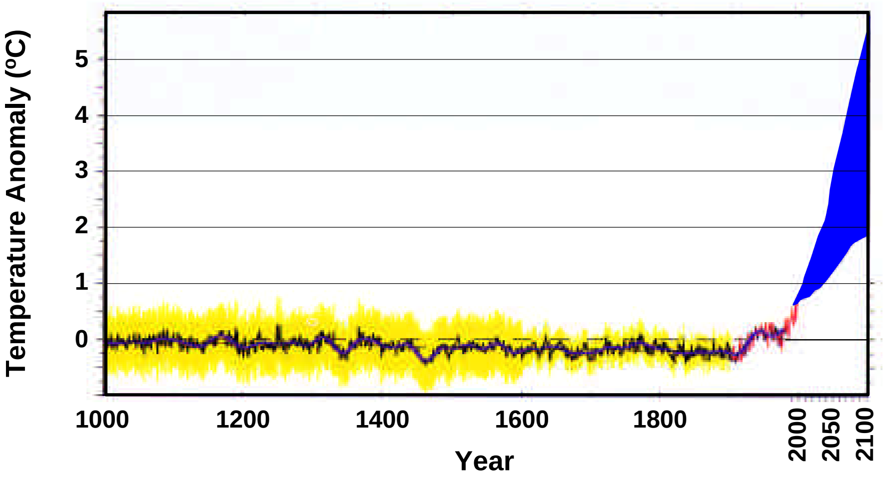


Source: Matt Simmons
EIA History - Natural Gas Monthly - January 2002,
Oil & Gas Split Rig Count - Baker Hughes

Issues Facing Energy

- Local/regional environmental
- Energy security
- **Global supply/environmental**

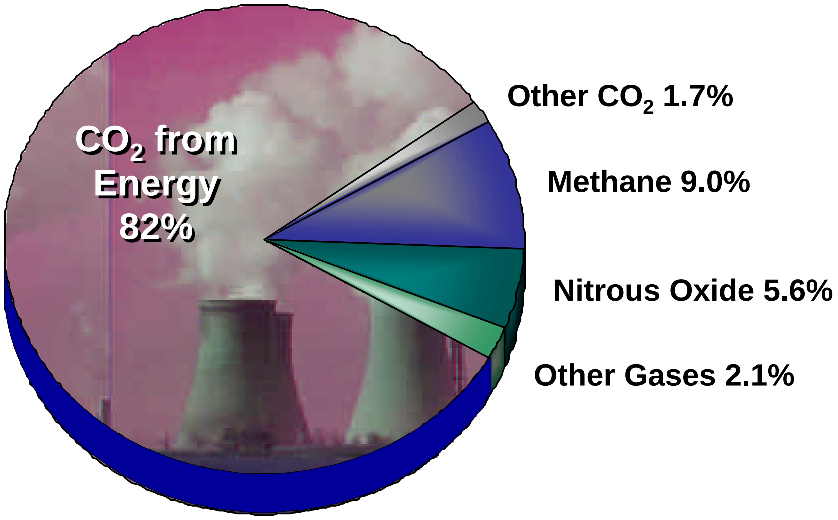
Mean Annual Temperature Variations
Northern Hemisphere



B. Eliasson, First National Conference on Carbon Sequestration, May 15-17, 2001

CO_2 From Energy Is Major Contributor

U.S. GHG Emissions Weighted by Global Warming Potential



EIA Report #EIA/DOE-0573
"Emissions of Greenhouse Gases in the U.S. 1999," Executive Summary (Oct. 2000)

Global Climate Change

Fact or Fiction?

- **Science unlikely to provide unequivocal causality answer**
- **Governments and markets likely to act on their perception of the science**
  - Interpreted with a slant towards their self-interest
- **Corporate boards increasingly expected to evaluate potential risks / benefits of climate change**
  - Enron effect

Portions based on Executive Action Brief
No. 23, June 2002,The Conference Board

Technological Carbon Management Options

Reduce Carbon Intensity
- Renewables
- Nuclear
- Fuel Switching

Improve Efficiency
- Demand Side
- Supply Side

Sequester Carbon
- Capture & Store
- Enhance Natural Processes

All options needed to:
- **Supply energy demand**
- **Address environmental objectives**

Vision 21

Ultra-Clean Energy Plant of Future

Energy Plants for Post-2015
- Coal and other fuels
- Electricity and possible co-products

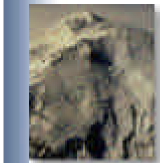
Goal

Eliminate Environmental Concerns from Use of Fossil Energy

Approach
- **Maximize efficiency**
- **Near-zero emissions**

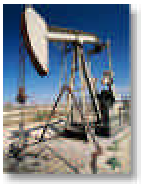
Approaches to Sequester Carbon

Capture and Storage



Unmineable Coal Seams

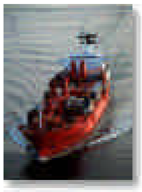
Deep Ocean Injection



Depleted Oil / Gas Wells, Saline Reservoirs

Enhance Natural Processes

Forestation



Iron or Nitrogen Fertilization of Ocean

Enhanced Photosynthesis

Hydrogen

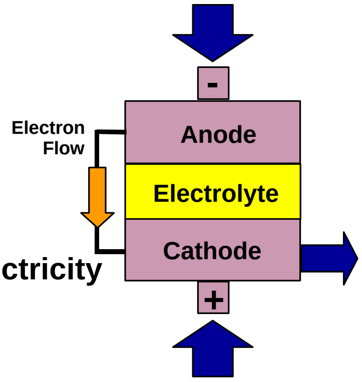
A Proposed Solution for Energy Issues . . .

- **Energy security**
- **Local environmental degradation**
- **Global environmental degradation**

Hydrogen Economy

Ability for consumers to use hydrogen energy devices for transportation, electric power generation, and portable power

Fuel Cells Are One Enabling Technology for Hydrogen Economy



Hydrogen

-

Electron Flow

Anode

Electrolyte

Cathode

Electricity

+

Pure Water

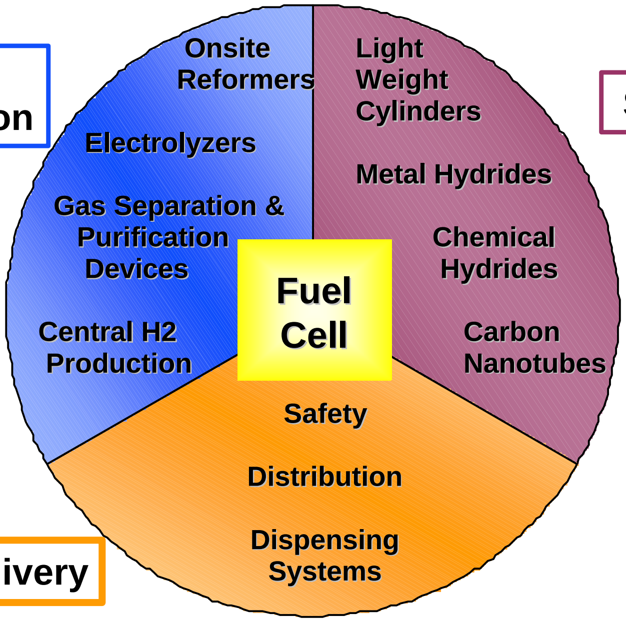
Oxygen from Air

Basically a battery with an external supply of fuel and oxidant

Cells stacked together for desired power

Issue: Cost
- Fuel cells cost $1,600 - $4,500 per kilowatt
- Internal combustion engines cost ≥ $35 per kilowatt

Infrastructure R&D Requirements



H_2 Production

Onsite Reformers

Electrolyzers

Gas Separation & Purification Devices

Central H2 Production

Storage

Light Weight Cylinders

Metal Hydrides

Chemical Hydrides

Carbon Nanotubes

Fuel Cell

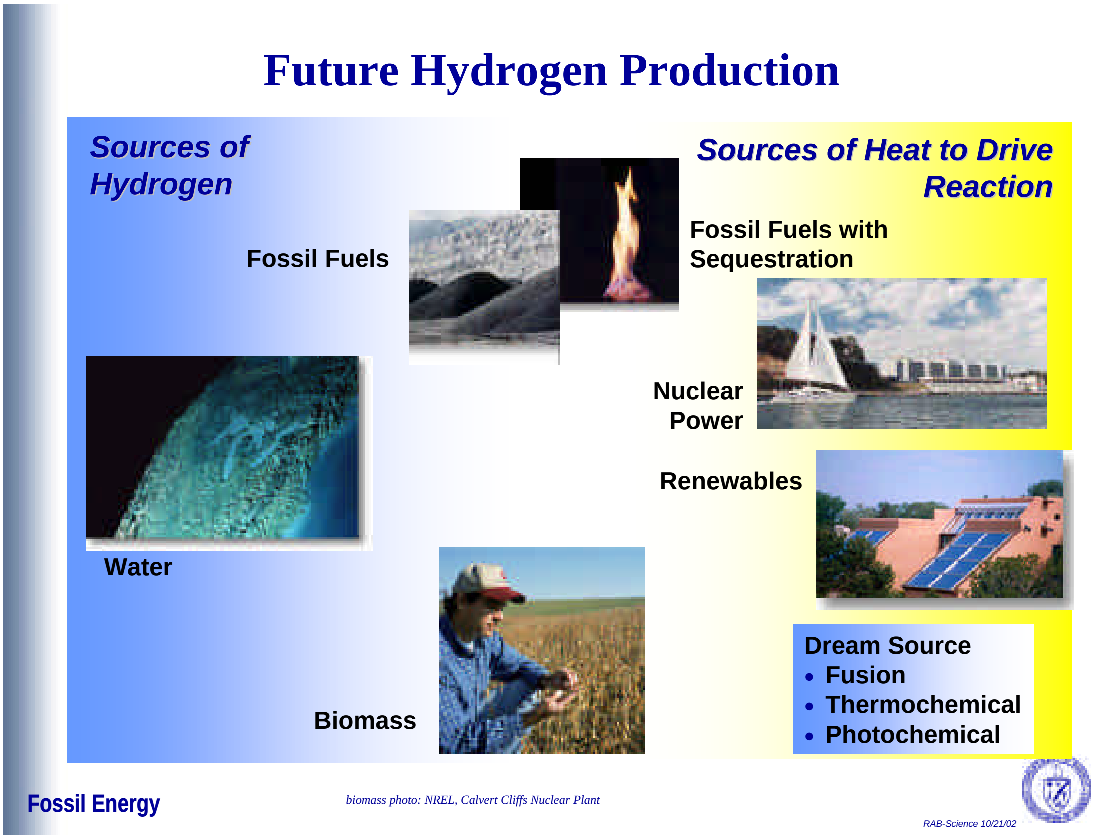
Delivery

Safety

Distribution

Dispensing Systems

Air Products



Future Hydrogen Production

Sources of Hydrogen

Fossil Fuels

Water

Biomass

Sources of Heat to Drive Reaction

Fossil Fuels with Sequestration

Nuclear Power

Renewables

Dream Source
- Fusion
- Thermochemical
- Photochemical

Fossil Energy

biomass photo: NREL, Calvert Cliffs Nuclear Plant

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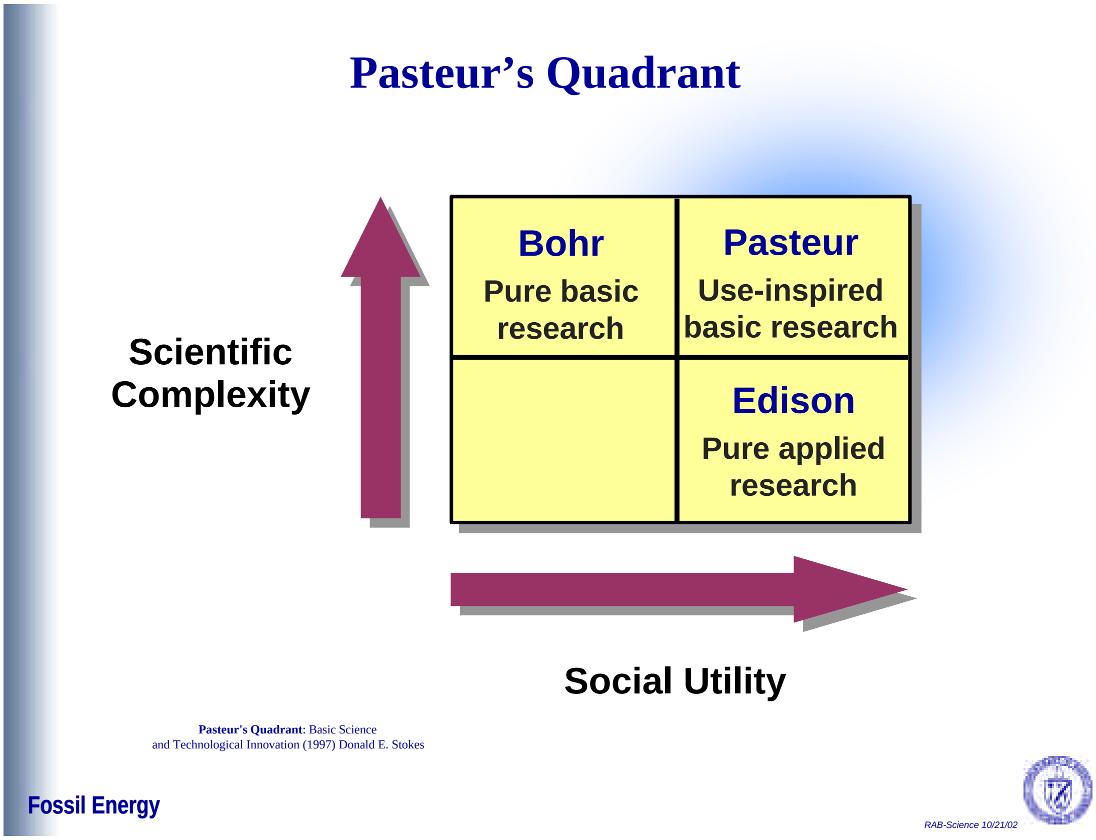

Pasteur's Quadrant

Scientific Complexity

Bohr Pure basic research	**Pasteur** Use-inspired basic research
	Edison Pure applied research

Social Utility

Pasteur's Quadrant: Basic Science and Technological Innovation (1997) Donald E. Stokes

Fossil Energy

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The Short List

Fossil Energy Basic Research Needs

- **Materials**
  - Alloys
  - Ceramics
- **Sensors & controls**
- **Self healing systems**
- **Robotic systems**
- **Computational techniques**
- **Geologic interactions**
  - Water
  - CO_2
  - Gas,oil, coal

Innovative Sequestration Approaches

Issue	**Approach**
• **Scarcity of innovative concepts in program** • **Traditional FE R&D performers more engineering oriented**	• **Engage best minds in nation!** • **National Academy of Science to assist in proposal preparation** – NAS roll-out meeting Feb. 03 • **National Lab involvement encouraged**

Seek Out of the Box Solutions!

Advanced Technologies Can Resolve the Environmental, Supply, and Reliability Constraints of Producing and Using Fossil Fuels

Fossil Energy

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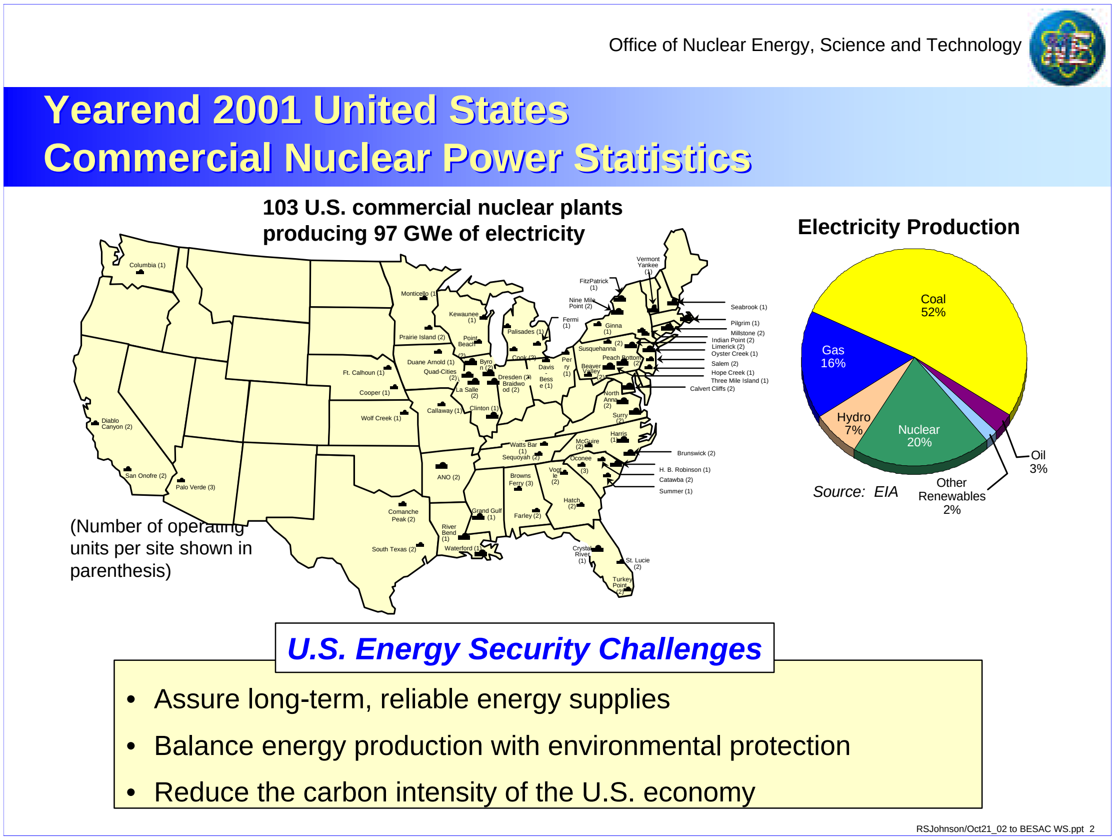
Basic Research Needs in Support of Advanced Nuclear Reactor and Fuel Cycle Technologies

Basic Energy Sciences Advisory Committee Workshop on
“Basic Research Needs to Assure a Secure Energy Future”
Gaithersburg, MD,
October 21, 2002

R. Shane Johnson
Associate Director for Advanced Nuclear Research
Office of Nuclear Energy, Science and Technology



Yearend 2001 United States Commercial Nuclear Power Statistics

103 U.S. commercial nuclear plants producing 97 GWe of electricity

(Number of operating units per site shown in parenthesis)

Electricity Production

Source: EIA

U.S. Energy Security Challenges

- Assure long-term, reliable energy supplies
- Balance energy production with environmental protection
- Reduce the carbon intensity of the U.S. economy

Nuclear Energy -- Practical, Achievable Solutions to Difficult Issues of the Future

Benefits of Nuclear

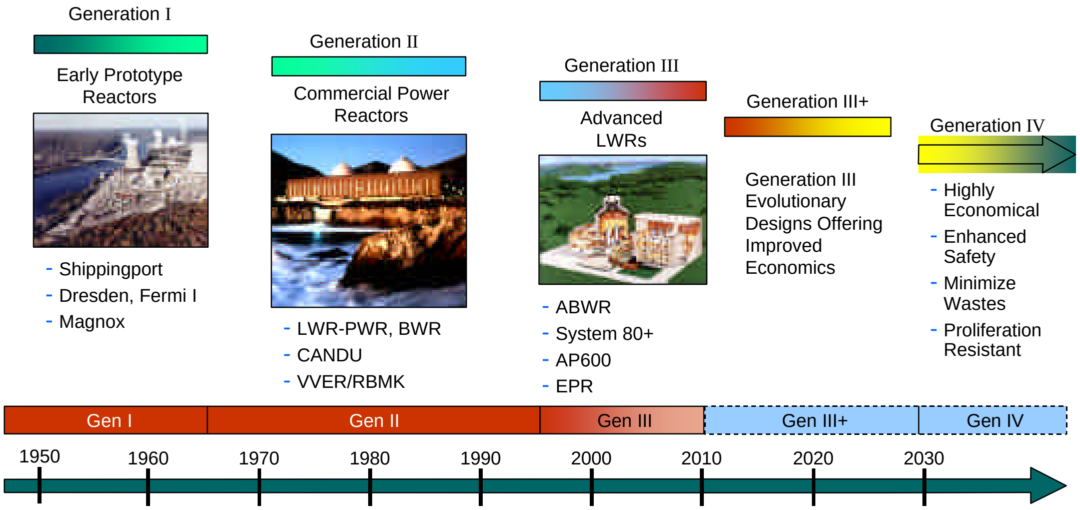
- **Clean – no CO_2, NO_x, SO_x emissions**
- **Low Generating Cost**
- **Compact, manageable waste stream**
- **Stable and secure fuel supply**
- **Sustainable – could be a thousand-year energy resource**
- **Potential for hydrogen production as a transportation fuel**

Challenges for New Nuclear

- **Innovative nuclear concepts push technological boundaries**
- **Higher temperatures, new coolants, new materials, new fuel cycle technologies**
- **U.S. nuclear R&D infrastructure weakened**
- **Bringing new, advanced nuclear technologies to reality will require government leadership**

Three Generations of Nuclear Energy - Thoroughly Demonstrated

The Evolution of Nuclear Power



Generation I

Early Prototype Reactors

- Shippingport
- Dresden, Fermi I
- Magnox

Generation II

Commercial Power Reactors

- LWR-PWR, BWR
- CANDU
- VVER/RBMK

Generation III

Advanced LWRs

- ABWR
- System 80+
- AP600
- EPR

Generation III+

Generation III Evolutionary Designs Offering Improved Economics

Generation IV

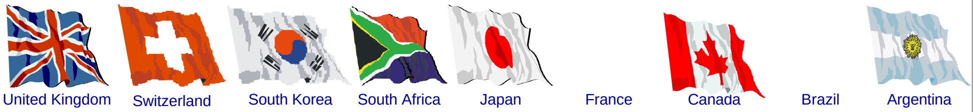
- Highly Economical
- Enhanced Safety
- Minimize Wastes
- Proliferation Resistant

Generation IV Technology Roadmap

- Identifies systems deployable by 2030 or earlier
- Specifies six systems that offer significant advances towards:
  - Sustainability
  - Safety and reliability
  - Proliferation resistance and physical protection
  - Economics
- Summarizes R&D activities and priorities
- Provides foundation for Generation IV R&D program plans

Generation IV Candidate Systems:

- Very-high-temperature gas-cooled reactor
- Gas-cooled fast reactor
- Supercritical-water-cooled reactor
- Lead-cooled fast reactor
- Sodium-cooled fast reactor
- Molten-salt reactor



U.S.A. United Kingdom Switzerland South Korea South Africa Japan France Canada Brazil Argentina

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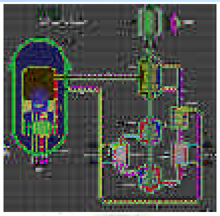
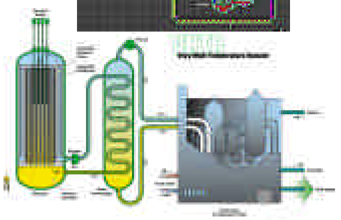
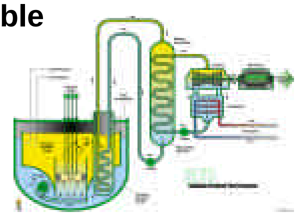
Generation IV Systems R&D Challenges

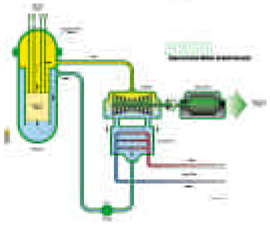


- New materials bearing up under new operating regimes, chemical environments, and fast-neutron irradiation
  - Alternative coolants
    - Supercritical water
    - Gas coolants such as helium, supercritical CO_2
    - Liquid metals such as sodium, lead, lead-bismuth
    - Molten salt
  - Higher pressure and temperature regimes
  - Greater fast-neutron damage



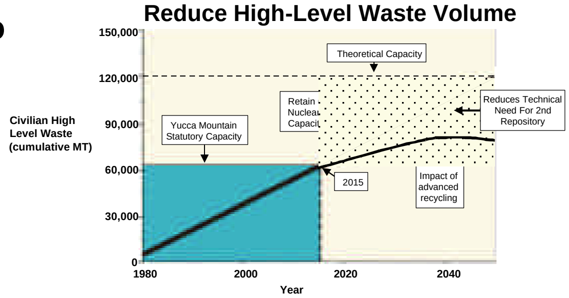
- New nuclear fuel forms capable of surviving power and temperature excursions
- New spent-fuel separation and recycling processes

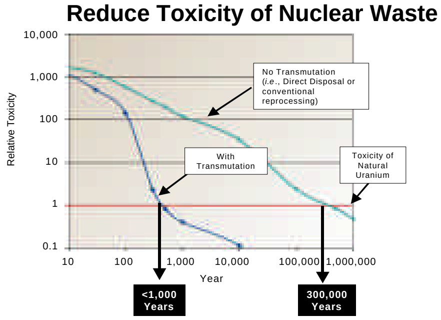




Advanced Fuel Cycle Research - Maximizing Energy From Nuclear Fuel

- **Develop the technologies to**
  - reduce commercial high-level waste by a factor of four by 2015
  - reduce long-term radiotoxicity and heat load of spent fuel by 2030
- **Reduce proliferation risk through destruction of plutonium in existing and future reactors**
- **Enable a decision to forgo a second repository while still supporting expanded nuclear power in the United States**


Reduce High-Level Waste Volume

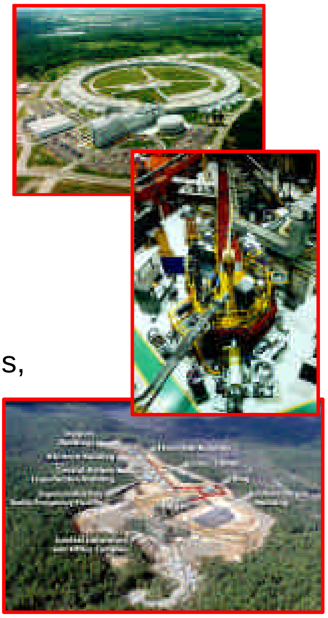

Reduce Toxicity of Nuclear Waste

Advanced Fuel Cycle R&D Challenges

- **Advanced separation chemistry and processes that:**
  - minimize waste volume
  - minimize losses
  - are proliferation resistant
  - minimize dose to workers
- **Advanced fuels for transmutation systems**
  - ceramic fuel in inert metal matrix (cermet)
  - dispersion fuel in inert matrix
  - ceramic, metal and particle fuels
- **Subcritical multiplier for accelerator transmutation**
  - demonstrate safety of configuration
  - materials and coolant for spallation target


Spallation Neutron Source

Basic Science Support



Foundations for Support

- Provide the fundamental understanding of materials and chemistry that support the development of next-generation reactor and fuel cycle systems
- Provide projects at the university level that engage students in R&D that showcase a relevance to advanced reactor development
- Maintain critical infrastructure for fundamental studies, including the ability to work on radioactive materials
- Encourage the development and application of advanced computational tools (e.g. multi-scale material modeling) toward advanced nuclear application

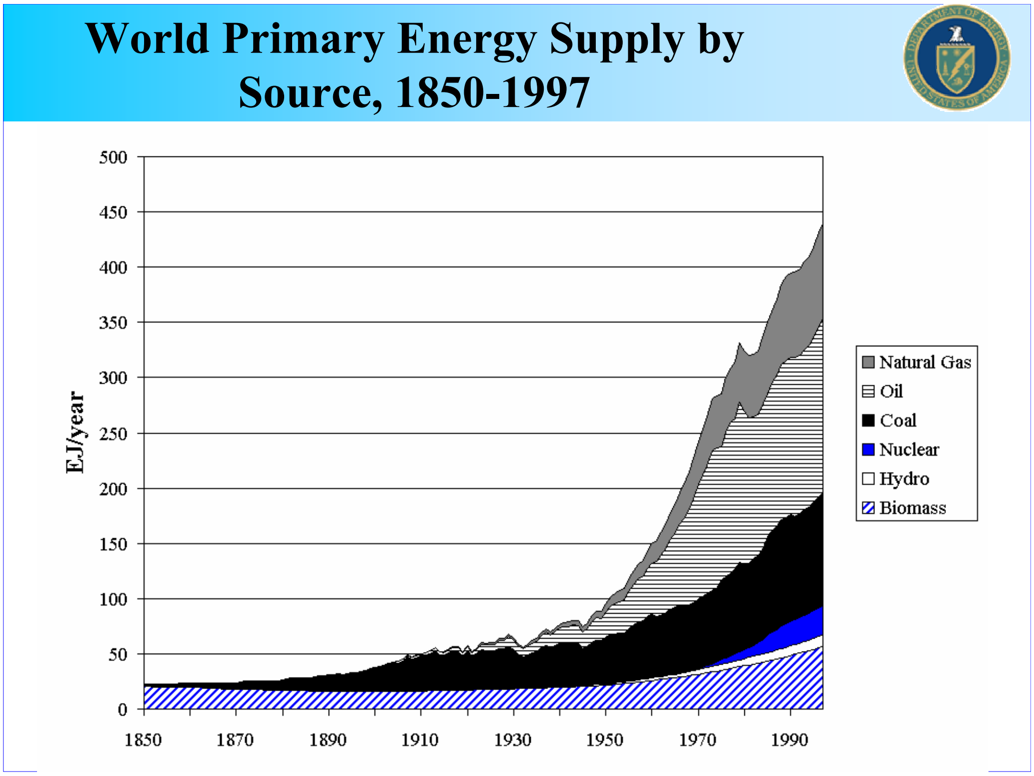
Basic Science Support

Specific Areas

- Radiation-stable materials for high temperature application (ferritic-martensitc alloys, ceramics and ceramic composites, refractory metals, coatings) to include welding and joining.
- Complex microstructural evolution in engineering materials (complex alloys) under irradiation
- Corrosion of structural materials in supercritical water undergoing radiolysis
- Corrosion of structural materials in lead and lead-bismuth.
- Advanced actinide chemistry that simplifies the number of processing steps (*e.g.,* group extraction using designer molecules)
- Materials for minimizing loss in the recycle process
- Fundamental understanding of the processing and physical properties of nitride fuel

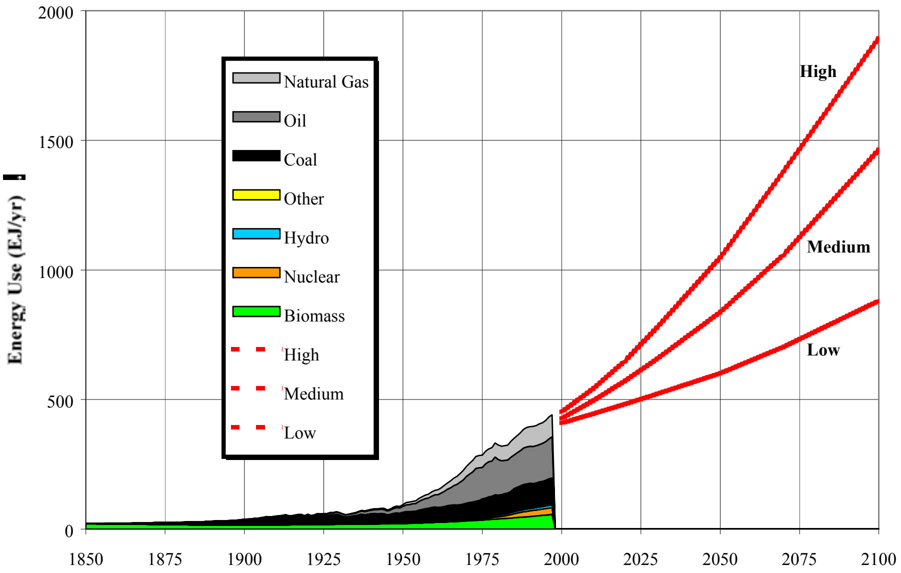
Science Issues in the Office of Energy Efficiency and Renewable Energy

Sam Baldwin
Chief Technology Officer and Member, Board of Directors
Office of Energy Efficiency and Renewable Energy
U.S. Department of Energy
October 21, 2002



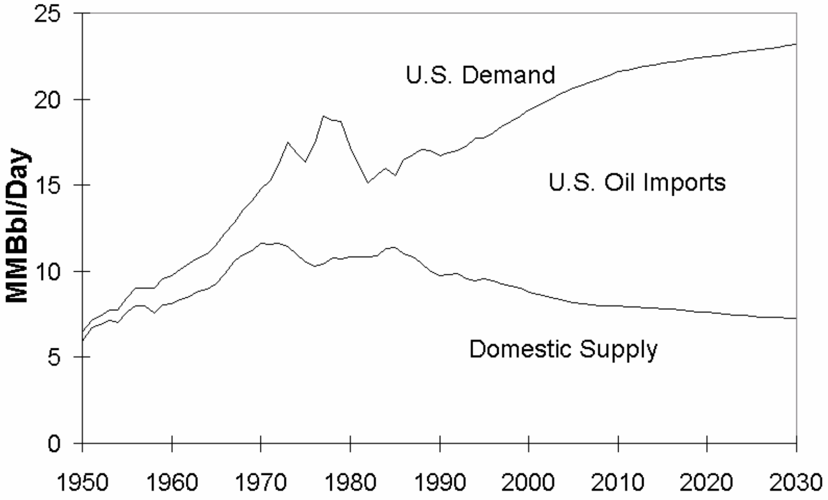
World Primary Energy Supply by Source, 1850-1997

Projections of Energy Use



The Oil Gap

(Business-as-usual)



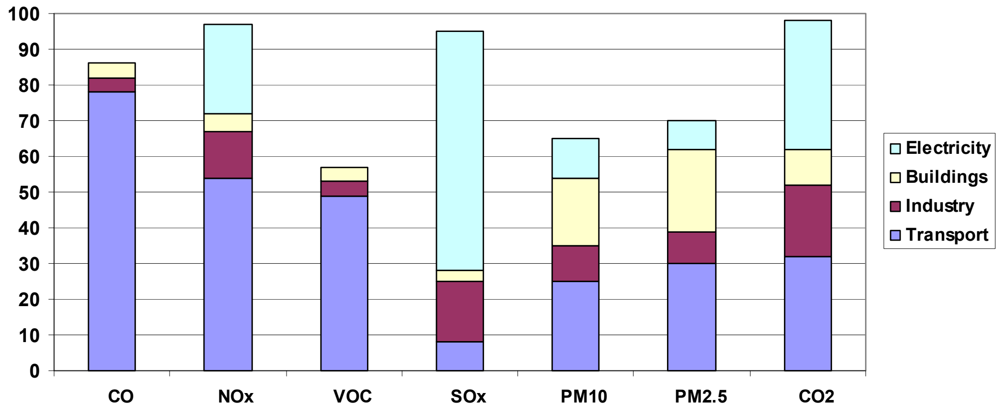
The Oil Problem

Nations that HAVE oil (% of Global Reserves)	
Saudi Arabia	26%
Iraq	11%
Kuwait	10%
Iran	9%
UAE	8%
Venezuela	6%
Russia	5%
Mexico	3%
Libya	3%
China	3%
Nigeria	2%
U.S.	2%

Nations that NEED oil (% of Global Consumption)	
U.S.	26%
Japan	7%
China	6%
Germany	4%
Russia	3%
S. Korea	3%
France	3%
Italy	3%
Mexico	3%
Brazil	3%
Canada	3%
India	3%

Source: EIA International Energy Annual 1999

U.S. 1998 Energy-Linked Emissions as Percentage of Total Emissions



EERE Vision, Mission, and Goals

Vision: A prosperous future where energy is clean, abundant, reliable, and affordable.

Mission: Strengthen America's energy security, environmental quality, and economic vitality through public-private partnerships that:

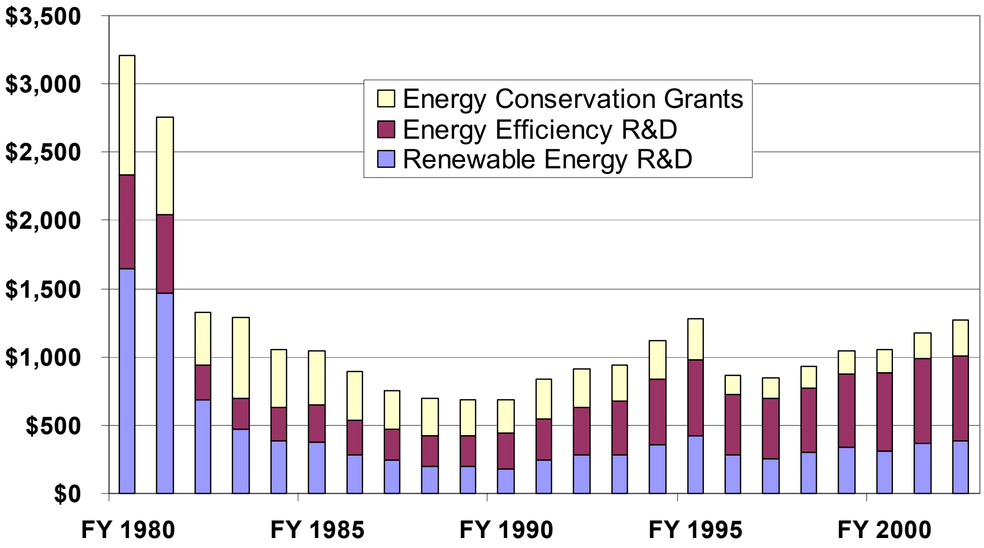
- Promote energy efficiency and productivity;
- Bring clean, reliable, and affordable energy technologies to the marketplace;&
- Make a difference in the everyday lives of Americans by enhancing their energy choices and their quality of life.

Goals:

1. End dependence on foreign oil.
2. Reduce burden of energy prices on disadvantaged.
3. Increase viability and deployment of renewable energy.
4. Increase reliability and efficiency of electricity generation.
5. Increase the efficiency of buildings and appliances.
6. Increase the efficiency/reduce the energy intensity of industry.
7. Create the new domestic bioindustry.
8. Lead by example through Government's own actions.
9. Change the way that EERE does business.

EERE Budgets 1980-2002

Millions of 2000$



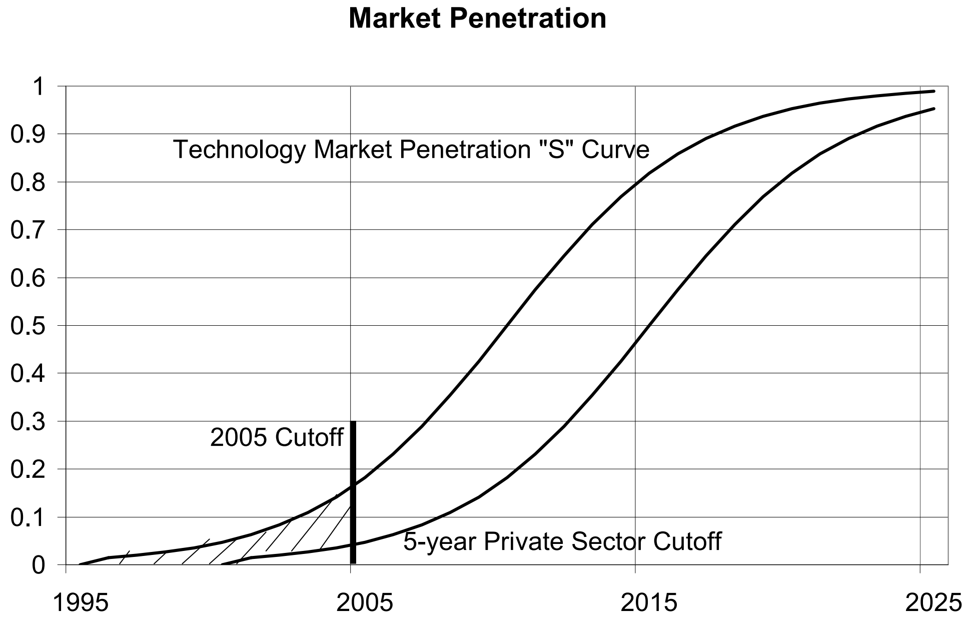
Strategic Program Review of EERE

- **Historic Performance**
  - Patents, Awards, Technical accomplishments
- **Performance-based**
  - Technology push to market pull; components to integrated systems
  - Competitive solicitations; Goals, metrics, milestones; Peer review; Graduations and terminations
- **Public-Private Partnerships**
  - Partnering
  - Contracting
  - Cost-sharing
- **Costs and Benefits**
- **Business Performance**

NRC Benefits/Costs Framework

	Realized **Benefits and Costs**	**Options** **Benefits and Costs**	**Knowledge** **Benefits and Costs**
Economic Benefits and Costs			
Environmental Benefits and Costs			
Security **Benefits and Costs**			

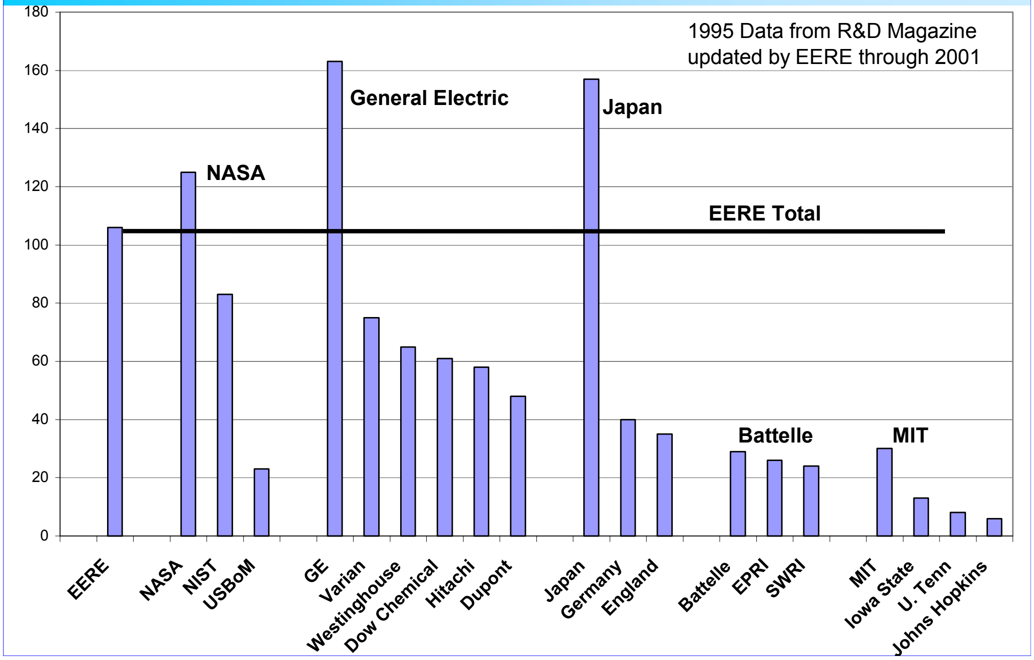
NAS Benefits Analysis Framework



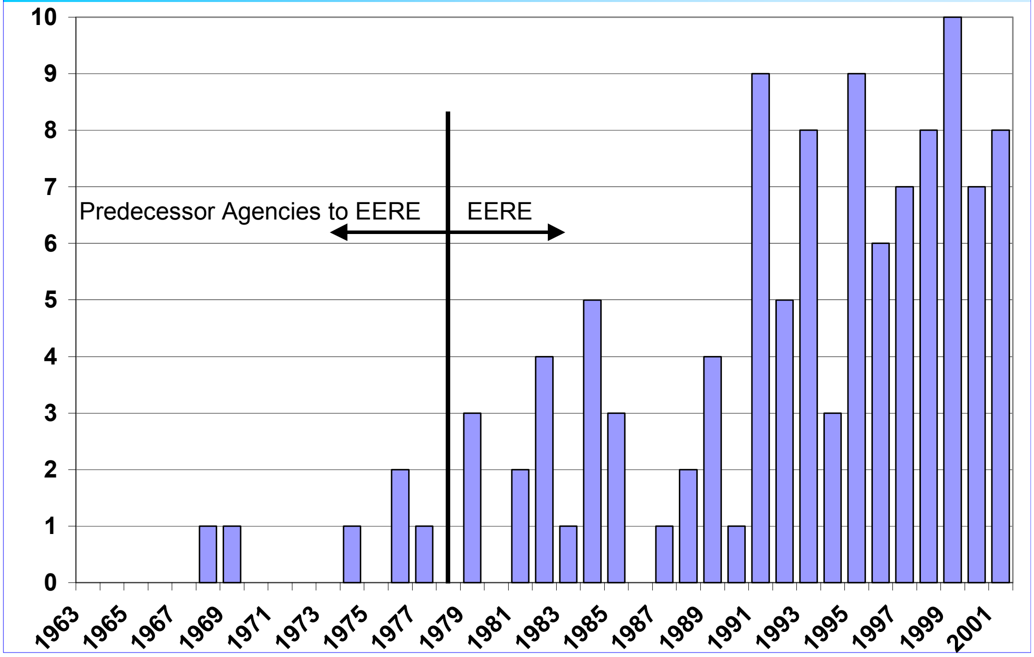
Benefits

- **NAS analysis**
  - $30 B net realized economic benefit on portfolio of $1.6B R&D;
  - NAS estimated additional environmental benefit of $3-$20 billion
- **Technologies to examine**
  - Buildings: Advanced refrigerators/freezers; Spectrally selective windows; Condensing Gas Furnaces; Flame Retention Head Oil Burner; DOE-2; Indoor Air Quality; Energy Star, Low-Income Weatherization; Codes and Standards: refrigerators/freezers, A/C, clothes washers, clothes dryers, dishwashers, water heaters, furnaces, electronic ballasts.
  - FEMP
  - Industry: Direct Steelmaking; Intermetallic Alloys, 140 technologies tracked
  - Transport: Catalytic converters for CIDI, heavy diesels, transportation materials—structural ceramics and lightweight materials; advanced batteries
  - Power: Biopower, Geothermal, Photovoltaics, Wind,

R&D100 Awards by Organization



R&D100 Awards for EERE Sponsored R&D



SPR Recommendations

- **Closures:** activities that should be closed because the work has been successfully completed and no significant further government role is needed (graduations), or does not provide sufficient public benefits (terminations).
- **Redirections:** activities that potentially provide appropriate public benefits but need redirection and/or redefinition to increase the probability of success.
- **Watch List:** activities that need close monitoring to ensure that they advance effectively and expeditiously.
- **Expansions:** activities not currently receiving adequate support in comparison to the benefits they can provide.
- **Best Practices:** actions to improve overall program performance.

Criteria for Judgments

- **Projected Benefits** (economic, environmental, security, options) vs investment
- **Projected potential for commercialization** by industry**.**
- **Whether industry could or would do the RD3 by itself**
- **Program effectiveness (**technical performance, business management, etc.)

http://www.eren.doe.gov/pdfs/strategic_program_review.pd

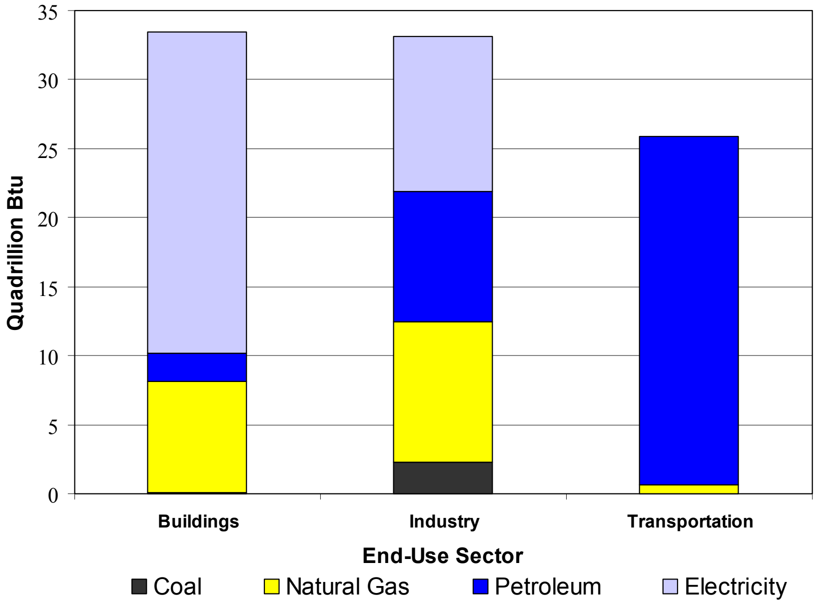
EERE Programs

- Solar
- Wind & Hydropower
- Geothermal
- Distributed Energy, Electricity Infrastructure and Reliability
- Biomass
- Industrial Technologies
- FreedomCAR & Vehicle Technologies
- Hydrogen, Fuel Cells & Infrastructure
- Building Technologies
- Weatherization & Intergovernmental Grants
- FEMP

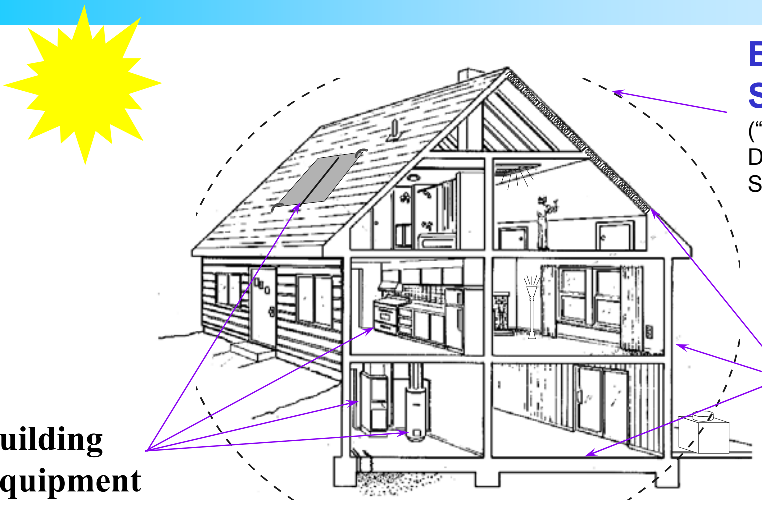
Budget by Program

	FY01	FY02	FY03 Req	FY03 House Floor	FY03 Senate Cmte
Biomass		111,581	108,944	114,944	125,439
Building Technologies		64,449	60,563	68,195	76,563
DEER		131,901	131,290	148,790	136,452
FEMP		20,321	26,425	21,925	26,425
FreedomCAR & Vehicles		181,352	153,563	195,963	181,253
Geothermal		27,098	26,500	26,500	28,300
Hydrogen & Infrastructure		76,317	97,381	96,476	100,500
Industrial Technologies		101,539	92,677	112,677	100,677
Solar		87,107	79,625	79,625	87,000
Weatherization & Intergov.		329,761	374,053	363,655	350,953
Wind & Hydro		38,598	48,986	51,489	56,489
Facilities & Infrastructure		4,870	5,000	5,000	6,800
TOTAL, EERE	1,175,236	1,282,635	1,318,651	1,377,585	1,369,803

Energy Consumption by End-Use Sector & Source - 1999



BUILDINGS



Building Systems
("whole-systems")
Design tools
System Integration

Building Equipment
Space conditioning
Lights
Appliances
BIPV, PEM-FC

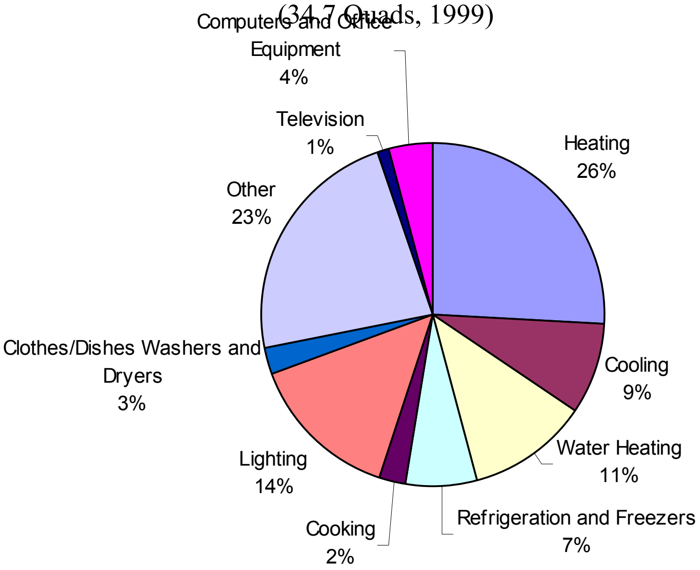
Building Envelope
Windows

Buildings consist of a complex system of interacting components facing variable input conditions

Materials Intensity

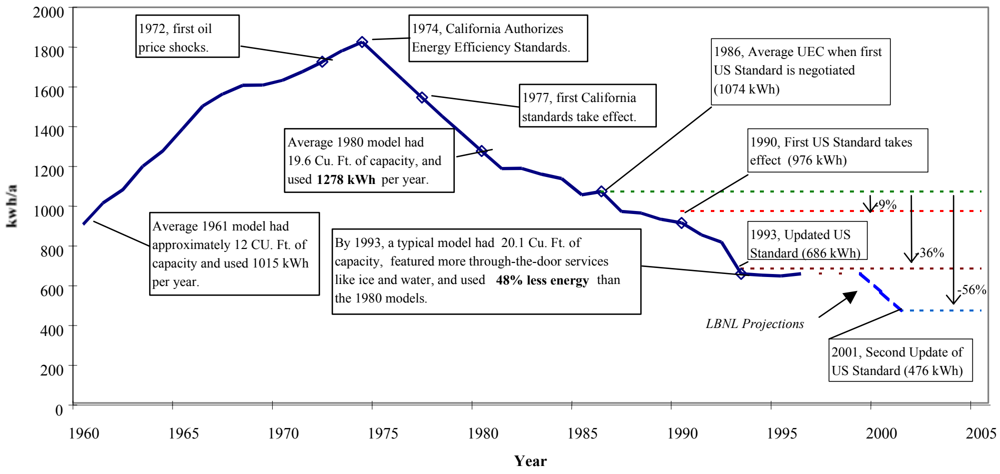
Residential and Commercial Building Energy Use

(34.7 Quads, 1999)



U.S. Refrigerator Energy Consumption

(Average energy consumption of new refrigerators sold in the U.S.)



1972, first oil price shocks.

1974, California Authorizes Energy Efficiency Standards.

1986, Average UEC when first US Standard is negotiated (1074 kWh)

1977, first California standards take effect.

Average 1980 model had 19.6 Cu. Ft. of capacity, and used **1278 kWh** per year.

1990, First US Standard takes effect (976 kWh)

Average 1961 model had approximately 12 CU. Ft. of capacity and used 1015 kWh per year.

By 1993, a typical model had 20.1 Cu. Ft. of capacity, featured more through-the-door services like ice and water, and used **48% less energy** than the 1980 models.

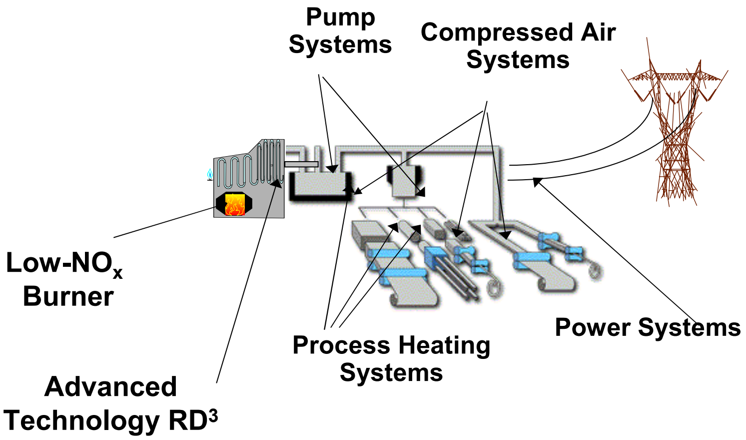
1993, Updated US Standard (686 kWh)

2001, Second Update of US Standard (476 kWh)

Science In the Buildings Sector

- **Advanced Refrigeration, Air Conditioning (FCVs):** (CFCs=>HFCs)
  - Magnetocaloric effect with Gd-Si-Ge alloys; Nd-Fe-B permanent magnets
- **Advanced Lighting**
  - LEDs, OLEDs, multiphoton phosphors (no Hg), nanostructured filaments
- **Windows**
  - Spectrally selective coatings, electrochromics
- **Power Electronics, Sensors, Controls**
  - Low-loss electronics
- **Water Heaters**
  - UV-, temperature-, and pressure-resistant polymers

Industry



Pump Systems

Compressed Air Systems

Low-NO$_x$ Burner

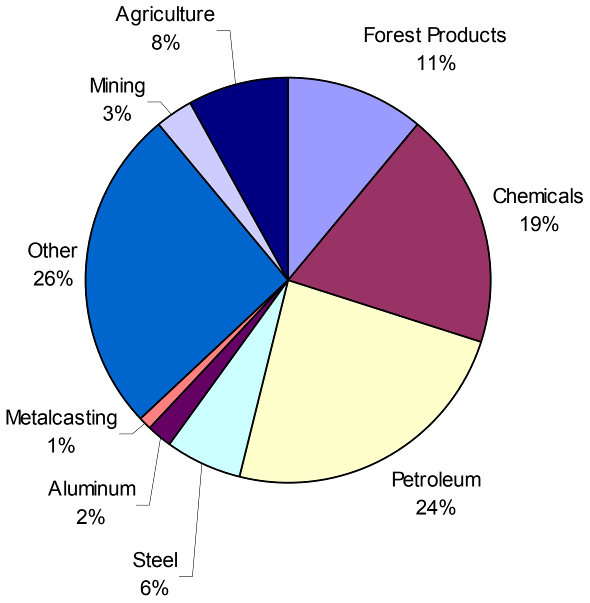
Advanced Technology RD^3

Process Heating Systems

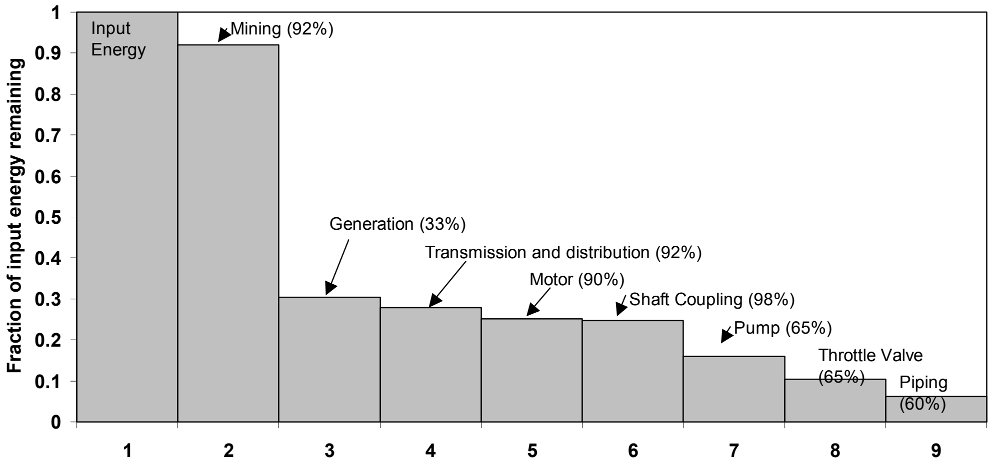
Power Systems

Industrial Energy Use

(35 Quads, 1999)



System Energy Use



Science Needs

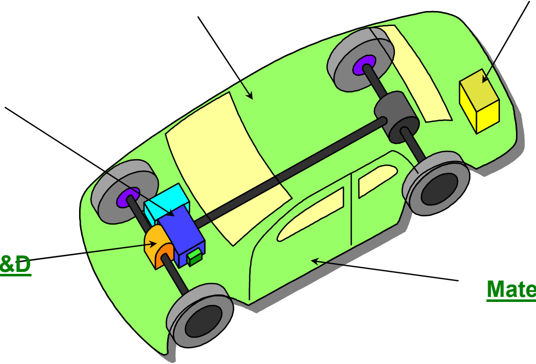
- **Resource extraction:** Remote Sensing (3-D Seismic), Hard materials (PCD drill bits)
- **Generation:** Combustion, Ceramics, Fuel Cells
- **T&D:** Efficient transmission lines; low-loss transformer cores (aSiFe)
- **Motors:** Magnetic materials (NdFeB)
- **ASDs:** Power electronics, sensors, controls
- **Pumps, piping:** Computational fluid dynamics.

Leverage

Science in the Industrial Sector

- **Advanced Materials; Advanced Processes**
  - Longer lifetimes, substitutes; advanced processing techniques
- **Efficient, high temperature separations**
  - High temperature membranes, filters; Separation in multicomponent systems
- **Improved process control**
  - Sensors (high operating temperatures, sensitivities)
- **Chemical, petroleum refining operations**
  - Heterogeneous catalysis/surface chemistry; homogeneous catalysis/metalorganic chemistry; separation science; materials properties/synthesis; diagnostics
- **Boilers, furnaces, gasifiers**
  - Efficiency, emissions, gas cleanup: Combustion science; chemistry
- **Industrial process flows, heat transfer, etc.**
  - Multiphase flows, heat transfer, etc.: Computational fluid dynamics.
- **Metal castings**
  - Alloys: alloy chemistries, properties, processing: Materials Science
  - Rapid, non-destructive evaluation of alloy chemistry/properties: Diagnostics

Transportation Technology



Hybrid Systems R&D

Heavy Vehicle Systems R&D

Fuels Utilization R&D

Biofuels

Advanced Combustion Engine R&D

Fuel Cell R&D

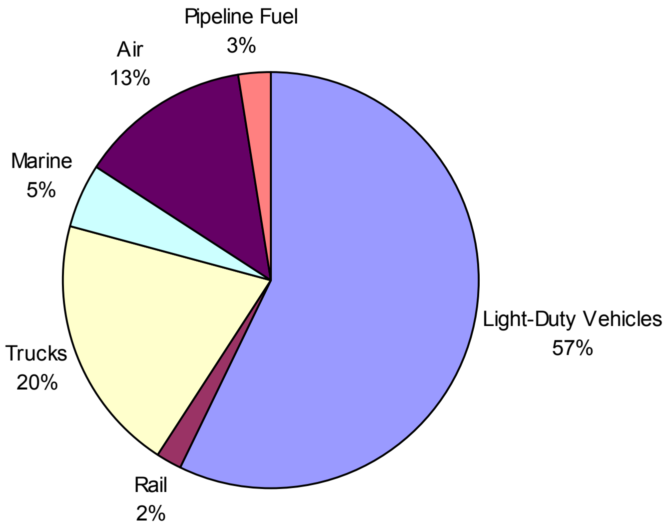
Electric Vehicle R&D

Material Technologies

Transportation Technology Assistance

Transport Energy Use

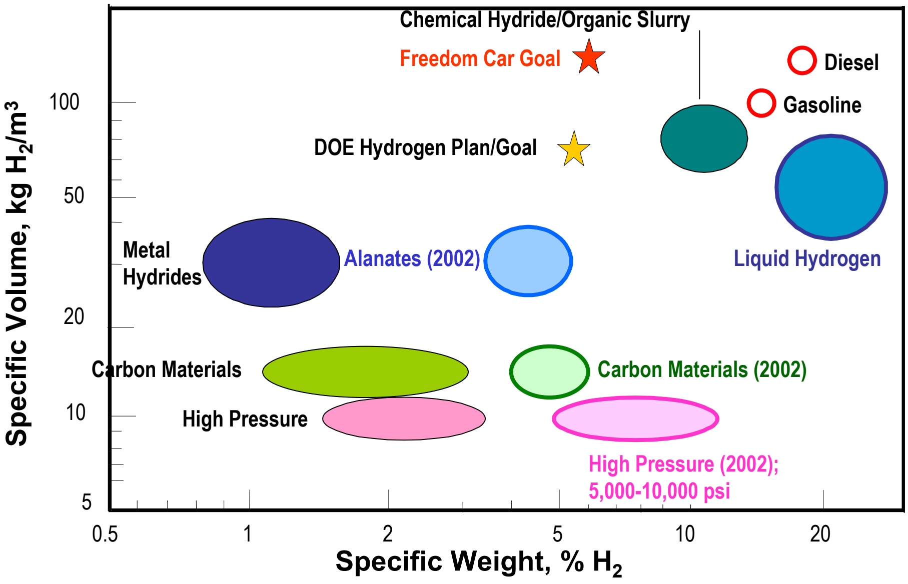
(26 Quads, 1999, 96.7% petroleum)



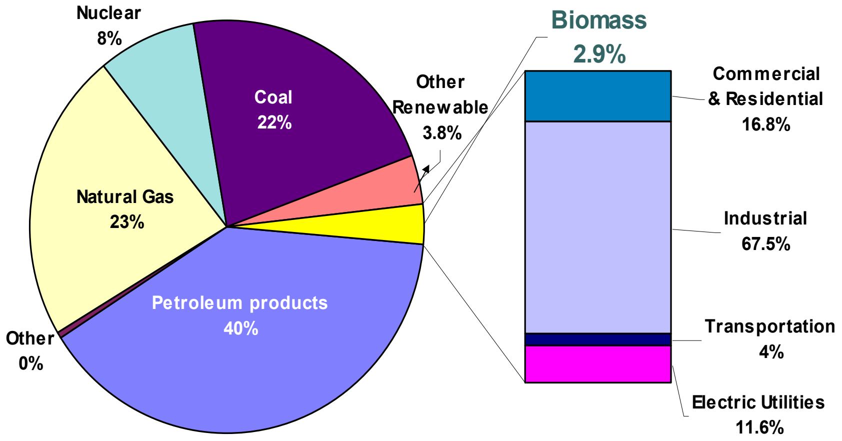
Science in the Transport Sector

- **Advanced Fuels:** petroleum-based, biomass-based
- **Hydrogen production and storage**
  - Fossil fuels; biomass; nuclear; solar; solar thermochemical (S-I, other cycles)
  - Carbon nanostructures, chemical hydrides.
- **Fuel Cells:** Cost, platinum loading, fuel processing/reformers, water/air mgmnt
  - Electrocatalysis, ionic transport in polymer electrolytes, fuel processing catalysis
- **High performance engines**
  - Real-time, high sensitivity multispecies measurements => Diagnostics.
  - Soot formation and evolution => Chemistry
  - Lean NOx catalysts w. high conversion rate over a wider exhaust temp range
  - Low speed flows; turbulence; multiphase flows => CFD
- **Aerodynamic drag**
  - Low speed flow; turbulence => CFD
- **Frames**
  - Composite materials => Materials Science
- **High Power Energy Storage**: Cost ($300), Life (15 yrs), Abuse Tolerance
  - Electrochemistry
- **Advanced Motors/Power Electronics**: Cost ($4/kW, $7/kW), Reliability (15y)

Hydrogen Storage Goals



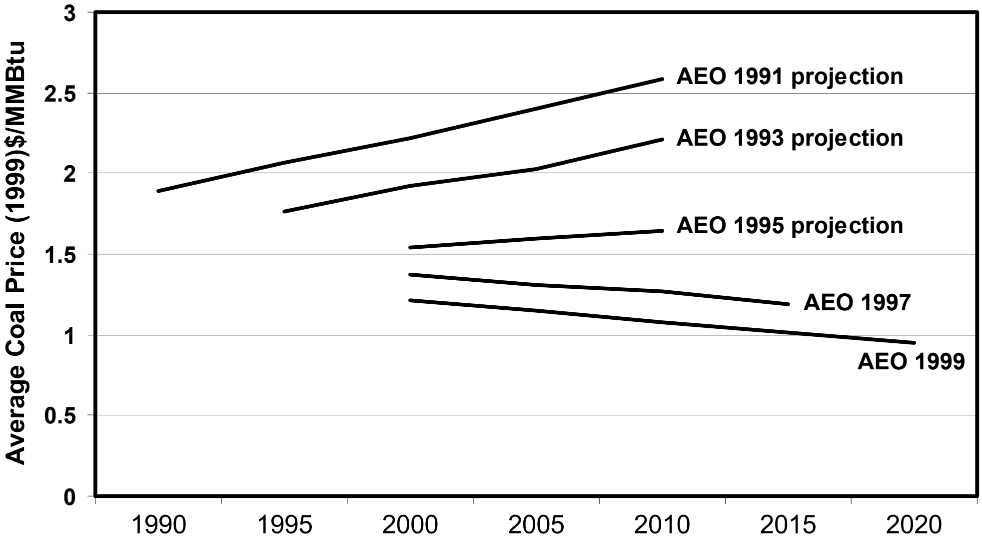
Bioenergy



Total Consumption = 96 Quads
Biomass = 2.9 Quads

Research Design

EIA AEO Coal Price Projections



Biorefinery

Biomass Feedstock

- Trees
- Forest Residues
- Grasses
- Agricultural Crops
- Agricultural Residues
- Animal Wastes
- Municipal Solid Waste

Conversion Processes

- Acid Hydrolysis/Fermentation
- Enzymatic Fermentation
- Gas/liquid Fermentation
- Thermochemical Processes
- Gasification/Pyrolysis
- Combustion
- Co-firing

USES

Fuels:
Ethanol
Renewable Diesel
Methanol
Hydrogen

Electricity

Heat

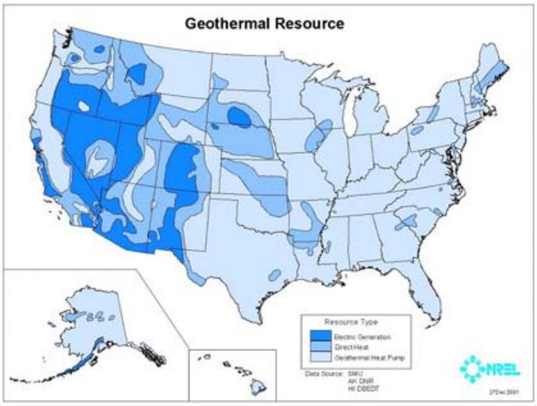
Products
- Plastics
- Foams
- Solvents
- Coatings
- Chemical Intermediates
- Phenolics
- Adhesives
- Fatty acids
- Acetic Acid
- Carbon black
- Paints
- Dyes, Pigments, and Ink
- Detergents
- Etc.

Science in Bioenergy & Bioproducts

- **Feedstock production**
  - Plant growth and response to stress (and on marginal lands)**;**
  - Higher productivity at lower input (water, fertilizer, etc.)
  - Production of certain components and/or new components
  - => Functional genomics; biochemistry; physiology; cellular control mechanisms; respiration; photosynthesis, metabolism, nutrient use, disease response
- **Biochemical pathways**
  - => Biocatalysis: enzyme function and regulation; enzyme engineering; catalyst reaction rates and specificity
- **Thermochemical pathways**
  - => Product-selective thermal cracking of biomass; CFD modeling
- **Bioproducts**
  - => New and novel monomers and polymers;
  - Biomass composites; => adhesion/surface science
- **Combustion**
  - => NOx chemistry; CFD modeling

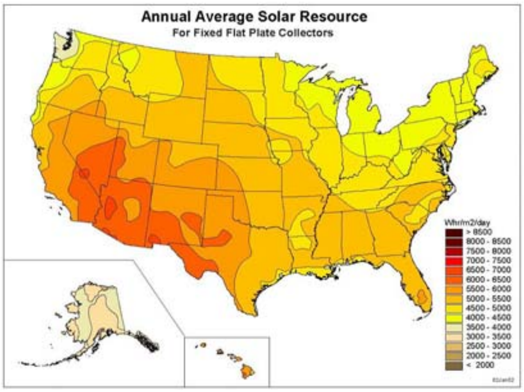
U.S. Geothermal Resource

- **R&D has reduced cost of geothermal power from 15 cents per kilowatt-hour in 1985 to a range of 5-8 cents per kilowatt-hour today.**
- **2007 target: 3-5 cents per kilowatt hour.**

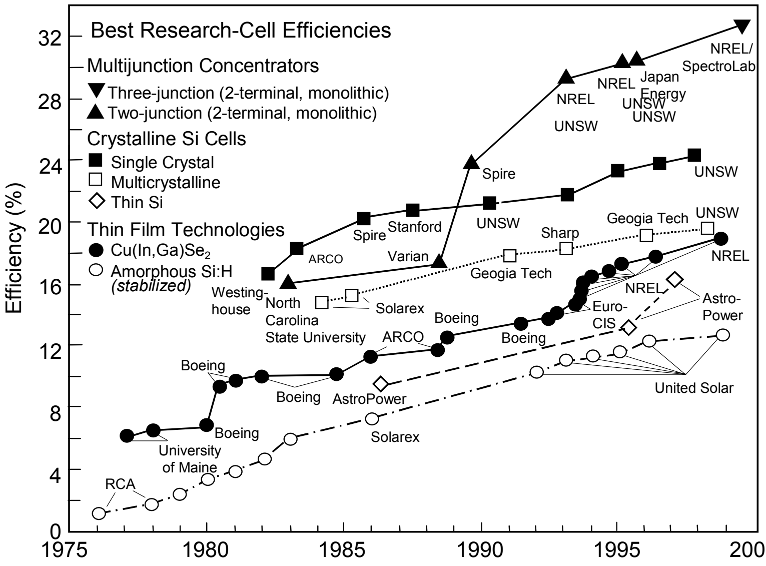


U.S. Solar Resource (PV)

- **R&D has reduced of PV power from $2.00 per kilowatt-hour in 1980 to the current range of 20-38 cents per kilowatt-hour.**
- **2020 target: 5 cents per kilowatt-hour.**

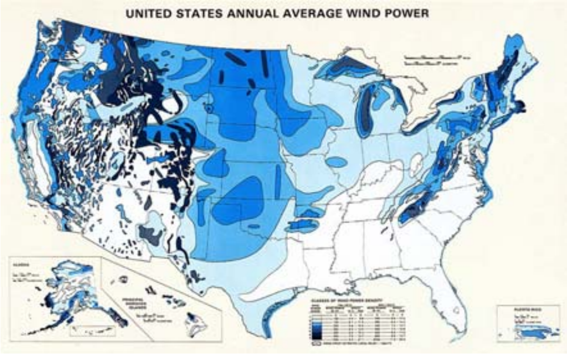


BEST RESEARCH CELL EFFICIENCIES



U.S. Wind Resource

- R&D has reduced cost of wind power from 80 cents per kilowatt-hour in 1979 to a current range of 4-6 cents per kilowatt-hour (Class 6).
- 2010 target: 3 cents per kilowatt hour (in Class 4 and above regimes.
- New R&D focus: low speed wind tech.; x20 resource; x5 proximity



Science in the Power Sector

- **Photovoltaics**
  - Materials, growth, characterization,
  - multi-junction thin films—interface chemistry, physics, defects, materials compatibility; Quantum dot cells, multiple quantum well devices, etc.
- **Geothermal**
  - Geoscience: formation/flow of fluids through fractured media; characterizing geology; geochemistry; remote sensing
- **Wind**
  - Computational fluid dynamics to model turbulent flow for wind turbine design
  - Modeling meso-scale atmospheric phenomena for wind forecasting for utilities
  - Composite materials—materials strength, fatigue properties
- **HTS**
  - Materials, cryogenics
- **Remote sensing**
  - algorithms for determining atmospheric and surface properties (aerosol optical depth, surface insolation, surface winds, bioenergy resources)

Time Constants

Consensus building	**~ 2-20+**
Science	**~10+**
Technical R&D	**~10+**
Production model	**~ 4+**
Financial	**~ 2+**
Market penetration	**~10-20+**
Capital stock turnover	**~15-100+**
– Cars	15
– Appliances	10-20
– Industrial equipment/facilities	10-30/40+
– Power plants	40
– Buildings	40-80
– Urban form	100’s
Lifetime of Greenhouse Gases	**~100’s-1000’s**
Reversal of Land Use Change	**~100’s**
Reversal of Extinctions	**Never**

APPENDIX E

SUMMARY PRESENTATIONS

Topical Team Summary

Fossil Energy

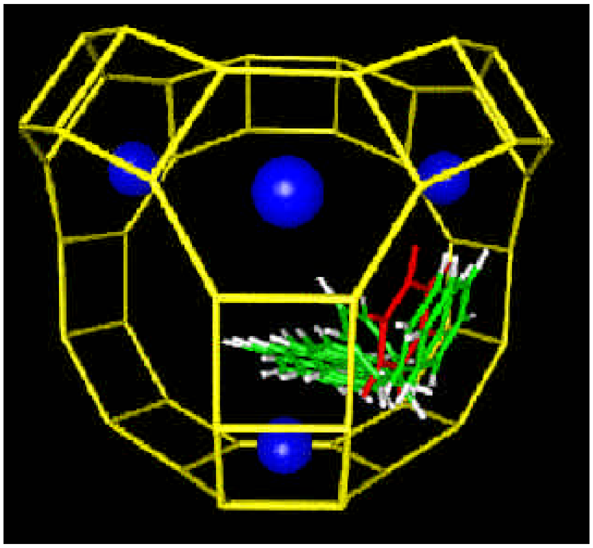
Fossil Energy Topical Team

Marvin Singer (Chair)
Tim Armstrong, ORNL
Tof Carim, BES
Cindy Dogan, Albany Res Lab
David Keith, CMU
Tina Nenoff, SNL
Eric Suuberg, Brown U
Anbo Wang, VPI
John Wimer, NETL
Mike Bockelie, Reaction Eng.
Bob Carling, SNL
Brian Gleeson, Ames/U of Iowa
Larry Myer, LBNL
Doug Ray, PNNL
Roger Turpening, BES
Nick Woodward, BES

Proposed Research Directions

1. Reaction Pathways of Inorganic Solid Materials: Synthesis, Reactivity, Stability
2. Advanced Subsurface Imaging and Manipulation of Fluid-Rock Interactions
3. Development of an Atomistic Understanding of High Temperature Hydrogen Conductors
4. Development of Predictive Fuel Conversion Models

Reaction Pathways of Inorganic Solid Materials: Synthesis, Reactivity, Stability



Benefits: inorganic solid materials with predicted properties

Status: “Edisonian” Approach

Obstacles: reaction pathways (kinetics, binding energies, thermodynamics) are not well understood

Challenges: governing rules for behavior of inorganic solids

Exploit the synergy **between experimentation (inelastic neutron scattering) & theoretical simulations (QM and Monte Carlo methods) in heterogeneous catalysis.**

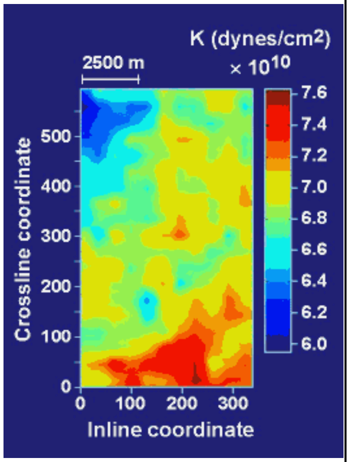
Advanced Subsurface Imaging and Manipulation of Fluid-Rock Interactions

Benefits: Increased production of domestic oil and gas resources along with the ability to tap unconventional gas reservoirs

Status: Production in continuous decline

Obstacles: Poor images of the subsurface, poor in information content, poor in resolution, and poor in registration. Most of the hydrocarbons remain trapped in the pore space.

Challenges: Imaging challenge--deployment of sensors, of all techniques, in the subsurface. Modify interfacial surface energies.



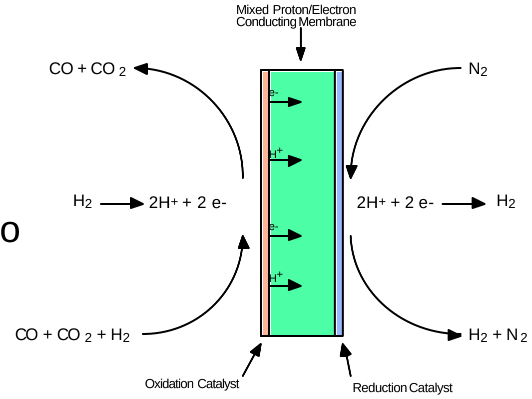
Development of an Atomistic Understanding of High-Temperature Hydrogen Conductors

Benefits: high flux, stable proton conductors

Status: Current proton conductors suffer from low conductivity and poor chemical stability - current approaches “Edisonian”

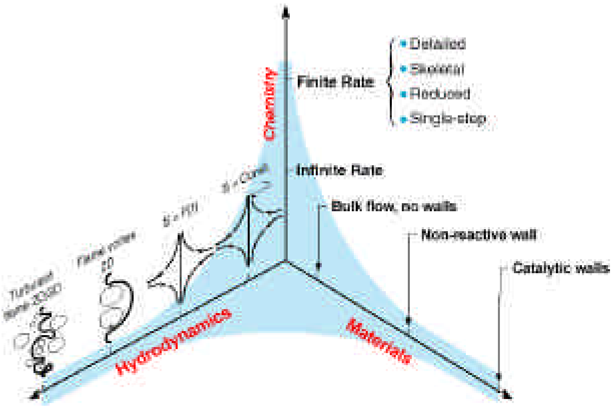
Obstacles: Need new materials, models to guide development and characterization methods to determine conduction mechanisms

Challenges: Development of models to predict H_2 conduction in materials



Development of Predictive Fuel Conversion Models

Combustion operates at the intersection of chemistry, hydrodynamics, and transport with approximations made along each axis



Benefits: Improved combustion devices

Status: Current models don’t adequately describe today’s experimental results

Obstacles: New codes to capture time-dependent events

Computer resources

Challenges: Development of the science base for simulation and validation

Topical Team Summary

Nuclear Fission Energy

Nuclear Fission Energy Topical Team

John Ahearne, Sigma Xi (chair)*
Allen Croff, ORNL (acting chair)
Ralph Bennett, INEEL*
Bob Gottschall, DOE/SC-BES
Andy Klein, Oregon State
Frank Goldner, DOE/NE
John Taylor, EPRI*
Neil Todreas, MIT*
Todd Allen, ANL-W

Jim Beitz, ANL
Bill Millman, DOE/SC-BES
Jack Richards, Cal Tech
Rob Versluis, DOE/NE
Brian Wirth, LLNL
Bill Weber, PNNL
Mike Kassner, Oregon State

*Did not attend workshop

Background

- Nuclear fission currently provides 20% of U.S. electricity safely and reliably
- In light of expected population growth and energy demand and the expected need for large quantities of hydrogen produced without contributing to adverse climate change, nuclear fission is expected to be a critical component of the future energy mix

Background

- Current light water reactors are the first generation of commercial nuclear fission based technology. Technological improvements are desired in the areas of:
    - Sustainability-waste impact and fuel utilization
    - Safety and reliability
    - Economics
    - Proliferation resistance and physical protection

Background

- Generation IV initiative has identified six technologies that have the potential to meet the four goals
- Successful deployment of these technologies relies on significant advancements in
    - Materials-high temperature, unique coolants
    - Actinide chemistry-support recycle
    - Fuels-high temperature, support recycle
    - Heat transfer

Key Issue-1

Issue: Decade-long under-investment in science relevant to nuclear fission resulting from lack of interest in nuclear fission

Response: Need to invest in nuclear-related physical science topics, further incorporating available and emerging state-of-the-art tools and approaches: neutron scattering, light sources, advanced computing

Key Issue-2

Issue: Commonality of science investments across nuclear fission and other energy sources

Response: One size does not fit all

- Some areas have much commonality, e.g., fluid flow, hydrogen production cycles
- Other apparently similar areas are very different, e.g., materials degradation because of the effects of radiation and unique hostile environments

Approach to identifying PRDs-1

Review technology issues stemming from the “big four” nuclear fission issues: proliferation, cost, waste disposal, safety and environment

Round-table definition of potential PRDs based on previous topical group input and participant views

Discuss potential PRDs; refine and combine where appropriate

Approach to identifying PRDs-2

Select “top several” based on vote excluding DOE/SC staff

Sanity check: Any major problem with what is below the cut line

Documentation

- PRD write-up
- Coordination disposition of potential cross-cuts

First Priority PRD

Materials degradation: mechanical and chemical degradation of cladding, reactors, and waste package components. Examples

- Multiscale modeling of the complex microstructural development of alloys and ceramics and the relationship of these highly non-equilibrium changes to mechanical, dimensional stability, and corrosion properties
- Fundamental understanding of intergranular cracking in irradiated components
- These challenges amplified by the extreme environments envisioned by Generation IV
- Multiple year stability of nuclear waste packages.

Second Priority PRD

Actinide and fission product chemistry: to support a sustainable recycle system. Examples:

- Designer molecules for selected proliferation resistant group extractions
- Green chemistry to minimize waste impact
- Development of deliberately designed ligands (ion channels of biological membranes or carbon nanotubes) for improvements in mining and extraction techniques

Third Priority PRD

Fuel behavior: for advanced high temperature fuels

- Behavior of novel fuel forms to harsh environments (high temperature, radiation, stress). These include nitride fuels, metallic fuels, dispersion fuels, and non-fertile (inert matrix) fuels.
- Influence of recycle products on fuel behavior including radiation response
- Multiscale modeling of fuel behavior (similar to materials issues in PRD 1)

Fourth Priority PRD

Heat transfer: Examples

- Eliminate use of engineering correlation by developing a first principles understanding of multi-phase heat transfer and fluid flow mechanisms (including supercritical water, lead-alloy coolants, molten salts)
- Understanding of fluids with dispersed particles (i.e. nanofluid suspensions)

Other Cross-Cutting Candidates

Hydrogen generation chemical cycles
- Chemical cycles that work at lower temperatures

Welding and joining
- For high-temperature, high-strength materials

Multifunction materials
- Self-monitoring or self-healing

Direct energy conversion
- Processes and materials

Potential PRDs Considered

11	Actinide and fission product processing chemistry
11	Materials degradation: mechanical
11	Materials degradation: chemical
7	Heat transfer
5	Fuel behavior
5	Hydrogen generation
3	Welding and joining
2	Fundamental effects of radiation on biological organisms
2	Processes/materials for direct energy conversion to electricity
2	Evaluation and condition monitoring in harsh environments
1	Educating the public
0	Remote, non-invasive sending
0	Sub-critical transmutation systems
0	Beneficial uses of depleted uranium
0	Multifunctional materials
0	Human factors and advanced instrumentation
0	Small reactors
0	Integrated power supplies
0	Extraction of energy from waste repositories
0	Synergistic energy sources
0	Infrastructure support

Topical Team Summary

Renewable and Solar Energy

Renewable and Solar Energy Topical Team

George Crabtree, ANL (Chair)	Extra Attendees
Sam Baldwin, EE	Tom Baker, LANL
John Cooke, ORNL	Dan Ginosar, INEEL
Jerry Hunt, ANL	Mack Kennedy, LBNL
Lonnie Ingram, Univ. of Florida	Joe Paladino, NETL
Lary Kazmerski, NREL	Sharlene Weatherwax, DOE-BES
Nate Lewis, Cal Tech.	Jane Zhu, DOE-BES
Jeff Mazer, EE	
Arthur Nozik, NREL	
Jay Spivack, GE	

Key Issues

Total energy/yr in 2000: 13 TW

Carbon free energy/yr required in 2050: 10-30 TW

Grand Challenges in basic research

> enable renewable use at this level

Proposed Research Directions

- Develop functional genomics and biochemistry for the tailoring of plants and microorganisms to increase the production of fuels and chemicals by 100-fold.
- Develop methods for solar energy conversion that result in a10-50 fold decrease in the cost-to-efficiency ratio for the production of fuels and electricity.
- Develop the knowledge base to enable the widespread creation of geothermal reservoirs.
- Effectively convert solar, wind and geothermal energy into stored chemical fuels.
- Cross cutting: Design and synthesize new classes of complex materials, including hybrids that integrate organic, inorganic and biological to revolutionize the development of renewable technologies.

Develop functional genomics and biochemistry for the tailoring of plants and microorganisms to increase the production of fuels and chemicals by 100-fold.

Genetic tailoring for materials, fuels, and chemicals

- understand limitations of plant efficiency
- improve energy efficiency - less water, nutrients, and land
- greater range of cultivation- salt tolerance and stress resistance
- rational design of enzymes for depolymerization of plant constituents
- simplify bioconversion process
- engineering of plants and microbes to produce renewable biomaterials and chemicals

Develop methods for solar energy conversion that result in a 10-50 fold decrease in the cost-to-efficiency ratio for the production of fuels and electricity.

Robust for 20 -30 years

Cost of installed photoconversion : $0.20/peak watt of solar radiation

- raise mobility of inexpensive photoconversion materials- polycrystalline, organic semiconductors
- interpenetrating networks- nanoscale charge separation and collector elements
- multiple junctions match solar spectrum, prevent carrier thermalization: efficiency 32% -> 65%
- quantum dots, quantum wells, and organic dyes

Develop the knowledge base to enable the widespread creation of geothermal reservoirs.

Entire western U.S. has high thermal gradient and untapped potential

Developed geothermal reservoirs limited to sites with surface hot water

Challenge: create geothermal reservoir where no fracture network exists

- create fracture network remotely
- map fracture network remotely
- understand interaction of injected fluid with fractured rock matrix
- develop materials and coatings for drilling above 300°C and 500-1000°C

Effectively convert solar, wind and geothermal energy into stored chemical fuels.

Solar, wind, and geothermal sources produce electricity far from end use

- convert electricity to storable fuels H_2 and O_2 from water, reduce CO_2 to methanol, ethanol or other C-based fuels
- direct conversion of solar photons to fuels or chemicals from H_2O, CO_2, N_2
- photoactive organic, inorganic, or biological molecules
- absorb solar irradiation and drive chemical reactions

Design and synthesize new classes of complex materials, including hybrids that integrate organic, inorganic and biological to revolutionize the development of renewable technologies

Entirely new classes of materials must be developed to bring renewables on line.

- nanostructures: single wall nanotubes for simultaneous bandgap and charge collection media, hybrid nanotube/metal materials, etc.
- semiconductor quantum dots as photovoltaic media
- organic semiconductors as inexpensive photovoltaics
- p -type transparent conducting oxides
- photocatalysts and photoelectrodes for water splitting
- engineered biosystems that carry out physical processes such as bugs that split water

Proposed Research Directions

- Develop functional genomics and biochemistry for the tailoring of plants and microorganisms to increase the production of fuels and chemicals by 100-fold.
- Develop methods for solar energy conversion that result in a10-50 fold decrease in the cost-to-efficiency ratio for the production of fuels and electricity.
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- Cross cutting: Design and synthesize new classes of complex materials, including hybrids that integrate organic, inorganic and biological to revolutionize the development of renewable technologies.

Topical Team Summary

Fusion Energy

Fusion Energy Topical Team

C.Baker, UCSD (chair)
S. Berk, OFES/DOE
A. Hassanein, ANL
R. Jones, PNNL
E. Rohling, BES/DOE
S. Willms, LANL
S. Zinkle, ORNL

Additional contributors-
M. Abdou/N.Morley, UCLA
R. Bangerter, LBNL
J. Dahlburg, GA
P. Efthimion, PPPL

Fusion Energy Proposed Research Directions

- Multiscale modeling of microstructural stability of irradiated materials
- Deformation and Fracture Modeling
- BES Research Opportunity in Plasma-Surface Interaction
- Thermofluids and “Smart Liquids”
- BES Research Opportunity in Plasma Aerodynamics

Multiscale modeling of microstructural stability of irradiated materials

- **Brief statement of proposed research topic:** Fundamental research is needed to identify the key physical processes that will enable materials to maintain microstructural stability during prolonged fusion neutron irradiation.
- **New scientific opportunities:** By utilizing physically-rigorous bridging of the gaps between different spatial and temporal modeling regimes (nanoscale to continuum), a comprehensive predictive capability for modeling the stability of prospective advanced nanoscale materials can be attained.
- **Relevance & impact to Fusion Energy and other applied programs:** The successful development of fusion energy will require materials that are capable of withstanding exposure to intense radiation fields over a broad range of temperatures.
- **Estimated time scale:**
  - ~10 years: development of improved interatomic potentials
  - ~ 10 years: multiscale microstructural evolution and nanoscale solute segregation models
  - ~10 years: development of improved physics-based models of radiation-induced or – enhanced solute segregation to interfaces
- **Additional Information:**
  - Development of improved interatomic potentials, including directionality effects, magnetic effects (very important for ferritic steels)
  - Numerous recent molecular dynamics (MD) simulations (using interatomic potentials of dubious quantitative accuracy) have predicted the possibility of long range one-dimensional transport of matter via self-interstitial crowding bundles.
  - Development of physically rigorous multiscale microstructural evolution models based on Molecular Dynamics, kinetic Monte Carlo and kinetic rate theory techniques.
  - Phase stability under irradiation
  - Transport and clustering of He

Deformation and Fracture Modeling

- **Research direction:** New opportunities exist to understand and predict the effects of radiation on deformation and fracture. Multi-scale modeling involving atomistic simulations, mesoscopic simulations, and continuum simulations coupled with greatly expanded computational capabilities allow us to understand phenomena and predict behavior beyond that which has been possible with experimental approaches.
- **New Scientific Opportunities:** The current understanding of radiation effects on deformation and fracture of new materials is inadequate. New multi-scale modeling capability has the potential to make breakthroughs in understanding and designing these new materials.
- **Summary:** Some examples covering both new materials and a description of some well known problems are given below.
  - Nanoscale reinforced materials
  - Advanced radiation resistant ceramic composites
  - Flow localization
  - Atomistics of crack initiation and growth (radiation embrittlement)
  - Initiation and growth of subcritical sized flaws
  - High-temperature deformation mechanisms

BES Research Opportunity in Plasma-Surface Interactions

- **Research Direction:** To increase the basic understanding of critical issues related to plasma-surface interactions including photon radiation transport, “potential” sputtering, and material erosion under intense power loadings.
- **New Scientific Opportunities:** Development deeper understanding and models for key plasma-surface interactions involving intense particle and heat loads.
- **Relevance to DOE Mission:** One of the most important issues concerning the basic feasibility of fusion as an energy source, and a major issue for present-day high-temperature plasma confinement experiments, is the interaction of intense heat and particle fluxes with plasma-facing components. These interactions need to be understood in terms of the basic phenomena so they can be controlled. Potential impacts include contamination of the plasma and short lifetimes of the components.
- **Summary:**
  - ➢ One important area that determines many of the plasma-surface interaction effects is photon radiation transport in both optically thin and optically thick plasmas with intense line populations.
  - ➢ Another important topic is a recently new physical phenomenon that is not well understood is called "Potential Sputtering".
  - ➢ Understanding fundamental models of material erosion and destruction under intense power applications is another vital topic.

Thermofluids and “Smart Liquids”

- **Research Direction:** The proposed research is to develop a fundamental understanding of flowing, electrically conducting fluids in complex environments which include electromagnetic fields. Magnetohydrodynamic forces can affect liquid motion from the largest, integral scales down to the fine scales of turbulence. Ultimately, fluid properties can be tailored so that such “smart liquids” can be shaped and steered in a novel fashion using fields.
- **New Scientific Opportunity:** Computation methods for 3-D direct numerical solution and other methods of incompressible, turbulent, free-surface fluid flow in strong electromagnetic fields
- **Relevance and Impact:** Fusion energy seeks to contain star-like conditions within physical barriers. The environment includes elevated temperatures, radiation and kinetic debris. To solve the resulting materials problems, increasing attention is being given to liquid walls in both magnetic and inertial fusion. Liquids can be pumped through the harsh reactor environment and out to a benign area where liquid refurbishment can be performed. “Smart liquids” may enable unique solutions to directing flow, especially free-surface flow, in complex, fusion reactor geometries.
- **Summary -- Specific Suggestions that might be of interest to BES include the following:**
  - Numerical simulation of the effect of magnetohydrodynamic forces on turbulence in incompressible liquid conductor flows and their related transport of heat and mass, especially at solid and free interfaces.
  - Control of liquid metal flow motion and velocity profiles via applied magnetic and electric fields and currents.
  - Modification and control of fluid properties and behavior via complex chemical doping and micro-additives.

BES Research Opportunity in Plasma Aerodynamics

- **Research Direction:** To developed the basic understanding of the application of weakly ionized plasmas in aerodynamics for control of shock, turbulence, heat fluxes, drag, and related phenomena.
- **New Scientific Opportunity:** Develop new methods to control aerodynamic flows.
- **Relevance:** Weakly ionized air plasmas have a high potential for impact on advanced aerodynamics. Specifically, plasmas and MHD processes may be capable of mitigating peak thermal loads, extracting high levels of power, reducing drag, reducing observability, reducing sonic boom, and suppressing noise.
- **Summary:**
    - Because the plasmas are so expensive in power to establish and sustain, one of the critical areas to understand is the time scale of the phenomena.
    - In many of the plasma aerodynamic applications the presence of instabilities may become a serious limitation.
    - Mechanisms for the efficient creation of air plasmas also need to be understood.
    - Perhaps the most difficult issue is the establishment of scalability relations.

Topical Team Summary

Distributed Energy, Fuel Cells, and Hydrogen

Distributed Energy, Fuel Cells, and Hydrogen Topical Team

Lutgard C. De Jonghe, U. California Berkeley,Chair
Meilin Liu, Georgia Institute of Technology
Joan Ogden, Princeton University
Vitalij Pecharsky, Iowa State University
Philip N. Ross, Lawrence Berkeley National Laboratory
Subhash Singhal, Pacific Northwest National Laboratory
John Turner, National Renewable Energy Laboratory
Douglas Wheeler, UTC Fuel Cells
Mark Williams, National Energy Technology Laboratory

Key BES Topics

- Hydrogen synthesis
- High capacity hydrogen storage
- Novel Membranes
- Designed Interfaces

Hydrogen Synthesis

- Photocatalytic Synthesis of Hydrogen
  Challenge: coupling of light harvesting systems with catalysis to produce hydrogen.

- Thermochemical Water Splitting Driven by Solar or Nuclear Heat
  Challenge: feasible redox cycles

- Fossil Hydrogen Production
  Challenge: advances in catalysis, membranes, gas separation

Photocatalytic Synthesis of Hydrogen

Approach:

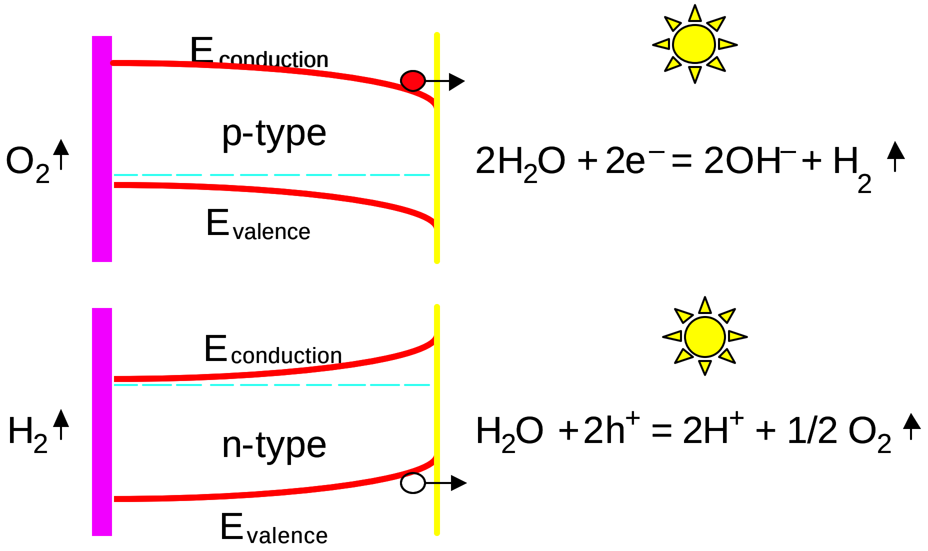
1) semiconductor materials that have appropriate light absorption characteristics and are stable in aqueous solutions.

2) catalytic coatings on semiconductor surfaces.

3) Identification of environmental factors (e.g., pH, ionic strength, solution composition, etc.) that affect the energetics of the semiconductor, the properties of the catalysts, and the stability of the semiconductor.

Photocatalytic Synthesis of Hydrogen

Band Edges of p- and n-Type
Semiconductors Immersed in Aqueous Electrolytes to Form Liquid Junctions



$2H_2O + 2e^- = 2OH^- + H_2$ ↑

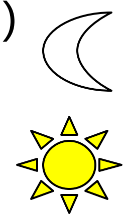
$H_2O + 2h^+ = 2H^+ + 1/2\ O_2$ ↑

Thermochemical Water Splitting

Approach: Thermochemical cycles (typically at ~700-900 C) driving a set of hydrogen producing redox reactions.

Example:

ZZn + H_2O ➔ H_2 + ZnO (dark/cold)
ZZnO + heat ➔ Zn + O_2 (sun)



Range of possibilities:

- Cycling between various oxidation states
- S-I cycles (corrosion issues!)

High Capacity Hydrogen Storage Materials

Challenge:
materials with 10+ percent mass and volume of hydrogen storage capacity

Approach:
replace C in CH_4 with light elements from which hydrogen can be more readily removed and reattached

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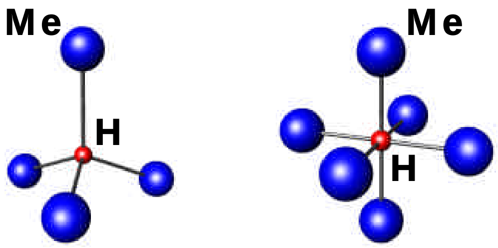
High Capacity Hydrogen Storage

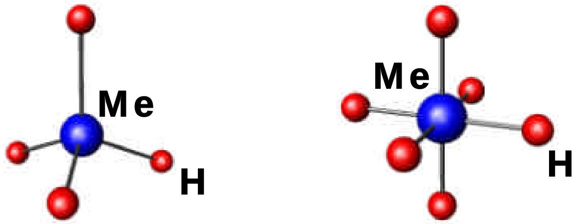


Metal hydrides

From encapsulating hydrogen

to encapsulating **by** hydrogen

Complex metal hydrides
Alanates, Borohydrides….



Novel Membranes

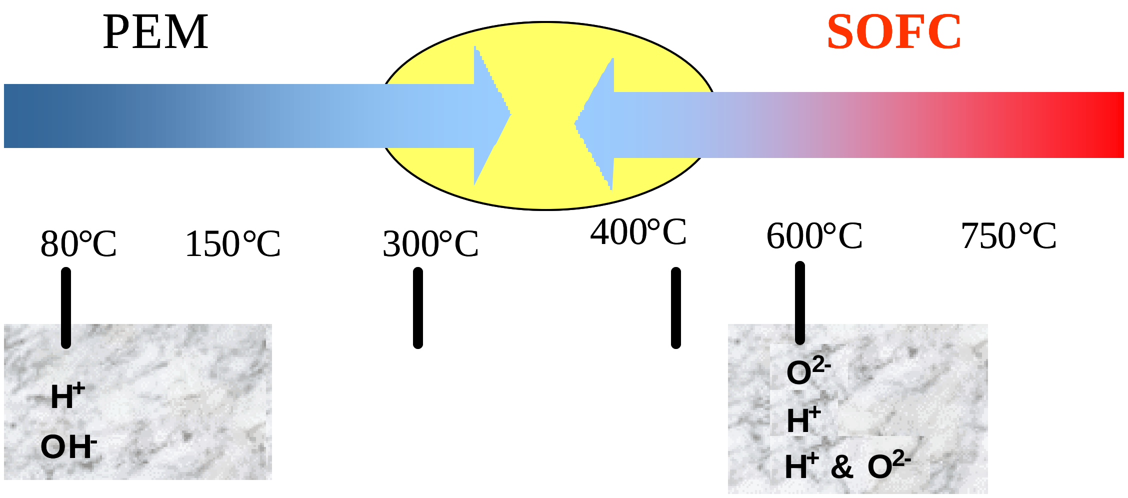
Challenge:

Design ionic and mixed-conducting membranes with high conductivity, stability, and selectivity over a broad temperature range.

Impact:

Increased efficiency and reduced cost of fuel cells, batteries, hydrogen separation/purification, oxygen separation, reforming/partial oxidation of hydrocarbon fuels, contaminant removal, gas sensing, and other processes relevant to energy storage and conversion.

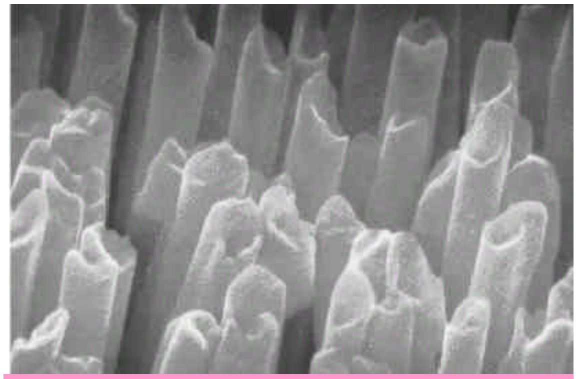
Ionic Membranes for Fuel Cells



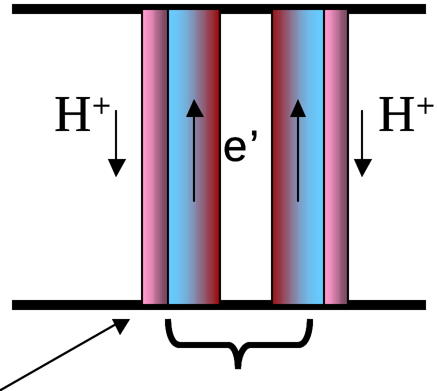
CO-poisoning
Thermal Management
Water Management

Cost Reduction Longer Operations Life Potential for mobile applications

Proton-Electronic Membranes



Proton transport along surfaces of nanotubes

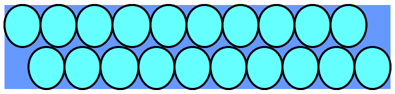


Nanotube for electron transport

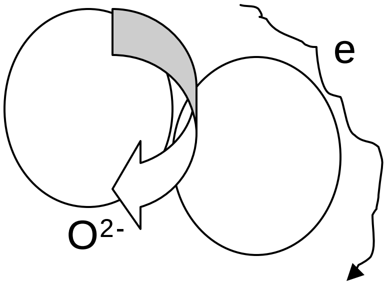
- Hydrogen separation/purification
- Electrodes for fuel cells based on proton conductors

Oxygen Ion-Electronic Membranes

Templated self-assembly of precursors
to form functional membranes and interfaces



Ionic and electronic transport along interfaces



- Oxygen separation
- Reforming/partial oxidation of hydrocarbon fuels
- Cathodes/anodes for SOFCs
- Contaminants removal

Designed Interfaces

Challenge:

The generation and utilization of hydrogen or carbon-containing fuels depends critically on interfaces that need to fulfill specific and often conflicting functions. Among these functions are structural, dimensional and chemical stability, electron, ion, and mass transfer, catalysis, and electrocatalysis, under a wide range of temperature, temperature changes, and gas partial pressures variations. So far the approach has been largely Edisonian. Basic science must develop a reliable roadmap to designing solutions in this multidimensional space.

Proposed approach:

We propose the development of a computational equivalent of combinatorial synthesis, drawing on a multidisciplinary, theory–based approach.

The impact of the combinatorial science is broad. The approach can be of exceptional value in a wide range of energy conversion and generation, separation technology, hydrogen production, and energy storage.

Topical Team Summary

Transportation Energy Consumption

Transportation Energy Consumption Topical Team

Jan Herbst, GM R&D (Chair)
Channing Ahn, California Inst. Tech.
Tarasankar DebRoy, Penn State Univ.
Jim Eberhardt, EE
Ed Grostic, ORNL
Oren Hadaller, The Boeing Company
Kenneth Hass, Ford Motor Company
Joseph Heremans, Delphi Research Labs
Chris Sloane, General Motors

Extra Attendees:
Iver Anderson, AMES
Suresh Baskaran, PNNL
Bill Kirchhoff, DOE-BES
Paul Lessing, INEEL
Paul Miles, SNL
Kevin Ott, LANL
Matesh Varma, DOE- BES

Integrated quantitative knowledge base for joining of lightweight structural materials for transportation applications

- Maximum benefits of lightweight transportation materials will not be achieved without an integrated knowledge base on joining.
- No integrated model exists of the various physical processes that constitute joining such as heat transfer, fluid flow, mass transport, gas sorption, vaporization, solidification, phase transformations, etc.
- Significant advances in computational hardware and models now permit integration of constituent models for the prediction of the response of new materials systems to a selected joining process.
- Integrated models will allow full incorporation of novel materials into future transportation systems with significant gains in fuel efficiency and, hence, enhanced energy security.

Vehicular energy storage

- Widespread use of hydrogen-powered and electric vehicles requires materials having greatly improved energy storage capability
- Current materials are limited in volumetric and/or gravimetric energy density relative to hydrocarbon fuels
  - ➢ H_2 @ 700 atm contains < 14% energy of equivalent volume of diesel fuel and the advanced Ni-M hydride battery only about 10% of that.
- Fundamental understanding of the phase stability, thermodynamics, and kinetics of both hydride and battery materials is needed to enable the discovery and development of new materials that satisfy system requirements.

Fundamental challenges in fuel cell stack materials

- Fuel cells have long been seen to offer the opportunity for high efficiency, pollution-free propulsion to meet the nation’s transportation needs, but persistent technical barriers remain: membrane performance & durability, cathode kinetics, tolerance to contaminants, alternatives to noble metal catalysts,...
- Materials for fuel cells have been developed empirically.
- Achieving higher performance membranes and electrodes requires
  - ➢ Fundamental theoretical understanding and experimental validation of relationships among composition, structure and properties
  - ➢ Accelerated design, novel synthesis and characterization of improved materials
  - ➢ Integrated, predictive, computational chemical & materials models with adequate fidelity for subsequent system optimization

Integrated Heterogeneous Catalysis for Transportation

- Catalytic processes are central to transportation fuel production, storage, utilization, and emissions abatement today and => enhanced US energy security in the future
  - H_2 production (coal, petroleum, natural gas => electrolytic, photolytic, biomass)
  - Liquid fuels (coal, petroleum, nat. gas => biomass, biofuels, tailored high density naphthenic aviation fuels)
  - Fuel cell electrocatalysts (Pt => base metal catalysts, more rapid cathode kinetics, bioinspired O_2 manipulation)
  - Hydrogen storage materials (catalytic uptake and release at appropriate pressures, temperatures, rates in materials of high hydrogen content)
- U.S. energy security will require integrated experimental, theoretical thrusts to enable rational design of heterogeneous catalysts
  - Fundamental, detailed knowledge of active site structure and reactivity: need access to emerging and development of new local structure tools
  - Multiple experimental techniques, high throughput experimentation, modeling and simulation tools
  - Fusion of complementary experimental information to yield coherent description of catalyst active site(s)
  - => Accelerate heterogeneous catalyst design (similar to capabilities available to homogeneous catalysis researchers today)

Thermoelectric materials and energy conversion cycles for mobile applications

- Thermoelectric materials (TEs) offer dual use in transportation systems:
  - Waste heat recovery: potential for ~20% increase in fuel economy
  - Cooling/air conditioning: greenhouse gas free; potential to exceed efficiency of vapor compression
- Realization of high-efficiency TEs requires
  - Improved theoretical understanding of electrical & thermal transport in semiconductors, esp. nanostructures and low thermal conductivity systems
  - Discovery and synthesis of materials with high Seebeck coeff. and electrical conductivity, low thermal conductivity
- Opportunities for new TE module configurations

Complex Systems Science for Sustainable Transportation

- Sustainability of US transportation system
  - Challenging problem: petroleum dependence, complex interdependencies among system components
  - System = fuels + vehicles + infrastructure + policies + behaviors…
  - Technological advances alone may not be good enough
- Complex systems science
  - Building conscilience among disparate fields (including physical, biological, computer, economic, behavioral sciences – e.g., genetic computer algorithms)
  - Emphasis on nonlinear, holistic, nonequilibrium behaviors
- Long-term basic research required to develop fundamental concepts, tools, and cross-disciplinary insights into non-traditional energy/transportation problems
  - An immediate example is the creation of a robust strategy for transporting nuclear waste from distributed sources to the Yucca mountain disposal site

Topical Team Summary

Residential, Commercial, and Industrial Energy Consumption

Residential, Commercial, and Industrial Energy Consumption Topical Team

Millie Dresselhaus (MIT, Chair)
Sam Baldwin (EE)
Hylan Lyon (Marlow Industries)
Gerald Mahan (Penn State Univ.)
Anne Mayes (MIT)
Steve Selkowitz (LBNL)
Jerry Simmons (SNL)
Harriet Kung (BES)
Aravinda Kini (BES)

Panel Members with Phase I Task:
Paul Alivisatos (UC, Berkeley)
Sam Bader (ANL)
Terry Michalske (SNL)

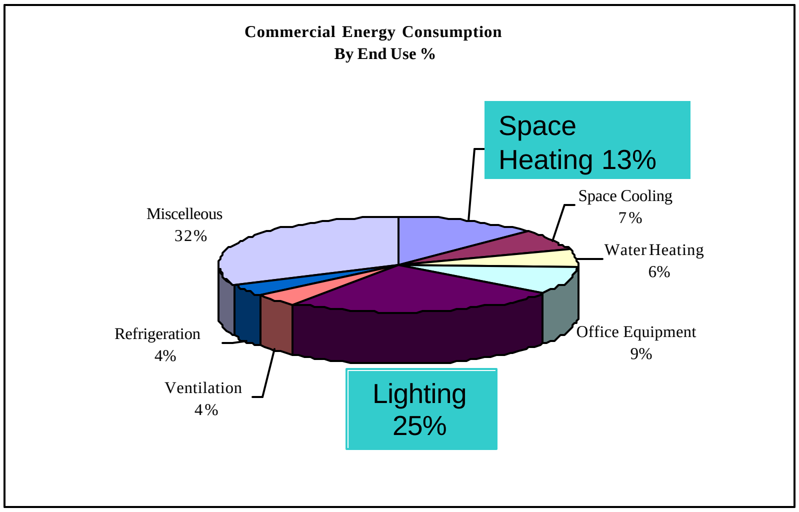
Speakers:
Dr. Anil Duggal (GE)
Dr. Jerry Simmons (SNL)
Prof. Woods Haley (UMN)
Dr. Ron Judkoff (NREL)
Dr. Ertugrul Berkcan (GE)
Dr. Dickson Ozokwelu (DOE/EE)
Prof. Vitalij Pecharsky (Ames/Iowa State)

Considerations for Selection of PRDs

- Importance of problem for energy security
- Potential of PRD to have impact on solving identified problem
- Potential of PRD to have impact on solving other problems of interest to DOE
- Potential for advancing science broadly
- PRD should lead to a new revolutionary technology

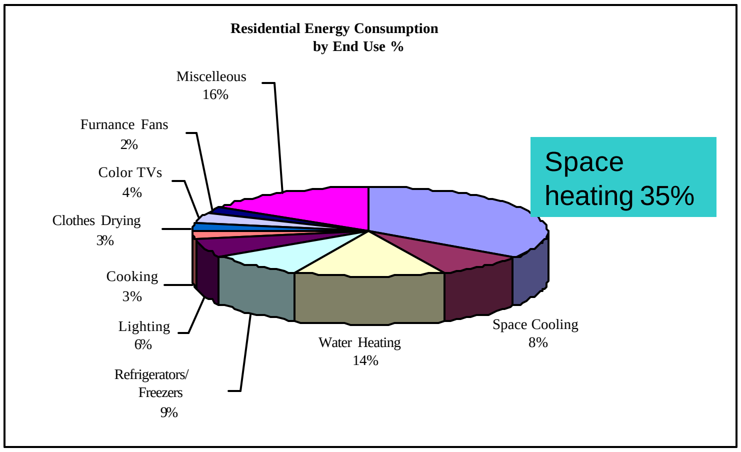
Commercial Energy Consumption

- Lighting is largest usage
- Second is space heating

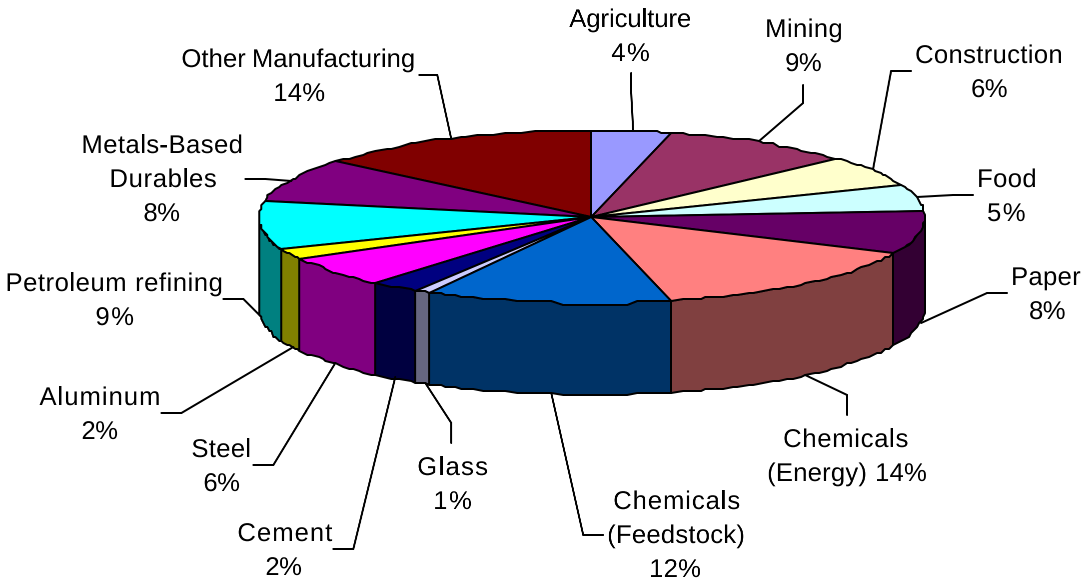


Residential Energy Consumption

- Space heating 35%
- Appliances 29%
- Lighting 6%



Industrial Sector Energy Use (%)



Key Proposed Research Directions

Four broad research themes were identified:

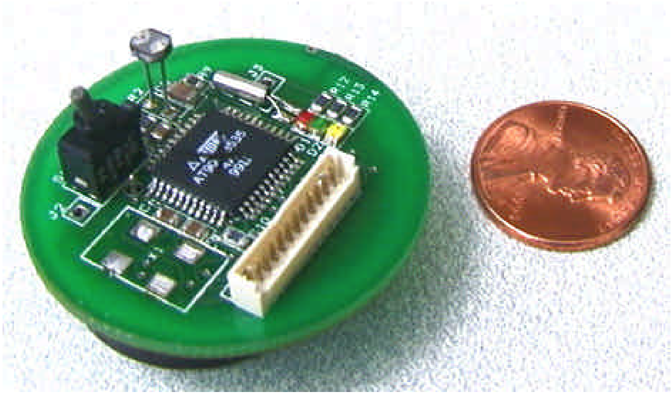
- Sensors
- Solid State Lighting
- Innovative Materials
- Multilayer Thin Film Materials and Deposition Processes

Sensors

- Ubiquitous, dense wireless sensor network, potential for large reduction in energy usage
- Sense and control energy flows, temperature, pollutants,…
- Equipment: e.g. smart dishwasher with turbidity sensor
- Buildings: Systems integration, diagnostics, comfort, safety….

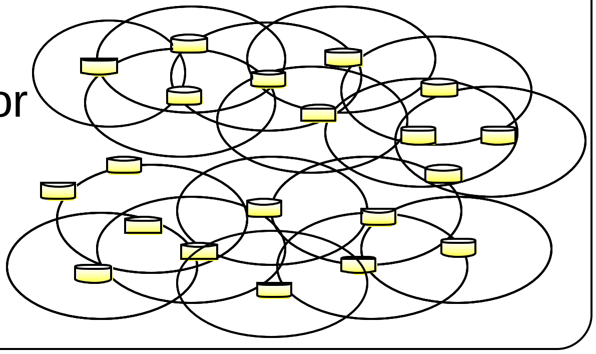
Smart Sensors

- Small self-powered sensors
- Robust, low cost
- Specific to each sensing function
- Sensors available for many different sensing functions
- Integrated signal processing for wireless transmission



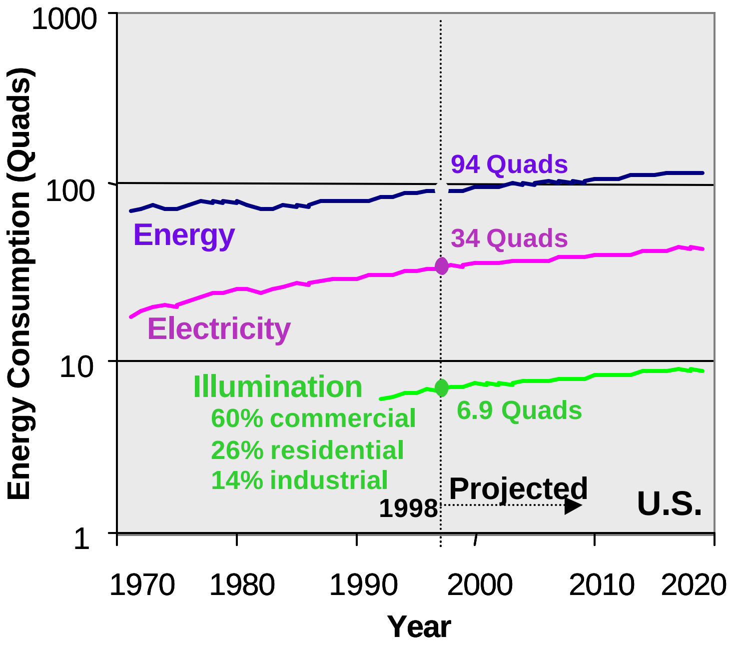
Smart Networks

- System integration of inputs from many sensors
- Information technology infrastructure for data collection
- On-chip signal processing linking sensors to actuators
- Wireless Communications protocols
- Self-organizing networks
- Adaptive logic, neural nets for real time control
- Optimization of linked sensors, actuators, controls



Solid-State Lighting

Lighting is large fraction of energy consumption, and very low efficiency

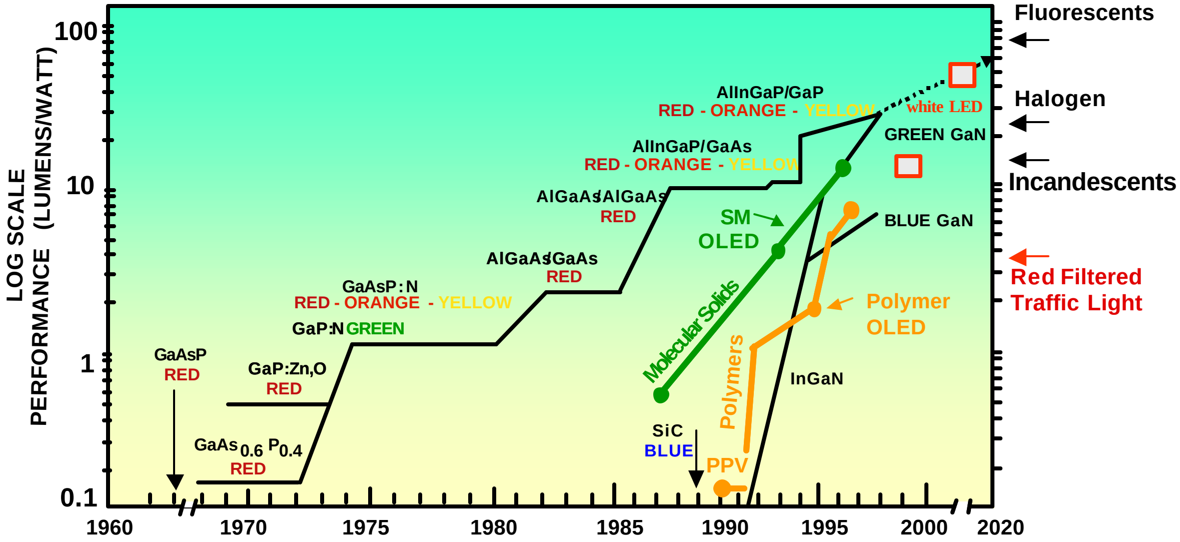


Efficiencies of energy technologies in buildings

Heating:	70 -80%
Electrical motors:	85-95%
Incandescent Lighting:	5-6%
Fluorescent Lighting:	20-25%

~20% of U.S electricity consumption is for general illumination

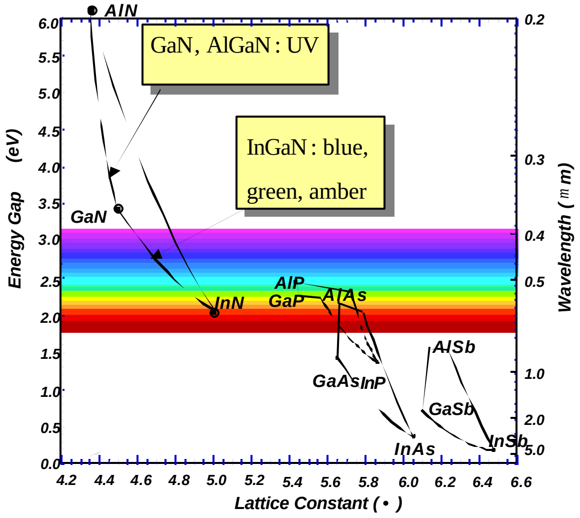
LEDs have been increasing in efficiency (and dropping in cost) at phenomenal rates



RED: lumens/Watt has improved at 30X/decade, cost has decreased at 10X/decade.

BLUE: Recently blue Nitride-based LED materials have appeared.

AlGaInN blue & UV LED materials are very new, considerably different from other III-Vs, and little understood



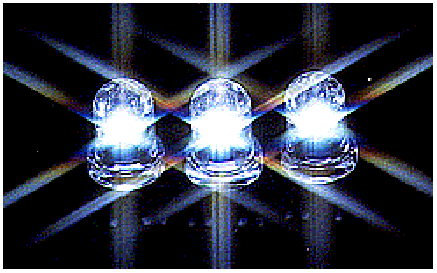
Nitride materials challenges:

- No lattice-matched substrate is known (dislocations therefore results)
- AlGaN not lattice-matched to GaN (dislocations and cracking)
- Mg p-type doping problematic (poor activation, high resistance)
- Growth process is poorly understood and difficult to control

Optical & electrical properties dependent on defect concentrations

Organic LEDs are potentially low cost, large area light sources

Inorganic LEDs



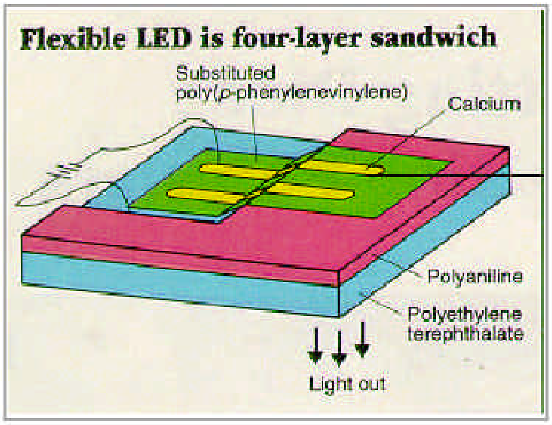
- High brightness point sources
- Spot lighting applications:
    - Flashlights
    - Traffic lights
    - Projection lamps
- More like incandescent

Organic LEDs

- Large area extended sources
- Diffuse lighting applications:
    - Backlights
    - Signs
    - General illumination
- More like fluorescent

Organic LEDs have several “simple” unanswered questions

- What is so special about the few “magic” materials? (Alq3, Polyfluorene)
- What is really going on at material interfaces?
- What controls the singlet-triplet exciton formation ratio in conjugated materials?
- Is it possible to make effective materials that are intrinsically stable to water?
- What are the mechanisms that lead to material degradation?
- Why is it so hard to make blue devices?

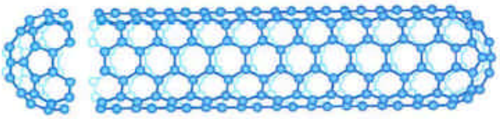


Innovative Materials- Independent Control of Multiple Materials Properties

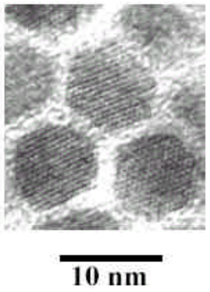
- Available new nanoscale building blocks
- Large scale rapid synthesis methods
- Ability to control processing
- Utilize organic, inorganic, and biological elements

Nanoscale Patterning- some examples of new building blocks

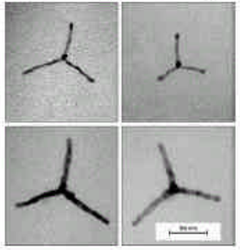
- Nanotubes



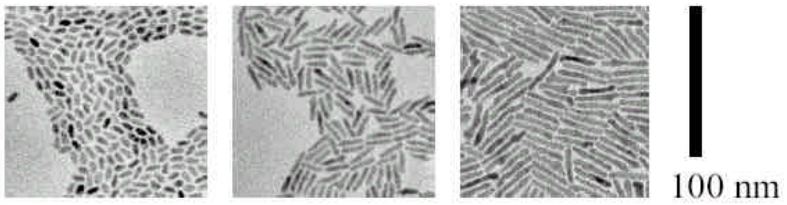
- Nanocrystals



(semiconductor Tetrapods!)



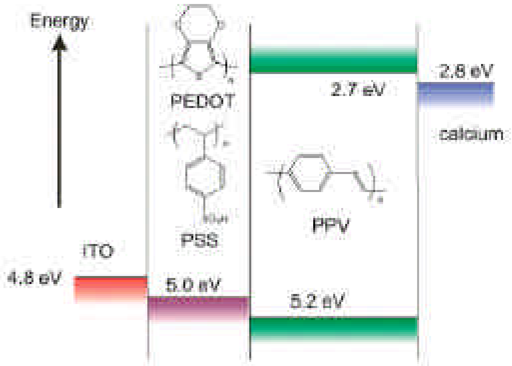
- Nanorods



Solar_Cell

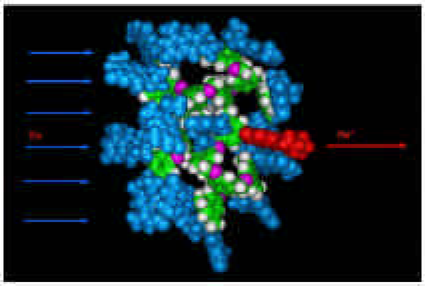
More Building Blocks

- Electronic Polymers and Organics

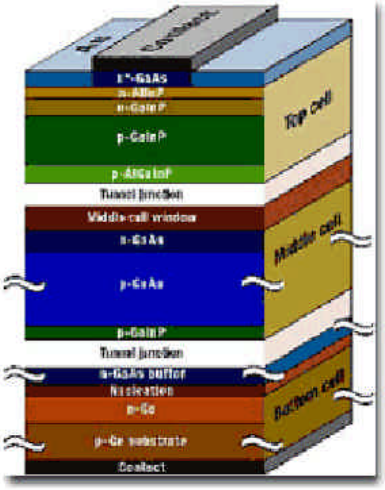


- Block Polymers

- Dendrimers



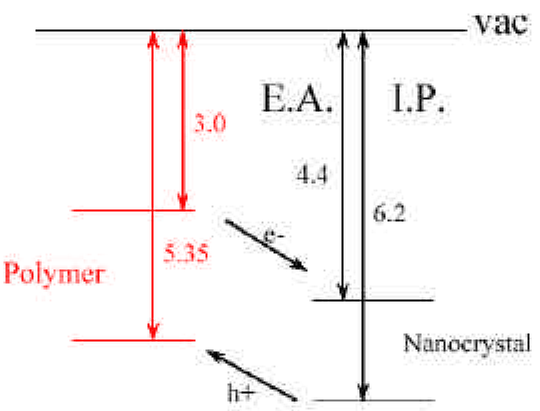
High end multi-gap tandem solar cells made by molecular beam epitaxy and used in satellites

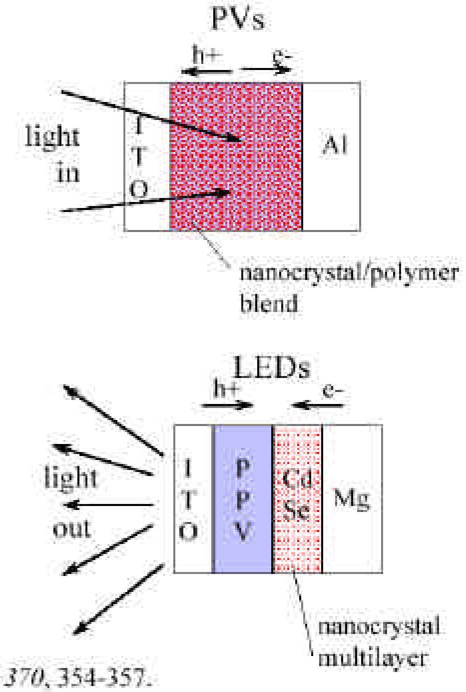


This cell has achieved 34% conversion efficiency under a concentration of 600 suns.

- Proof of concept 36% efficiency.
- Processing impractical for wide areas.
- Same materials can be assembled from inexpensive mass-produced colloidal nanorods.

Semiconductor Nanocrystals and Polymers Band Offsets and Electrical Devices

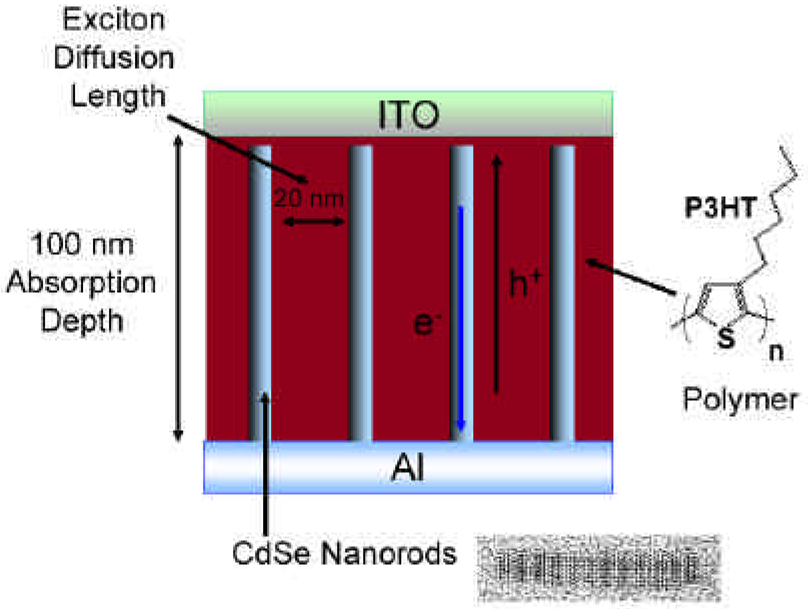




Colvin, V. L.; Schlamp, M. C.; Alivisatos, A. P., *Nature* **1994**, *370*, 354-357.

Schlamp, M. C.; Peng, X.; Alivisatos, A. P., *J. Appl. Phys.* **1997**, *82*, 5837-5842.

Self-assembled Nanorod-Polymer Photovoltaics



Absorption

Exciton Diffusion

Charge Transfer

Charge Transport

Transport: Bicontinuous Network

Some Applications of Innovative Materials

- New LED for solid state lighting(50% efficiency)
- New low cost organic solar cells(30% efficiency)
- Thermoelectrics for self-powered sensors
- New sensor materials for selectivity
- New phase change materials for thermal storage

Multi-layer Thin Films

- First successful nano-dimensioned “products”, 5-50nm thick
- Ex: Low E coatings
  - 30% energy savings on 4% of U.S. total energy use
  - 40million sq.m/yr

- Broad potential applicability for new advanced coatings in buildings
- Needs - “New Materials technologies” and “Low-cost deposition technologies”

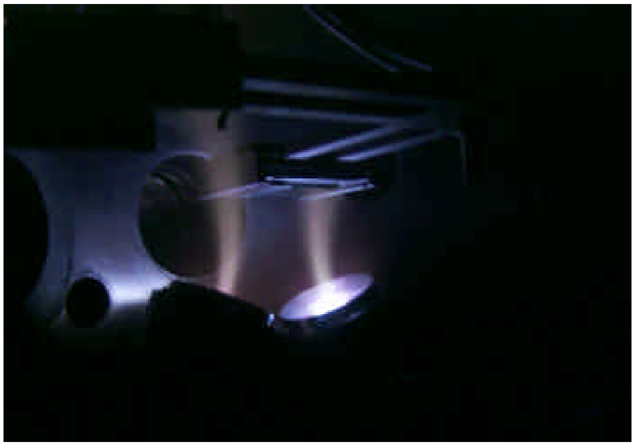
Opportunities for Novel Approaches to Materials

- Electrochromic window coatings - change in optical density with applied voltage
- Bendable, Transparent, conductive coatings
- Dynamic redirection of daylight

Opportunities for Novel Deposition Processes

- Modeling process parameters and film growth chemistry and kinetics
- Prediction of coating properties vs present “tweak and look” approach
- Energetic Deposition for improved rate and properties

e.g., plasma-assisted sputtering



Topical Team Summary

Cross Cutting Research and Education

Cross-Cutting Research Topical Team

Rick Smalley, Rice Univ. (Chair)
Ivan Bekey, Bekey Designs
Kwan Kwok, DARPA
Gerry Lavin, DuPont
John Mankins, NASA
Yoram Shoham, Shell
Jeff Tester, MIT
Nathan Lewis, CalTech
Art Green, ExxonMobil

Agenda

Nate Lewis (Terrawatts)	1:10 – 1:30
Jeff Tester (HDR)	1:45 – 2:30
John Mankins (Solar Satellites)	2:45 – 3:15
Kwan Kwok (Darpa's approach)	3:30-3:40
New & Old Cross-Cutting Issues	
inputs and discussion	3:45-4:30
Workshop Summary & Closing	4:30-5:00 pm

Cross-Cutting PRDs

1. Education / Workforce
2. Nanomaterials –
   - Carbon nanotubes
   - etc.

Development of Proposed Research Directions

Education / Workforce

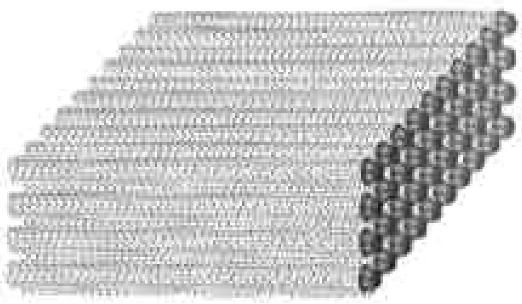
The 10-50 TW BY 2050 ENERGY CHALLENGE

Launch an Education Program within DOE to educate the public on the real problems in World energy supplies.

And how these can only be solved by Breakthrough research in the Garden of the Physical Sciences.

Single Crystal Fullerene Nanotube Arrays

A multifunctional supermaterial



- extreme strength / weight
- high temperature resistance
  (600°C in air, 2000°C in space)
  (for BN tubes ~900°C in air)
- unidirectional thermal conductor
- electromechanical structural component
- unidirectional electrical conductor
  - 0.7 to 1 eV direct band-gap semiconductor
  - or metallic conductor
  - or (for BN tubes) a 6 eV band-gap insulator

The Promise and the Challenge of Space Solar Power

23 October 2002

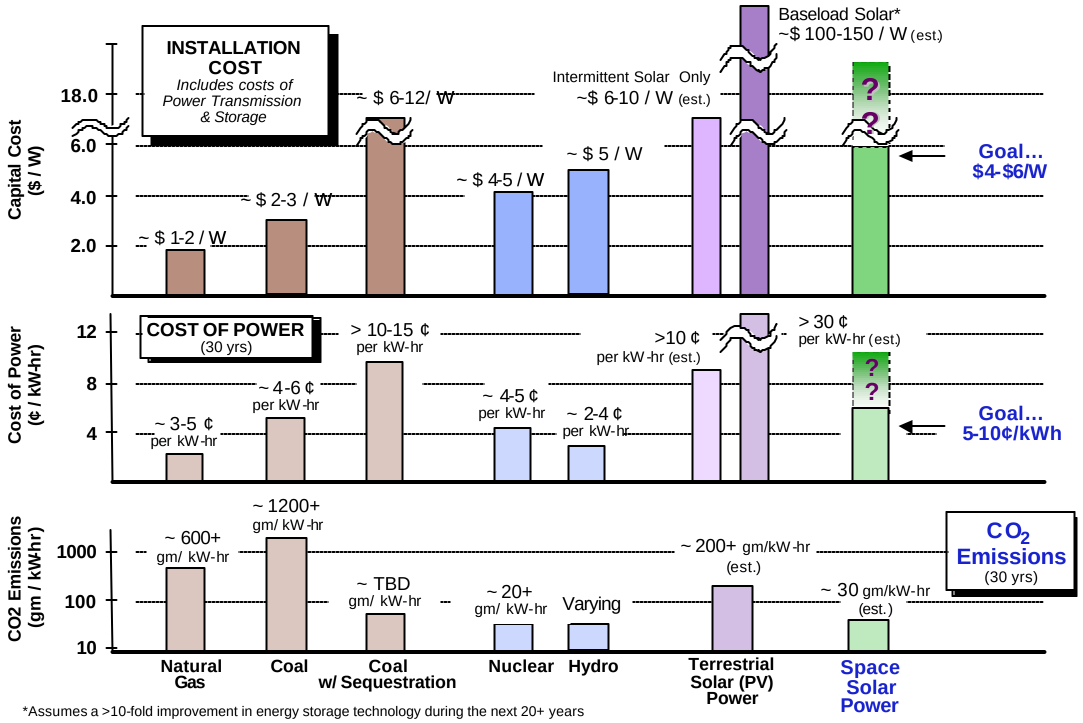
John C. Mankins
Chief Technologist, Human Exploration & Development of Space
NASA Headquarters
Washington, DC, USA

Executive Summary

- **Global climate change caused by accumulating concentrations of greenhouse gases in the atmosphere is a growing concern**
  - Continuing improvements in efficiency are being more-than-offset by rapidly growing global demand for new power plants
- **Stabilizing the carbon dioxide-induced component of climate change <u>is</u> an energy problem**
- **By 2050-2100, ~ 15TW to 40TW of Carbon-neutral energy must be available if CO2 levels are to be stabilized at 2- to 4- times pre-industrial levels**
- **Only a handful of baseload power options exist that can make a meaningful contribution to that level of generation capacity**
- **Space Solar Power (SSP) is one of those options**
- **A constellation of large Space Solar Power Satellites (SSPS) deployed in a family of geosynchronous Earth orbits has the potential to deliver 10s to 100s of Terawatts to markets worldwide**

What are the Options?

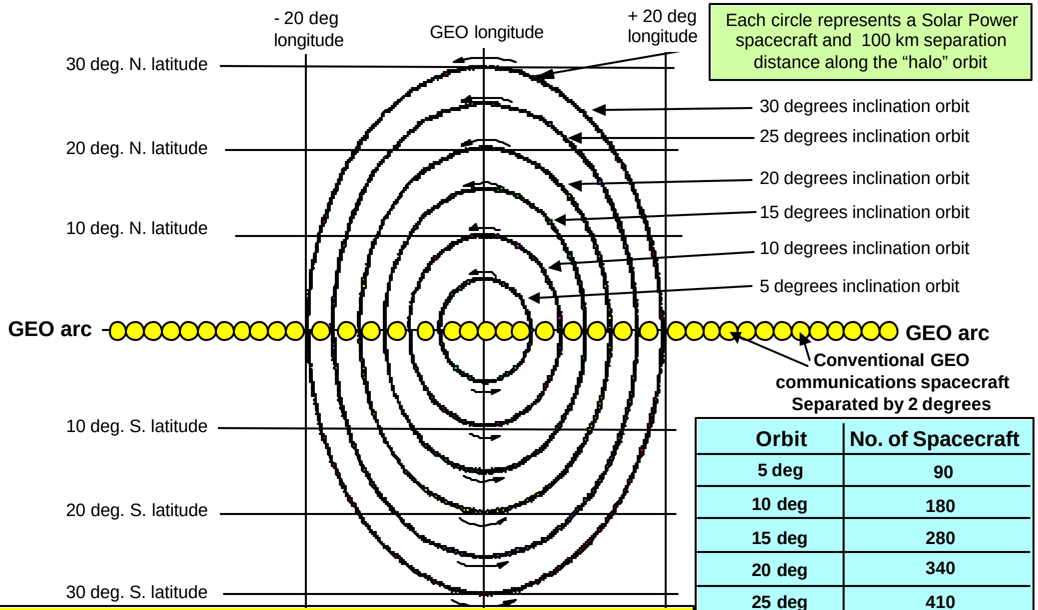
Comparison of Some Baseload Power Alternatives



*Assumes a >10-fold improvement in energy storage technology during the next 20+ years

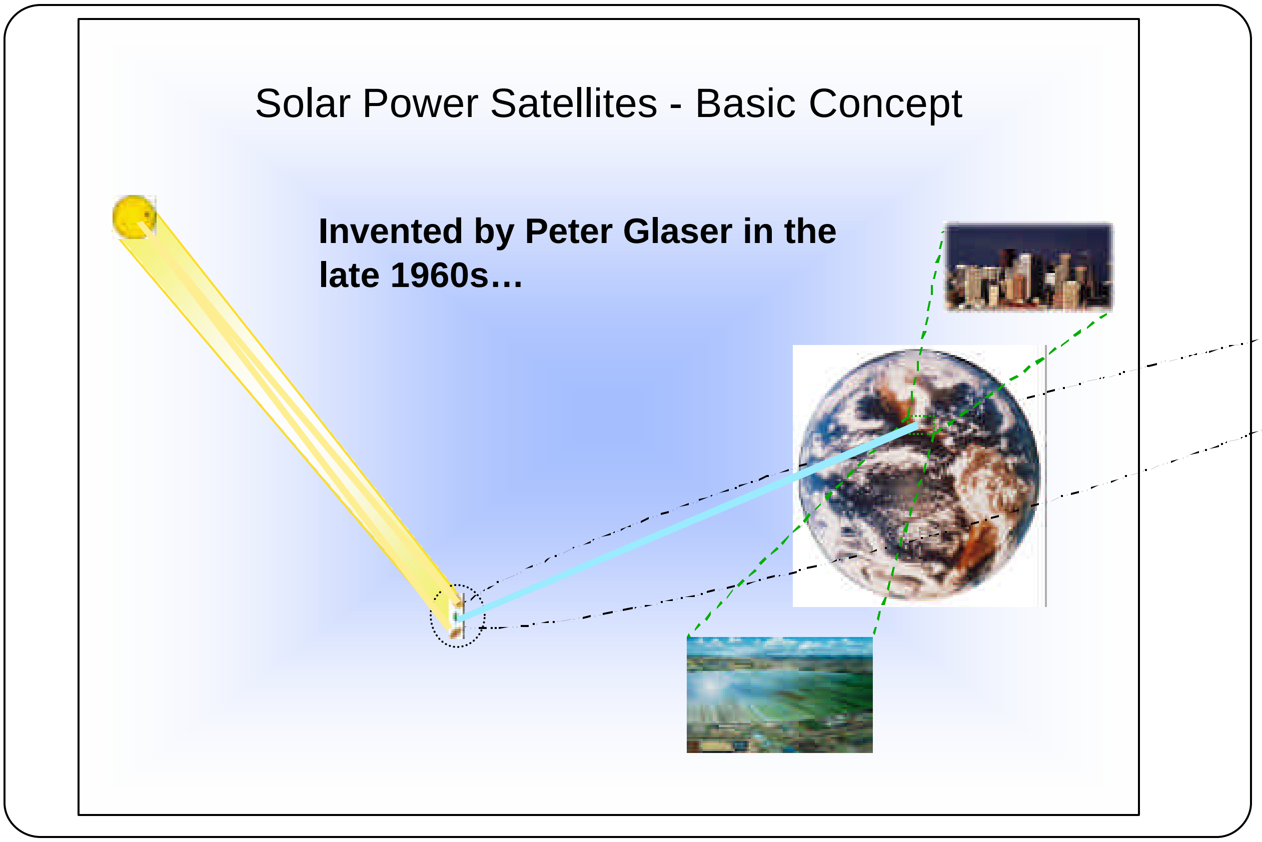
POWER CAPACITY OF GEOSYNCHRONOUS ORBITS

Space Solar Power Spacecraft placed into just 6 of hundreds of possible circulating "halo" orbits provide 18 Terawatts of power



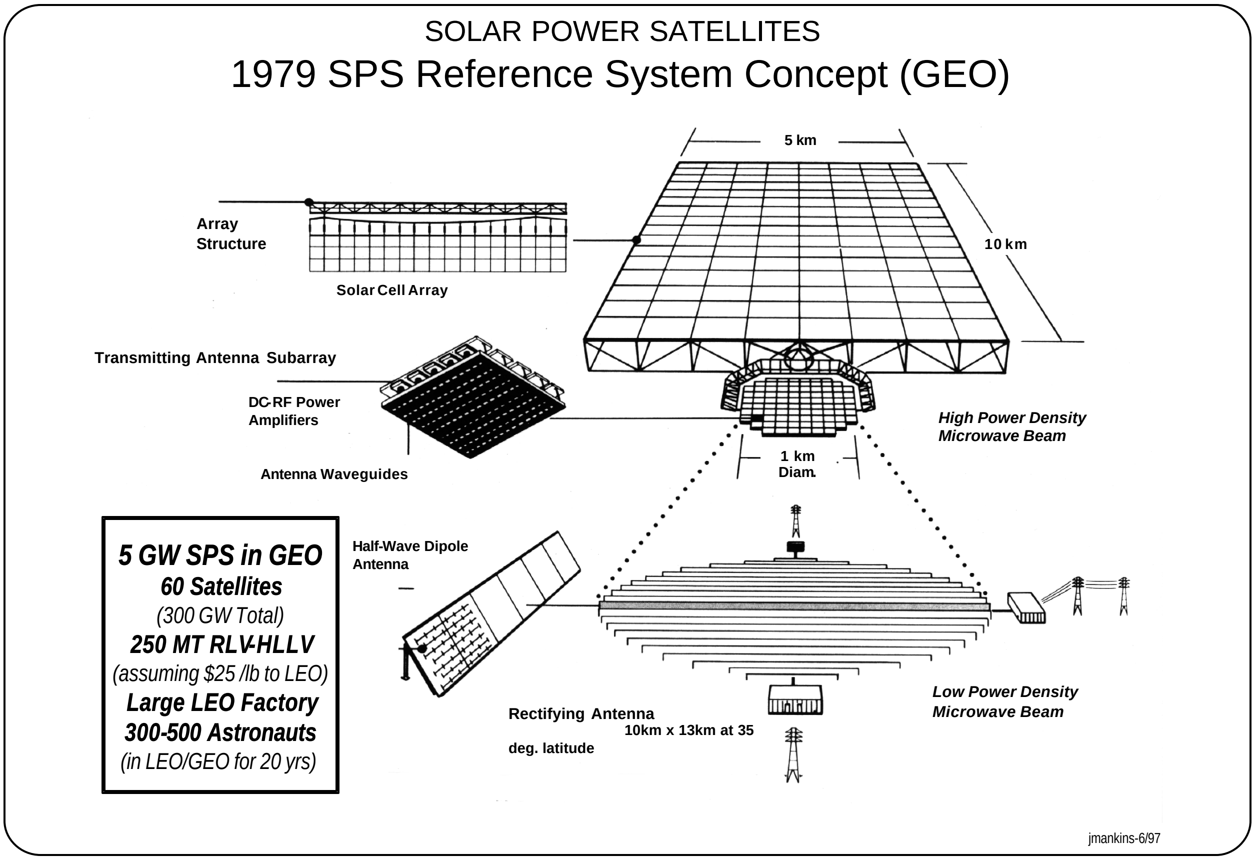
Orbit	No. of Spacecraft
5 deg	90
10 deg	180
15 deg	280
20 deg	340
25 deg	410
30 deg	500
TOTAL	1,800

Since each spacecraft supplies 10 Gigawatts, the total capacity of just these 6 orbits is 18 Terawatts. Since there are hundreds of orbits available their capacity exceeds 2,000 Terawatts



Solar Power Satellites - Basic Concept

Invented by Peter Glaser in the late 1960s…



SOLAR POWER SATELLITES

1979 SPS Reference System Concept (GEO)

5 GW SPS in GEO
60 Satellites
(300 GW Total)
250 MT RLV-HLLV
(assuming $25 /lb to LEO)
Large LEO Factory
300-500 Astronauts
(in LEO/GEO for 20 yrs)

jmankins-6/97

SOLAR POWER SATELLITES

2000 Integrated Symmetrical Concentrator Concept

Incident Sun Light in GeoStationary Earth Orbit @ 1358 W/m^2

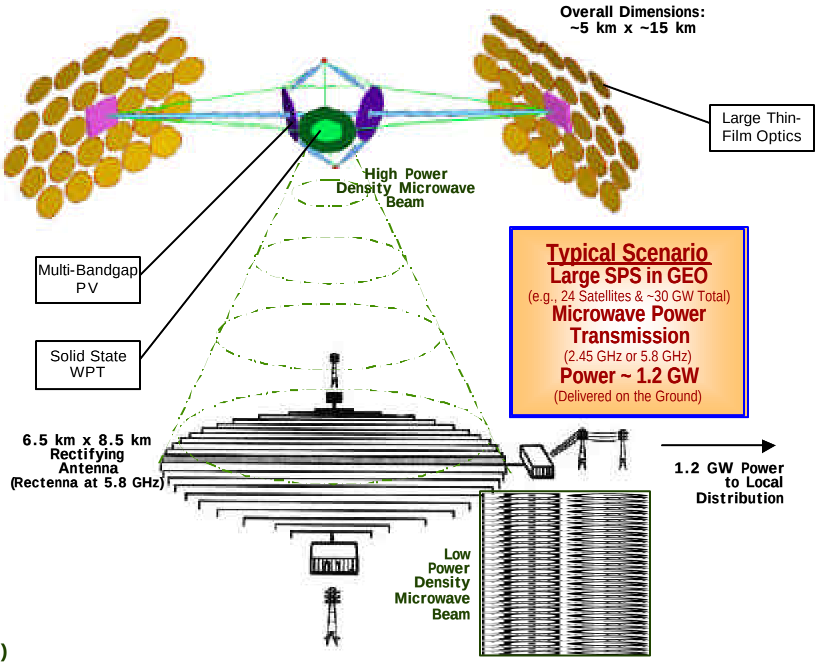
Photovoltaic (PV) Conversion @ 35-50% Efficiency and ~1000 W/kg

Phased Array Conversion to Microwave RF Beam @ 2.45 GHz or 5.8 GHz and >80% Efficiency Goal

Wireless Power Transmission from Space to Earth @ ~90% Efficiency Goal

Rectifying Antenna Conversion of RF to Voltage @ >85% Efficiency Goal

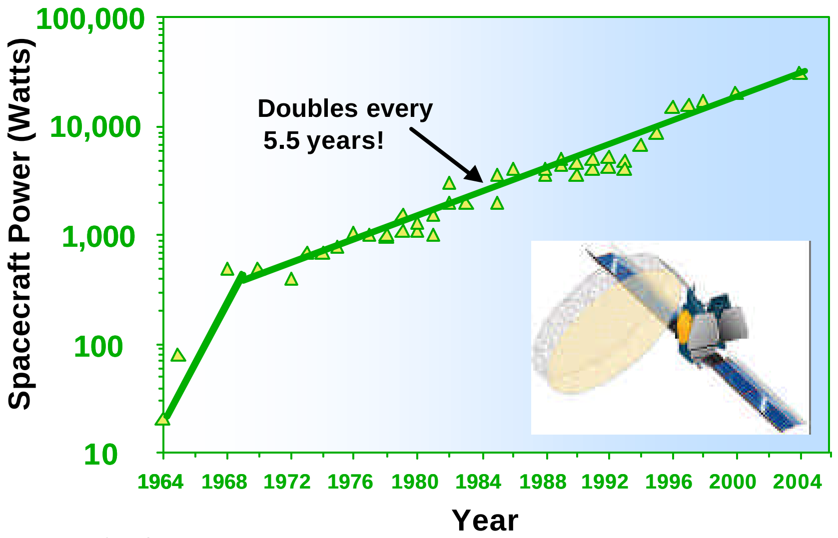
Management & Distribution of Baseload Power to Local Grid (e.g., 1.2-4.8 GW, 1-10 Beams)



Typical Scenario
Large SPS in GEO
(e.g., 24 Satellites & ~30 GW Total)
Microwave Power Transmission
(2.45 GHz or 5.8 GHz)
Power ~ 1.2 GW
(Delivered on the Ground)

Space Solar Power

Communications/National Security Satellite Power Trends



Courtesy of Boeing

Future National Security Needs

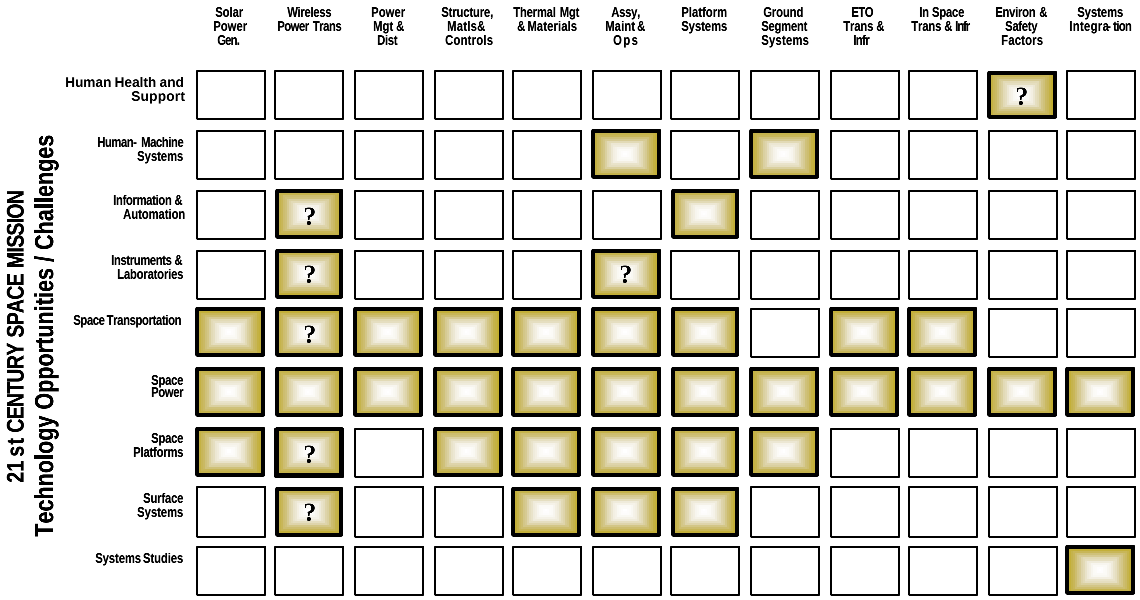
SBR: on critical roadmap for >25kW power needs

SBL: Increased power identified as a top enabler

NRO: > 100kW

SMC/XR (Don Gasner): >100-200kW

21st Century Space Mission Challenges and … SSP Technology Areas

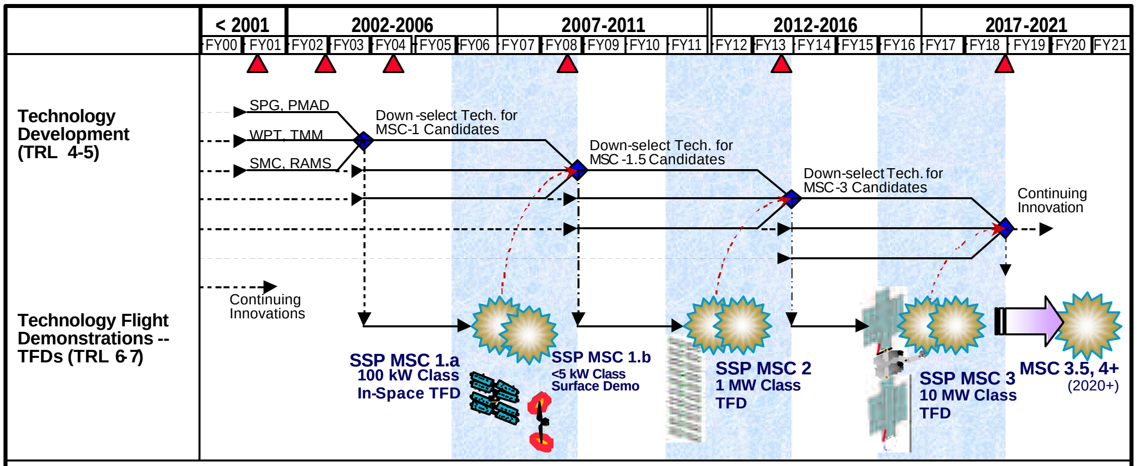


SPACE SOLAR POWER
Technology Roadmap Areas

21 st CENTURY SPACE MISSION Technology Opportunities / Challenges

	Solar Power Gen.	Wireless Power Trans	Power Mgt & Dist	Structure, Matls& Controls	Thermal Mgt & Materials	Assy, Maint & Ops	Platform Systems	Ground Segment Systems	ETO Trans & Infr	In Space Trans & Infr	Environ & Safety Factors	Systems Integra-tion
Human Health and Support											?	
Human- Machine Systems						■		■				
Information & Automation		?					■					
Instruments & Laboratories		?				?						
Space Transportation	■	?	■	■	■	■	■		■	■		
Space Power	■	■	■	■	■	■	■	■	■	■	■	■
Space Platforms	■	?		■	■	■	■	■				
Surface Systems		?			■	■	■					
Systems Studies												■

Space Solar Power
Strategic Research & Technology Roadmap



Schedule of Milestones

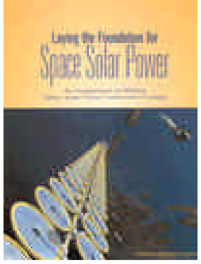
▶	'99-'00	Complete initial Space Solar Power Exploratory Research and Technology (SERT) Program
	2001	Identify/refine top 2-3 systems concepts/architectures for each MSC Demonstration opportunity; refine interim applications
▶	2002/3	Establish/Integrate SSP test beds at participating organizations
	2003	Down-select technologies for initial 100kW class TFD
▶	2004/5	>200 W/kg Solar Power Generation (Array Level) in a Test Bed High-efficiency WPT (>10kW level) in a Test Bed
	2005	50 M class structures & controls flight experiments
	'06-'08	100KW Space-to-Ground & Space-to-Space SPG/WPT Demo
▶	2008	>400W/kg Solar Power Generation (Array Level) in the Lab 50 kW Solar Electric Propulsion/Generation Flight Test High-efficiency WPT (>100kW level) in a Test Bed
	2008	Down-select technologies for 1 MW class TFD
	'11-'13	1 MW Class Space to Space SPG/WPT Demo
▶	'12-'13	>600W/kg Solar Power Generation (Array Level)
	2013	Down-select technologies for initial 10MW class TFD
▶	2017	>1000W/kg Solar Power Generation (Array Level)
	'16-'18	10 MW CLASS INTEGRATED SSP SYSTEM FLIGHT DEMO

LEGEND ◆ Strategic Research and Technology Decision Point ▲ Major Technology Development Milestone ✹ Major Technology Flight Demonstration

Space Solar Power Background
Results of the US NRC SSP Review (1 of 2)

- **During 2000-2001, the Aeronautics and Space Engineering Board (ASEB) of the NRC assessed the technology investment strategy of the "Space Solar Power" Program to determine its technical soundness and contributed the roadmap by…**
  - Critiquing the overall technology investment strategy in terms of the plan's likely effectiveness in meeting the program's technical and economic objectives
  - Identifying areas of highest technology investment necessary to create a competitive space-based electric power system
  - Identifying opportunities for increased synergy with other research and technology efforts
  - Providing an independent assessment of the adequacy of available resources for achieving the plan's technology milestones, and
  - Recommending changes in the technology investment strategy
- **Findings?**
  - "SERT program has provided a credible plan for making progress toward the goal of providing space solar power for commercially competitive terrestrial electric power despite rather large technical and economic challenges
  - "Current SSP technology is aimed at technical areas with important commercial, civil, and military application
  - "Dedicated NASA team has defined a potentially valuable future program…
  - "Current SSP program is operating on minimal budget and significantly higher funding and program stability will be necessary to attain aggressive goals of program
  - "Funding plans during the first five years (leading to first flight test demonstration) are reasonable…"

Space Solar Power Background
Results of the US NRC SSP Review (2 of 2)



- **Findings? (continued)**
  - "Concern in committee that investment strategy is based on modeling efforts and individual mass, cost, and performance goals that may guide management toward poor investment decisions
  - "Significant technical breakthroughs necessary to achieve final goal of cost-competitive terrestrial baseload power
  - "Ultimate success of terrestrial power application critically depends on dramatic reductions in cost of transportation from Earth to GEO
  - "Leveraging of technological advances made by organizations external to NASA must be done."
- **The SSP R&T panel also made a series of recommendations for improving the management and focus of future program efforts, including**
  - Need to prepare a formal technology plan
  - Need for improvements in systems and cost modeling, including increased use of expert critique and review
  - Continued use of technology flight demonstrations
  - Early emphasis on environmental, health and safety issues
  - Key technologies:
    - Solar Power Generation
    - Wireless Power Transmission
    - Space Power Management and Distribution
    - Assembly, Maintenance and Serving
    - In-Space Transportation

But…

- **Despite our best efforts, we are NOT there yet…**
  - We have a better understanding of the issues and the challenges
  - We have an extensive database of options and alternatives
  - We have an strong, peer-reviewed Strategic R&T road map
  - We have made progress on many key technologies
    - Except the key area of very low cost access to space…
- **We have NOT yet gotten to clear economic viability**
  - Don't buy stock in an "SPS Start-Up Company" just yet…
- **What will a viable concept be like? --** "Concept-X"

A Visionary Idea: "Concept-X"

What Might It Be Like?

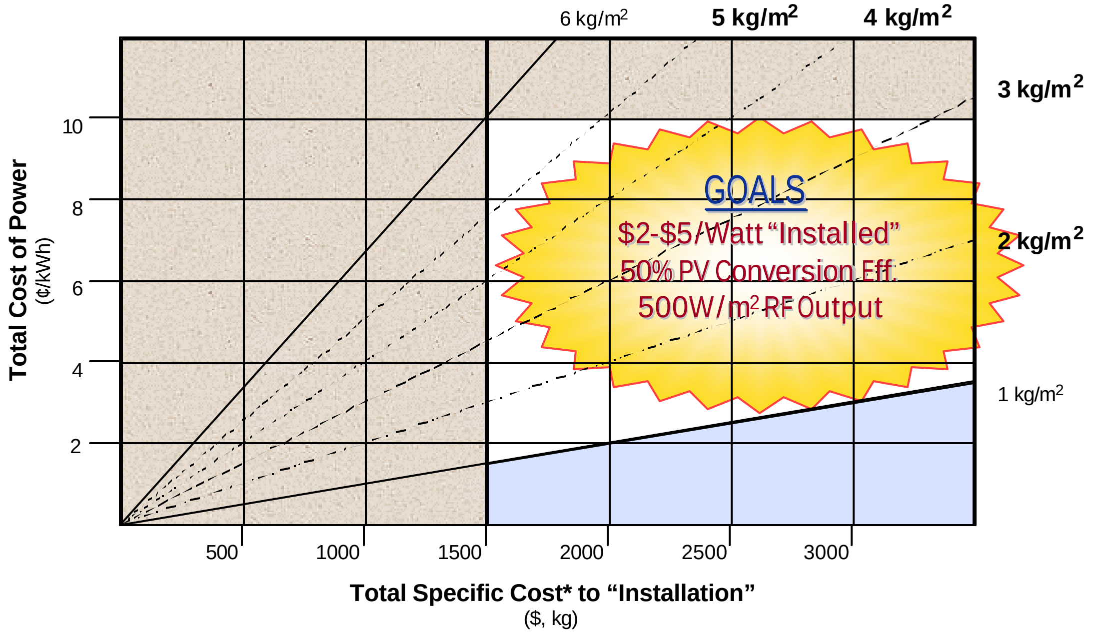
- **Most probably some version of the ISC/Sandwich approach**
  - Use of solar flux redirecting optics (e.g., large thin-film mirrors)
- **In the RF Case…***
  - Phased array must be very low mass per square meter…
  - All thermal should be local…
  - All PMAD should be local…with no converters…
  - Diameter of transmitter should be large, but send beam to multiple ground sites…
    - Reducing size of ground station
  - Find some way to avoid using a full 10:1 Gaussian distribution

***** *Solar-pumped laser based concepts may also prove promising, but are not yet sufficiently mature to allow the definition of a "Concept-Y"*

A Visionary Idea: “Concept-X”
What Might It Be Like?

- **Ambitious Goals must be achieved…**
  - Sandwich or ISC -like Optics (< 10% of total system mass)
  - PV Energy Conversion
    - Efficiency: > 50%
  - RF transmitter:
    - ~ 5 km diameter at 2.45 GHz (or another frequency…choice is not critical)
    - Efficiency: > 80%
    - RF Power Output per square-meter: ~ 500 W
    - Total Power Output: >10 GW
  - Ground Rectenna:
    - 10-20 stations at < 2 km diameter each (and @< 500 MW output)
    - Cost per Receiving Station: < $2/W

A Visionary Idea: “Concept-X”
What Should We Seek to Achieve?



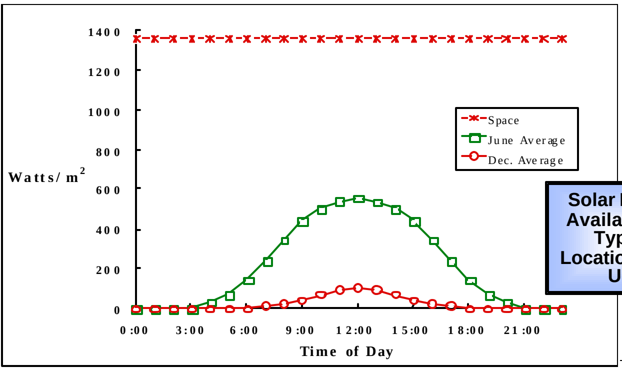
*Including cost of Money, H/W, Launch, etc.…

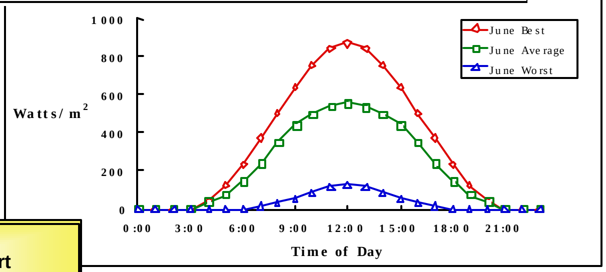
SSP Research and Technology
Some Key Directions

- **Continuing advances in / applications of intelligent systems and robotics -- pursuing the goals of self-assembly, large and self-sufficient "communities" of systems, etc.**
  - Including modular/distributed avionics -- e.g., wireless network avionics (massively redundant)
- **Higher strength-to-weight materials and structural concepts applicable in the space environment**
  - Both thin film / deployable and rigid structure / assembled
- **Higher temperature solid state devices of various types, including PV cells, FET amplifiers, phase shifters, etc.**
- **MEMS / μ-device thermal management, etc.**
- **Various Options, including**
  - Laser wireless power transmission (electric and solar-pumped)
  - High-voltage and/or HTc power management and distribution
  - Others…
- ***PLUS…***
  - Very low cost space transportation

…Terrestrial Solar Power?

- **There must be terrestrial solar…**
- **For baseload power, however, the challeng facing ground solar power are in many ways harder than th for space-based systems**
- **The total solar energy available at a typical site on the Earth's surface is much less than in space**
- **Moreover, the energy available varies widely — seasonally and daily**
- **"Baseload" using ground solar requires substantial over-capacity and costly large-scale energy storage or global distribution networks…**



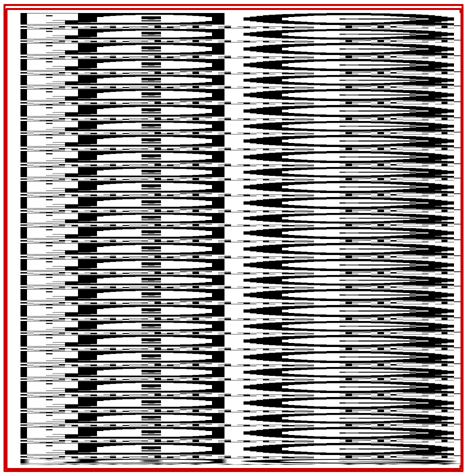


Solar Energy Available at a Typical Location in the U.K.

BASIC TRADE:
WPT + Space Transport
Versus
Ground Solar + Energy Storage

…the Safety of Power Beaming?

- **There is a continuing concern regarding the health & safety issues associated electromagnetic radiation**
  - These must be treated seriously
  - At microwave frequencies, the only known physical effect on living tissue is thermal heating
- **The US Standard Limit for microwave exposure is = 100 W/m^2, for = 6 minutes**
- **For SSP, power densities would vary greatly across an incoming beam; a 2.45 GHz, 5 GW beam would have densities of**
  - Beam Center ~ 230 W/m^2
  - Rectenna edge ~10 W/m^2
  - Fence edge ~ 1 W/m^2
- **Studies conducted in the late 1970s found that for exposure levels up to 500 W/m2 for 30 min., there was <u>no</u> discernable effect on honey bee test subjects (3000 subjects, over 2 trials)**
- **Further research in 2001-2002 indicates no effect on plants “outside the fence”**
- **Further research required to ensure that any possible health factors associated to SSP/WPT (people and animals) were within acceptable limits**



Summary

- **Space solar power appears to be a technically-viable option capable of delivering large (>100’s GW) essentially carbon-free electrical power globally**
  - No issues with any areas of fundamental physics
- **Significant advances have been made since the 1970s**
  - Concepts
  - Technology
  - Infrastructure
- **Technology developments needed in a number of areas…**
  - Materials, structures, devices, autonomy, robotics, others
- **Strategic R&T road maps for SSP have been developed and reviewed by the National Research Council**
  - “SSP technology … aimed at technical areas with important commercial, civil, and military application
  - “… a potentially valuable future program…
  - “… significantly higher funding and program stability … necessary
  - “Funding plans during the first five years (leading to first flight test demonstration) are reasonable…”

Topical Team Summary

Energy Biosciences Research

Energy Biosciences Research Topical Team

Mark Alper, LBNL
Heinz Frei, LBNL
Evan Hughes, EPRI
Laurie Mets, Univ. Chicago
John Shanklin, BNL
Chris Somerville, Stanford Univ.
Walt Stevens, BES
Lut De Jonghe, UCB

Other Attendees:
John Stringer, EPRI
Linda Horton, ORNL

October Workshop Suggested Need for Additional Discussion of Opportunities related to Biological Energy Research

- Team workshop held on January 13-14, 2003 in Palo Alto
- Presentations included:
  - World energy situation (Stringer)
  - Results from the October Workshop (Horton)
  - Current BES Biosciences research program (Stevens)
- Proposed Research Directions from the October workshop were included in the discussions
  - Renewable Energy; Transportation; Industrial Residential, Commercial; Distributed Energy

Proposed Research Directions

- Energy Biotechnology: Metabolic Engineering of Plants and Microbes for Renewable Fuels and Chemicals
- Genomic Tools for the Development of Designer Energy and Chemical Crops
- Nanoscale Hybrid Assemblies for the Photo-Induced Generation of Fuels and Chemicals

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Energy Biotechnology:
Metabolic Engineering of Plants and Microbes for Renewable Fuels and Chemicals

- Increase the efficiency of biomass production by plants by metabolic engineering
  - ➢ Control plant architecture and composition (lignin, cellulose, hemicellulose, starch and oils)
  - ➢ Enzyme design, metabolic modeling, and rational pathway engineering
- Increase the efficiency of microbial conversion of biomass to fuels and chemicals
  - ➢ Improved microbial biocatalysts
  - ➢ Understanding of the fundamental chemical and physical processes of fractionation and solubilization

100-Fold Increase in Contribution of Renewable Biomass

Genomic Tools for the Development of Designer Energy and Chemical Crops

- High yields of 3 to 5 times current energy crops are needed for economic viability and a major role for biomass energy
- High energy density and properties compatible for manufacturing the final product are critical
- Emerging genomic tools will enable high yields and other desirable properties within 10-20 years
  - Identify key genes that determine yields and important plant properties
  - Use genomic tools to breed plants that can be directly integrated into the energy conversion process (improve efficiency, cost effectiveness, etc.)
- Example genomic tools to be developed include single DNA molecule sequencing and mapping, improved bioinformatics for marker assisted breeding

Nanoscale Hybrid Assemblies for the Photo-Induced Generation of Fuels and Chemicals

- Nanoporous inorganic, organic, and biochemical hybrid structures
  - ➢Efficient synthesis of fuels (hydrogen, methanol) from renewable sources (water, CO_2) using sunlight energy
  - ➢Efficient photochemical energy storage
- Self assembly using the principles of molecular recognition
- Strategies for organizing nanoscale assemblies relative to one another to achieve concerted, macro-scale effects
- Dynamic analysis for time-resolved spectroscopy, diffractometry, computational approaches and molecular genetics

APPENDIX F

LIST OF ABBREVIATIONS AND TERMS

AFC	alkaline fuel cell
AFCI	Advanced Fuel Cycle Initiative
Alq3	a flexible, light-emitting polymer used for organic light-emitting diodes
ANL	Argonne National Laboratory
APS	Advanced Photon Source
ARIES-RS	a Tokamak design fusion power plant
ARIES-ST	a spherical torus design fusion power plant
ATP-ADP	adenosine triphosphate-adenosine diphosphate
BBO	billion barrels of oil
BES	Basic Energy Sciences Program of DOE
BESAC	Basic Energy Sciences Advisory Committee
BOP	balance of plant
Btu	British thermal unit
CFD	computational fluid dynamics
CHP	combined heat and power
cm	centimeter
COP	coeficient of performance
CRI	color rendering index
CVD	chemical vapor deposition
CVM	cluster variation method
DFT	density functional theory
DNA	deoxyribose nucleic acid
DNS	Direct Numerical Simulation
DOE	Department of Energy
DP	Defense Programs
dpa	displacement per atom
DT	deuterium and tritium
EE/FSU	Eastern Europe/Former Soviet Union
EE/RE	Energy Efficiency and Renewable Energy Program of DOE
EIA	Energy Information Administration
EJ	exajoule (10^{18} Joules)
EMI	electromagnetic interference
ES&H	Environmental, Safety and Health
EV	electric-drive vehicle
FC	fuel cell
FCEV	fuel-cell-powered electric vehicle
FE	Fossil Energy Program of DOE
FETC	Federal Energy Technology Center
FIRE	Fusion Ignition Research Experiment
ft	feet
GB	gigabarrels
gC/MJ	grams carbon per megajoule
GDP	gross domestic product
GFR	Gas-cooled Fast Reactor
GHG	greenhouse gas

GIF	Generation-IV International Forum
GJ	gigajoule (10^9 Joule)
GJ/s	gigajoule per second
GM	General Motors
g/MJ	grams per megajoule
GRI	Gas Research Institute
GW	gigawatt (10^9 Watt)
GWP	Global Warming Potential
HCCI	homogeneous charge compression ignition
HEV	hybrid electric vehicle
HTGR	high-temperature gas-cooled reactor
ICE	internal combustion engine
IEA	International Energy Agency
IEO	International Energy Outlook
IFE	intertial fusion energy
IAEA	International Atomic Energy Agency
IASCC	irradiation-assisted stress corrosion cracking
IGNITOR	magnetic fusion experiment led by Prof. Bruno Coppi at the Massachusetts Institute of Technology.
ITER	International Thermonuclear Experimental Reactor
IWG	Interlaboratory Working Group
J	Joule
JANAF	thermochemical tables database of National Institute of Standards and Technology
JET	Joint European Torus
J/s	Joule per second
kg	kilogram (10^3 gram)
kJ	kilojoule (10^3 Joule)
km	kilometer (10^3 meter)
kW	kilowatt (10^3 Watt)
kWh	kilowatt-hour (10^3 Watt-hour)
l	liter
lb/MBtu	pounds per mega (10^6) British thermal unit
LBNL	Lawrence Berkeley National Laboratory
LED	light-emitting diode
LES	Large Eddy Simulation
LFR	Lead-cooled Fast Reactor
LMJ	Laser Mega-Joule (fusion energy facility in France)
LNG	liquid natural gas
LPC	ultra-lean premixed hydrocarbon combustion
LWR	light-water reactor
m	meter
mA	milliamp
mbd	million barrels per day
MBtu	mega Btu (10^6 Btu)
McF	million cubic feet

MCFC	molten carbonate fuel cell
MD	molecular dynamics
MEA	membrane/electrode assembly
meV	milli-electron volt
MeV	mega-electron volt
MFE	magnetic fusion energy
MHD	magnetohydrodynamics
MJ	megajoule (10^6 Joule)
MJ/s	megajoules per second
MJ/s_e	megajoules per second, electrical
mph	miles per hour
MSR	Molten Salt Reactor
Mt	million metric ton
MtC	million metric tons of carbon
MW	megawatt (10^6 Watt)
NASA	National Aeronautics and SpaceAdministration
NE	Nuclear Energy, Science, and Technology (DOE Office of)
NEPDG	National Energy Poligy Development Group
NERAC	Nuclear Energy Research Advisory Committee
NETL	National Energy Technology Laboratory
NIF	National Ignition Facility (fusion energy facility)
nm	nanometer
NMR	nuclear magnetic resonance
NNSA	National Nuclear Security Administration
NRC	National Research Council
NRC	Nuclear Regulatory Commission
NREL	National Renewable Energy Laboratory
NSLS	National Synchrotron Light Source
OECD	Organization for Economic Cooperation and Development
OLED	organic light-emitting diode
OPEC	Organization of the Petroleum Exporting Countries
ORNL	Oak Ridge National Laboratory
OS	Office of Science
OTA	Office of Technology Assessment
PAFC	phosphoric acid fuel cell
PEMFC	proton-exchange membrane fuel cell
ppm	parts per million
PRD	proposed research direction
ps	picosecond (10^{-12} second)
psi	pound per square inch
PUREX	plutonium uranium extraction process
PV	photovoltaic
Quad	energy unit equal to 10^{15} Btu
R&D	research and development
RH	relative humidity

RTIL	room temperature ionic liquid
s	second
S/cm	unit of ionic conductivity, Siemens/cm
SCF	supercritical fluid
SCR	selective catalytic reduction
SCWR	Supercritical Water-cooled Reactor
SFR	Sodium-cooled Fast Reactor
SI	International System of Units
SNRA	Swedish National Road Administration
SOFC	solid oxide fuel cell
STM	scanning tunnelling microscope
swnt	single-walled nanotubes
TBtu	terra Btu (10^{12} Btu)
tC	ton of carbon
TcF	trillion cubic feet
TE	thermoelectric
TFTR	Tokamak Fusion Test Reactor
TW	terawatts (10^{12} Watts)
TWe	terawatt electric
TWh	terawatt-hour
UAV	unmanned aerial vehicle
UREX	simplified version of PUREX
USGS	U.S. Geological Service
UV	ultraviolet
VHTR	Very High Temperature (gas-cooled) Reactor
VLT	Virtual Laboratory for Technology
vmt	vehicle miles traveled
VOC	volatile organic carbon
W	Watt
yr	year
YSZ	yttria-stabilized zirconia
Z	atomic number
Z	thermoelectric figure of merit for converting heat into electrical energy
ZT	Z (thermoelectric figure of merit) times the average operating temperature