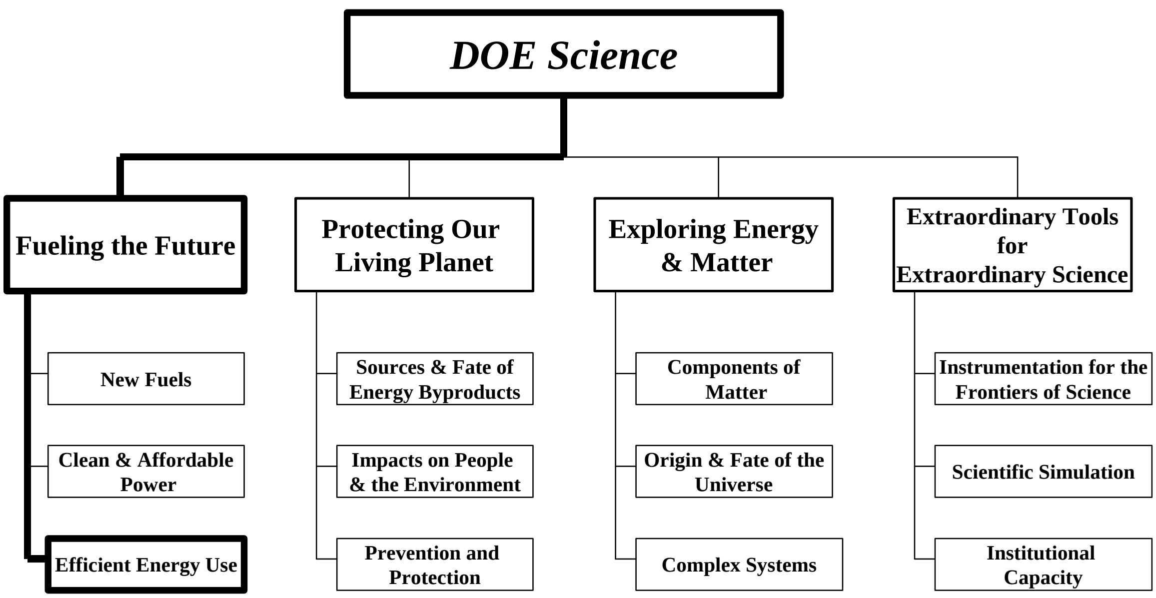
Chapter 4
Efficient Energy Use

Scientific Challenge: ***To understand the engineering, materials, and chemical processes to develop new energy efficient technologies.***



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Increasing the efficiency in the way we use energy has only positive effects. Energy efficiency lowers costs, making financial resources available for more productive use. It decreases our dependence on energy supplies from unstable regions of the world. It decreases the adverse affects on the environment from extracting, refining, transporting, and combusting fuels. Also, since the vast majority of the fuel consumed today is carbon based, efficiency is the quickest and most effective way to reduce the principal greenhouse gas—carbon dioxide—and local air pollutants such as particulates, SO_x, and NO_x.

There are many ways to increase efficiency. Some are very simple, such as increasing insulation and caulking leaks. More sophisticated and more difficult ways require substantial basic research and development. Increasing the temperature of heat engines will increase efficiency, but all of the degradation reactions, such as corrosion, increase exponentially with temperature. Understanding combustion reactions will lead to significant improvements in boilers and internal combustion engines. Lowering weight in automobiles and trucks will increase fuel economy, but low weight materials may not be very strong. A large amount of energy is used first to refine, melt, and cast parts only to grind way substantial amounts to create the final shape. Substantial efficiency could be gained with better materials and processes that could cast directly to final shapes. Vast amounts of energy are wasted because of inefficient separation and unspecific catalytic processes. New superconductors can eliminate electrical transmission losses and improve the efficiency of generators. A diverse portfolio of high-quality basic research projects enables the interdisciplinary work needed to solve the problems of efficient energy use. Office of Science research programs help guarantee that energy technology development is being conducted with benefit from advanced scientific knowledge and that basic research projects are focused in areas directly relevant to energy systems.

Combustion-Related Sciences

Description, Objectives, and Research Performers

The research program investigates, at the molecular level, chemical reactions in the gas phase, at surfaces, and at interfaces and the relationship between molecular scale phenomena and bulk phenomena. Research activities involve closely coupled experimental and theoretical efforts. Experimental projects include studies of molecular dynamics, chemical kinetics, spectroscopy, clusters, and surface science. The goal related to energy efficiency is to increase the efficiency of the combustion process.

Combustion-related chemical physics research is conducted at several national laboratories (including a single-purpose laboratory devoted to combustion, the Combustion Research Facility (CRF) at Sandia National Laboratory) and at a broad spectrum of universities. Cluster research is carried out at both national laboratories and universities, while work related to the solid-liquid interface and the relationship to environmental remediation issues is performed predominantly at national laboratories.

Research Challenges and Opportunities

Nearly 90% of the nation's energy needs are produced by combustion. Typical combustion reactions involve dozens, sometimes hundreds, of chemical reactions whose rates at combustion temperatures must be known. It is not practical to measure all of the rates of reactions that might be included in a computer model for a particular combustion system with a particular fuel and oxidant. One of the challenges of the chemical physics program is to provide data and techniques for producing or predicting the values of chemical reaction rates to be included in combustion models for predicting the efficiency and emission characteristics of combustion devices and for optimization and control of combustion devices.

Catalysis not only makes the production of chemical feed stocks and fuels economically feasible, it does so by reducing the demand for energy. Catalysts also find extensive use in pollution reduction. In contrast to those technical areas that are highly codified with a great deal of predictive capability, surface mediated catalysis is in a more Edisonian stage of development. The surface science and clusters projects in the chemical physics program are aimed at providing predictive capability for surface mediated catalysis through provision of explanatory theories relating surface structure to surface mediated chemistry.

Research Activities

A primary goal of the chemical physics program is to provide combustion-related data and techniques for producing or predicting the values of chemical reaction rates to be included in combustion models. Research activities focus on improving theory and obtaining confirmatory experimental measurements of the dynamics and spectroscopy of vibrationally and electronically excited species relevant to combustion systems to enable predictions of reaction rates under a wide variety of conditions, including high temperatures and pressures, energy transfer phenomena, and spectra for diagnostic probes. Models can then predict the efficiency and emission characteristics of combustion devices, and researchers can optimize and control combustion processes.

The surface science and clusters research is aimed at providing predictive capability for surface-mediated catalysis through provision of explanatory theories relating surface structure to surface-mediated chemistry. Clusters provide a means of relating surface structure to chemical activity because structure is a function of cluster size. The use of a chemical physics approach to investigate fundamental issues at the solid-liquid interface related to environmental remediation issues is also part of this program. The program comprises combustion-related chemical physics research, cluster research, and work related to the solid-liquid interface and this relationship to environmental remediation issues. Experimental techniques are used to determine the structures, while theory is employed to predict the dynamics of surface reactions.

Accomplishments

- Within the last three years a novel and elegantly simple experiment has been designed and refined that allows the interaction of chemistry and turbulence to be examined in quantitative and verifiable detail for the first time. Comparisons of these experiments with computational simulations have shown that the widely accepted chemical reaction mechanism for methane combustion is in error. Because of the simplicity of this experiment, it promises to be widely copied and in the coming years we can expect to see an acceleration in our ability to understand and control combustion processes.

- Scientists have demonstrated a new variant of laser frequency modulation spectroscopy that is specifically tailored to the detection of transient combustion species. Although frequency modulation has long been used to compensate for source fluctuations in spectroscopy, the new technique is simple to apply and likely to gain wide usage. It has already been applied to the study of the chemistry of NH_2 radicals. With this new technique, more rapid progress in the characterization of combustion reaction mechanisms can be expected.

- In studying water and organic solvents adsorbed on surfaces, scientists have observed a phenomenon they have dubbed "molecular volcanoes." The research is conducted to understand, at a molecular level, processes that control movement of organic solvents in soils and aquifers. The knowledge gained will contribute to the development of control and storage strategies for organic wastes.

Advanced Materials

Description, Objectives, and Research Performers

Research in advanced materials is concerned with the microstructural aspects of geometrical packing configurations of atoms in solids, defects and imperfections in those packing configurations, and the microscale morphology and composition of crystalline solids. The objective is to develop quantitative models and theories depicting the structure of materials because that structure, in turn, relates to and controls their behavior and performance. Advanced materials research also includes engineering behavior with a focus on the influence of synthesis and processing on materials structure and properties. Physical behavior of materials is concerned with understanding the mechanisms for various forms of physical behavior, particularly under conditions that interact with and change the bulk and/or surface structure of the material. The objective is to predict physical behavior by developing mechanistically rigorous computational models of materials response under imposed electrical fields and thermal and environmental stimuli, drawing upon fundamental structural models and theories as needed. The basic research program specifically targets the needs of the DOE technology programs and, therefore, has significant impacts on energy generation, transmission, conversion, and conservation technologies. This research is conducted at national laboratories and universities. Significant research that brings together basic and applied researchers takes place under the distributed Center of Excellence for the Synthesis and Processing of Advanced Materials.

Research Challenges and Opportunities

The challenge lies in improving the understanding of the structure of materials and the relationship of structure to behavior and performance to such a degree and extent that this understanding will form the basis for predictive models. These predictive models would then be used to improve the behavior and performance of existing materials or to design new materials with superior behavior and performance. Other challenges are to understand the mechanisms and dependencies of physical behavior and their responses to perturbing stimuli or fields such that valid predictive models or simulations can be developed. These models will help to accurately predict the physical behavior of materials under untested perturbing stimuli or for new and yet unknown materials. Sound predictive models or simulations are likely to guide research efforts toward more significant discoveries, and in a more cost-effective manner than is currently possible.

Research Activities

Activities include the synthesis and processing of materials with new or improved behavior and/or with reduced waste by-products; hard and wear resistant surfaces to reduce friction and wear; high-rate, superplastic forming of lightweight, metallic alloys for fuel-efficient vehicles; and high-temperature structural ceramics and ceramic matrix composites for high-speed cutting tools and fuel-efficient and low-pollutant engines. Quantitative, non-destructive analysis provides early warning of impending failure, prediction of remaining reliable service life, and on-line in-situ flaw detection during fabrication or production. Response of magnetic materials to applied static and cyclical stress in investigated. Research into plasma, laser, and charged particle beam surface modification may yield increased corrosion or wear resistance. Another advanced materials research area pertains to the processing of high-temperature, high-strength, yet fabricable intermetallic alloys; and to the welding and joining of alloys, ceramics, and dissimilar materials.

Predictive theory and modeling covers density functional, coherent potential, pseudopotential, linear combination of atomic orbitals, tight-binding, Monte-Carlo, cluster variation and other methods. Bulk metallic glasses, buckeyballs, dimensionally restricted structures and other forms of new materials are being investigated, and crystal growth, solidification and solid state phase transformation mechanisms. Crystalline defects are being characterized by existing and improved techniques of electron beam microcharacterization, atom-probe field ion microscopy, atomic force microscopy and positron annihilation spectroscopy; emphasis is on improving the precision, detectability, spatial resolution and range of validity of these techniques. Analysis and modeling are being employed to study grain boundaries, interfaces, and free surfaces. Surface phenomena are also being examined. Scientists are studying aqueous, galvanic, and high-temperature gaseous corrosion. Studies of photovoltaics and semiconductors and their junctions and interfaces are contributing to solar energy conversion, sensors, radiation detectors and other solid state devices. Scientists are studying the relationships between and among crystal defects, grain boundaries, and processing parameters to critical current density, fabricability, and other parameters of superconducting behavior for high-temperature superconductors. Phase equilibria and kinetics of reactions in materials are being studied in hostile or extreme environments such as the very high temperatures and reactive environments found in energy conversion processes and in systems that are far from thermodynamic equilibrium, e.g., steels, precipitation hardened or quenched alloys, glasses, spinodal systems, and composites; nanophase systems and finely divided powders; and diffusion and transport of ions in solid electrolytes for improved performance in batteries and fuel cells.

Accomplishments

- Very high quality films and crystals of controlled defect containing complex oxides have been grown that will improve power density and voltage in lithium-containing batteries.

- A breakthrough in understanding the processing of ceramic aerogel films has led to a new non-toxic, low temperature process to produce such films in an environmentally benign manner.

- A new understanding of how hard nitride films are formed has enabled a process to grow diamond-like cubic boron-nitride films, the second hardest known material. Unlike diamond, boron-nitride does not react with iron or steel, making it an ideal material for long-life high-speed cutting tools.

- A tenfold increase in the electrical conductivity of gallium arsenide semiconductors was achieved by creating vacant arsenic sites on the crystal lattice of gallium arsenide which act as "traps" for carbon ions. Carbon-doped gallium arsenide is a semiconductor that is attractive for application in electronic devices, such as diode lasers for reading compact discs or ultra-high speed transistors.

- A threefold increase in the fracture toughness of the structural ceramic silicon carbide was achieved by developing a sintering process that permitted a structure of interlocking plate-like grains to grow during the sintering process. This interlocking structure exhibits exceptionally high resistance to the passage of a crack, thereby increasing the fracture toughness.

- A record solar photovoltaic efficiency of 30% was achieved by acquiring a fundamental understanding of the conversion of solar energy to electrical energy by thin-film semiconductor structures, a newly developed film growth technique, and a tandem, two-stage design based on two complementary solar cells grown as one combined cell.

- Light bulbs, fluorescent tubes, and neon lights may soon become things of the past, replaced by more efficient and brighter lighting sources utilizing light emitting diodes (LEDs) based on gallium nitride semiconductors. A high-pressure spectroscopic method showed that the unexpected high excess of electrons in the manufacturing process for these semiconductors resulted from an oxidizing impurity in gallium nitride, providing a scientific basis for improving the manufacturing process for very efficient LEDs.

Engineering Sciences

Description, Objectives, and Research Performers

Research in engineering sciences is necessary to help resolve the numerous engineering issues that arise from energy production and use. Research includes work in three technical areas: (1) mechanical systems, including fluid mechanics, heat transfer, and solid mechanics; (2) systems sciences, including process control, instrumentation, and intelligent machines and systems; and (3) engineering analysis, including nonlinear dynamics, data bases for thermophysical properties, models of combustion processes for engineering applications and foundation of bioprocessing of fuels, and energy-related waste and materials. This research is conducted principally at national laboratories and universities.

Research Challenges and Opportunities

The research challenges are to extend the body of knowledge underlying current engineering practice so as to create new options for enhancing energy savings and production, for prolonging useful equipment life, and for reducing costs without degradation of industrial production and performance quality; and to broaden the technical and conceptual base for solving future engineering problems in energy technologies.

Research Activities

In mechanical systems, research activities include seeking a better understanding of diffusion at a flowing gas-liquid interface, experimental testing of the newly developed method for fracture mechanics, and a better understanding of the engineering of nanoscale systems. In systems sciences, ongoing research seeks to relate the operations of the system to the design process in complicated nonlinear chemical processing systems. In engineering analysis, porous silicon is being studied to enable its use in computer systems along with quantum dots as active elements. Scientists need to better understand the shot noise in nano-electronics and electron wave guides in nano-systems with a few electrons.

Accomplishments

- Methods to control the highly unstable chemical processes in very high-pressure reactors for low-density polyethylene production were developed; these methods are now used to prevent shutdowns of industrial reactors.

- Phenomenological understanding that relates large-scale behavior to small-scale interactions between phases led to improved methods for universal predictions of gas-liquid flow in pipelines. This will improve pipeline design and reduce failures.

- A very fast algorithm for many variables was developed for optimizing/minimizing a variety of industrially used systems; use of the algorithm for oil exploration earned an R&D 100 Award.

- A technique was developed to do a visualization of 3-D chaotic mixing. Results from the experiment compare favorably with computer simulations. Such diagnostics will be very useful for better understanding industrial mixing and will provide ways to lower costs in a diverse range of energy-intensive manufacturing processes.

- A new way to capture and focus light was developed, which founded a new field of optics. This led to better solar energy systems, such as a solar furnace operating at almost the temperature of the surface of the sun. Other practical benefits include safer and brighter tail lights on automobiles, a new light condenser for movie projectors twice as bright as previous ones, diodes that replace incandescent bulbs, protective counter measures for military aircraft and tanks, brighter screens for laptop computers and improved flat-panel TV screens.

Catalysis and Chemical Transformations

Description, Objectives, and Research Performers

Basic research in this area is related to the fundamental understanding of chemical transformations and conversions central to new or existing concepts of energy production and storage. The emphasis is on understanding the fundamental chemical principles. Catalysis is a chemical process found widely in nature and used extensively in industry because it removes energy barriers to chemical reactions. Catalysts used for refining petroleum or manufacturing chemicals are important because they reduce process energy, speed up production, and make possible the manufacture of new materials. Models for catalytic action are limited in scope and applicability. The catalysis program seeks to gain understanding of catalysis at the molecular level to allow the development of general theories and models of catalytic action. The program includes both heterogeneous (multiple phases such as liquid/solid) and homogeneous (single-phase) catalysis. Research in heterogeneous catalysis seeks to characterize the role of surface properties on molecular transformations and the structural relationships between oxide surfaces and reaction pathways, especially in the acid and redox catalysts commonly encountered in industrial applications. Research in homogeneous catalysis seeks to characterize the activation and subsequent reactions of carbon-hydrogen bonds and the role of bonding and molecular structure on the catalytic processes. The program constitutes the largest single component of the nation's basic research portfolio focused on chemical catalysis. This research is conducted at national laboratories and universities.

Research Challenges and Opportunities

New opportunities are in aqueous catalytic chemistry, understanding the interface between water and catalytic oxides, and in catalytic activation and conversion of chlorofluorocarbons. Another area is the development of catalysts and catalytic processes for the transformation of carbon dioxide, i.e., the development of chemistry for new or improved CO_2 mitigation concepts. The disciplines of organic, organometallic, inorganic, physical, and thermochemistry are central to these programs. Despite their importance, catalytic processes are not sufficiently well understood to allow rational design of new catalysts. Catalysts are crucial to energy conservation in creating new, less-energy-demanding routes for the production of basic chemical feedstocks and value-added products. The creation of new organometallic precursors has the potential provide materials that are synthesized by less-energy-intensive processes and function as energy-saving media themselves.

Research Activities

Of particular interest are research activities with the objectives of understanding the chemical aspects of catalysis, both heterogeneous and homogeneous; the chemistry of fossil resources, particularly coal, including characterization and transformation; the conversion of biomass and related cellulosic wastes; and the chemistry of precursors to advanced materials. Researchers use state-of-the-art methods to elucidate phenomena occurring at aqueous oxide interfaces with emphasis on the nature of species as they undergo the transition from solvation to surface adsorption. They determine new ways to create materials precursors, molecules that will allow the design of materials with specific physical and chemical properties. Researchers develop methods for detecting single molecular events. They create new multifunctional catalytic systems, bringing together the two basic disciplines of homogeneous catalysis and heterogeneous catalysis. Scientists study materials that are partially ordered, and understand the consequences of short-range order on molecular phenomena related to these materials. They develop tools to probe reaction-induced surface structure dynamics and develop combinatorial approaches to increase the efficiency of gaining fundamental understanding of catalytic processes.

Accomplishments

- There has been a marked improvement in understanding specific processes in catalysis over the past five years. This new fundamental knowledge has provided the basis for advances in alkane (C-H) activation, selective upgrading of methane via selective oxidation, new routes to value-added chemicals through selective oxidation of hydrocarbons, polymerization catalysis, CO and CO_2 conversion, and new catalyst concepts for emissions control which will perform under “lean burn” conditions, as required for advanced gasoline and diesel engines.

- Basic research on single site metalocene catalysts has enabled the development of a revolutionary new process for the industrial scale production of a new generation of polyolefin polymers with superior performance characteristics. The remarkable stereospecificity features of these new catalysts have led to a variety of new, advanced polymer products over a wide range of densities.

- A new nano-phase graphitic material capable of absorbing as much as three grams of hydrogen for each gram of carbon has been discovered by researchers studying catalyst deactivation. The discovery has high potential significance to hydrogen storage technology, and perhaps also to storage of other small gases.

- Fundamental studies on metal-catalyzed polymerizations have led to new materials applications. For example, a palladium-based catalytic system generates polyketone polymers used in gears for business machines, liners for flexible fuel hoses, and industrial molded parts. In another case, a low-cost, catalytic route for the manufacture of advanced polymer materials, namely, polyoxalate polymer resins, are now under study for use in making bioabsorbable sutures.

Portfolio Summary

This portfolio area, “Efficient Energy Use,” encompasses research from many programs and supporting activities that crosscut the research topics covered above. The table below summarizes specific programs that strongly support or moderately support Efficiency Energy Use, including combustion-related sciences, advanced materials, engineering sciences, and catalysis and chemical transformations. The funding totals for these areas are an analytic tool reflecting the highly crosscutting, leveraged aspects and implications for individual research areas within DOE’s science portfolio. **Because research areas may appear in multiple chapters, there will be significant instances of multiple counting, and the chapter totals will**

not sum to the overall science budget. Additional details on these research areas are presented in the Research Summary Matrix and the corresponding Research Summary Profiles.

Strongly Supportive RSPs (Combined Budget: $278.76 Million) Advanced Computing and Communications Facility Operations Advanced Computing Software and Collaboratory Tools Catalysis and Chemical Transformations Chemical Physics Research Engineering Behavior Laboratory Technology Research and Advanced Energy Projects Mechanical Behavior and Radiation Effects Mechanical Systems, Systems Science, and Engineering Analysis Physical Behavior of Materials Scientific Computing Application Testbeds Structure of Materials
Moderately Supportive RSPs (Combined Budget: $828.68 Million) Chemical Energy and Chemical Engineering Computer Science to Enable Scientific Computing Environmental and Molecular Sciences Laboratory (EMSL) Experimental Condensed Matter Physics Experimental Program to Stimulate Competitive Research (EPSCoR) General Purpose Plant & Equipment (GPP/GPE) High Performance Computer Networks Materials Chemistry Multiprogram Energy Lab Facilities Support (MELFS) Neutron and Light Sources Facilities Neutron and X-Ray Scattering Photochemistry and Radiation Research Science Education Support Separations and Analysis Small Business Innovation Research (SBIR) Program Small Business Technology Transfer (STTR) Program Theory & Simulations of Matter, Engineering Physics
NOTE: Please see Appendix A for more information on the budgets, the research performers, and other related information for each Research Summary.