Introduction

The GCEP portfolio was dynamic during 2005-2006 as new programs were approved for funding and some initial research efforts were completed. This technical report contains updates of the research activities currently funded and recently completed.

Progress made in current research activities funded by GCEP is described by topic area in Chapter 2. Investigators provide specific progress reports that may include background, methodology, results, publications, and future directions. Chapter 3 contains reports from completed GCEP research efforts. In 2006, major projects were completed in the areas of hydrogen, CO_2 storage, and advanced combustion.

In 2006, GCEP introduced an exploratory research program. The purpose of this program is to allow exploration of new ideas by supporting preliminary research or analysis. These scoping research activities are limited to $100K and a one year performance period. Currently three efforts are funded under this program. Their reports are provided in Chapter 4.

Research and analysis activities conducted by the GCEP systems analysis staff are discussed in Chapter 5. The analysis staff, working with students, builds tools that enable the creation of energy models to allow quantitative comparisons of energy technologies

The GCEP research portfolio continues to evolve under the broad topic areas shown below.

1. Hydrogen production, storage and use
2. Solar energy
3. Biomass energy
4. Carbon sequestration
5. Carbon capture and separation
6. Advanced combustion
7. Advanced materials and catalysts
8. Integrated Assessment of Technology Options

As the GCEP portfolio develops over time, the research will expand and cover other aspects of various energy conversions.

While not an exhaustive list, each of these areas is expected to play an important and interconnected role in future energy systems and the reduction of greenhouse gas emissions (GHG). For example, hydrogen has been identified as a potential energy carrier in some energy scenarios. The research portfolio described here includes work on hydrogen storage as well as hydrogen production by microbes. Currently hydrogen is produced primarily from fossil fuels. Reduction of GHG emissions from that method of producing hydrogen would also require CO_2 capture and storage, another topic considered in this report.

Solar and biomass energy are renewable energy options that have the potential of low net emissions of CO_2. In particular biomass resources are being considered as potential alternative transportation fuels. However, research for renewable energy still needs to address issues of cost, intermittency, conversion efficiency, and energy density.

Combustion is currently, by far, the most common first step in converting the energy stored in chemical bonds to energy services for humankind. Because of its ubiquitous nature and its intimate coupling with carbon-based fuels, even small improvements to combustion technology can have significant impact on total greenhouse gas emissions whether they are from biomass or fossil resources.

If the CO_2 produced from the conversion of fossil fuels is captured and stored, a fraction of anthropogenic CO_2 emissions can be avoided. Fossil fuel combustion not only produces CO_2 but also a mix of other gases. Since the storage of CO_2 in the subsurface requires a relatively pure stream, CO_2 separation technology must be integrated into fossil fuel conversion systems. Furthermore, the capture system and storage reservoir should be located nearby to optimize the coupling of the processes. The primary geologic settings that have been considered for CO_2 storage are depleted oil and gas reservoirs, deep saline aquifers, and coal beds.

The development and advancement of materials is an encompassing need in systems that extract, distribute, store or use energy. The performance of these systems depends on the materials. Plastics, coatings, alloys and catalysts are some of the broad classes of materials used in current energy products. Advancements in these materials improve system efficiency and energy conversion processes, extend lifetime, and reduce CO_2 emissions.

Listed below are current and completed research efforts categorized by topic area. Detailed reports for each of the active projects are in Chapter 2. Completed projects noted with an asterisk (*) are in Chapter 3.

1. Hydrogen

    a. Biohydrogen Generation (Professors J. R. Swartz, Chemical Engineering and A. M. Spormann, Civil and Environmental Engineering) – develop an organism/bioreactor system employing a genetically engineered organism that will directly convert sunlight to hydrogen.

    b. Direct Solar Biohydrogen: Part II (Professors J. R. Swartz, Chemical Engineering and A. M. Spormann, Civil and Environmental Engineering) – following the successful expression of active oxygen-tolerant hydrogenase in cell-free reaction, this project investigates genetic engineering techniques to express it in *synechocystis* bacteria and couple it effectively to ferrodoxin

    c. Nanoengineering of Hybrid Carbon Nanotube-Metal Nanocluster Composite Materials for Hydrogen Storage (Professors K. Cho, Mechanical Engineering, B. M. Clemens, Materials Science and

Engineering, H. Dai, Chemistry, A. R. Nilsson, Stanford Synchrotron Radiation Laboratory) – develop optimized nanocomposite materials for high-density H_2 reversible-storage applications.

d. Hydrogen Effects on Climate, Stratospheric Ozone and Air Pollution (Professors M. Z. Jacobson, Civil and Environmental Engineering, D. M. Golden, Mechanical Engineering) – study the potential effects on global and regional climate, stratospheric ozone, and air pollution of replacing fossil-fuel-based vehicles and electric power plants with those powered by hydrogen fuel cells.

e. Solid-State NMR Studies of Oxide Ion Conducting Ceramics for Enhanced Fuel Cell Performance (Professors J. F. Stebbins, Geological and Environmental Sciences, F. B. Prinz, Mechanical Engineering) – develop new understanding of the atomic-scale structure and dynamics of the oxide ion conducting ceramic materials which are the heart of Solid Oxide Fuel Cells.

f. Modeling, Simulation and Characterization of Atomic Force Microscopy Measurements for Ionic Transport and Impudence in PEM Fuel Cells (Professor P. M. Pinsky, Mechanical Engineering, Professor D. M. Barnett, Materials Science and Mechanical Engineering) - examine the properties of solid polymer membranes through modeling of ion transport, impedance, diffusion and atomic force microscopy imaging.

*****g. Nanoscale Electrochemical Probes for Monitoring Bioconversion of Hydrogen (Professor F. B. Prinz, Mechanical Engineering) – develop nano scale sensors to monitor the electro-chemistry of hydrogen production in microbes. The sensors are designed to measure reduction-oxidation reactions, electron transfer reactions, and the broader kinetics of biochemical processing within the cell.

*****h. Understanding, Predicting and Measuring Conductivity in Fuel Cell Electrolytes (Professor F. B. Prinz, Mechanical Engineering) – delineate the relationship between electrocatalyst geometry and electrochemical behavior using platinum microelectrodes on a polymer electrolyte fuel cell. Develop the nanoscale technique of atomic force microscopy impedance imaging to allow highly localize measurements of electrochemical properties.

2. Renewable Energy – Solar

a. Nanostructures Photovoltaic Cells (Professor M.D. McGehee, Material Science and Engineering) – develop ordered bulk heterojunctions for efficient organic photovoltaic cells that could be deposited in reel-to-reel coaters.

b. Is Bioelectricity Possible (and Economically feasible?) (Professor F.B. Prinz, Mechanical Engineering) – explore the possibility of capturing electricity directly from living biological cells by inserting nano-scale electrodes into their chloroplasts.

c. Nanostructured Metal-Organic Composite Solar Cells (Professor M. Brongersma, Materials Science and Engineering) – develop organic multijunction photovoltaic cells that use metal nanoscale features to enhance both photon absorption and charge transport.

d. Inorganic Nanocomposite Solar Cells by Atomic Layer Deposition (Professor S.F. Bent, chemical Engineering) – design photovoltaic devices using nanostructured inorganic semiconductor composites deposited by Atomic Layer Deposition techniques.

e. Nanostructured Silicon-Based Tandem Solar Cells (Professor M.A. Green, University of the New South Wales) – develop multijunction thin-films based on polycrystalline-silicon and higher bandgap silicon compounds with embedded silicon quantum dots for enhanced photon absorption.

f. Advanced Materials and Devices for Low Cost and High Performance Organic Photovoltaic Cells (Professor Z. Bao, Chemical Engineering) – develop novel organic materials for efficient photon absorption in the infrared spectrum and enhanced exciton diffusion.

3. Renewable Energy – Biomass

a. Genetic Modification of Plant Cell Walls for Enhanced Biomass Production and Utilization (Professor C. R. Somerville, Biological Sciences) – increase the production of cellulose by increasing the expression of the genes encoding the components of cellulose synthase.

b. Directed Evolution and Genomic Analysis of Novel Yeast Species for More Efficient Biomass Conversion (Professor G. J. Sherlock, Genetics, Professor F. Rosenzweig, Biological Sciences, University of Montana) - develop novel, adaptively evolved, hybrid yeast strains capable of aggressively fermenting sugars at elevated temperatures and ethanol concentrations from pretreated forest and agricultural residuals.

4. CO_2 Sequestration

a. Assessing Seal Capacity of Exploited Oil and Gas Reservoirs, Aquifers and Coal Beds for Potential Use in CO_2 Sequestration (Professor M. D. Zoback, Geophysics) – develop tools to determine how changes in the state of stress in oil and gas reservoir rocks, coal beds, and aquifers with CO_2 injection affect the ability of those formations to retain the CO_2.

b. Subsurface Monitoring of CO_2 Storage (Professor J. M. Harris, Geophysics) – develop an appropriate suite of monitoring tools to detect movement of injected CO_2 in the subsurface.

c. A Numerical Simulation Framework for the Design, Management and Optimization of CO_2 Sequestration in Subsurface Formations (Professor H. A. Tchelepi, Professor L. J. Durlofsky, Professor K. Aziz, Petroleum Engineering) - build a numerical simulation framework that allows for the design, management and optimization of subsurface CO_2 sequestration operations.

d. Geologic Storage of CO_2 in Coal Beds (Professors J. M. Harris and M. D. Zoback, Geophysics, Professors A. R. Kovscek and F. M. Orr, Jr., Petroleum Engineering) – investigate geologic storage of CO_2 with a focus on the properties and geomechanics of deep coal beds as well as the prediction, simulation, and monitoring of CO_2 flow within the beds.

*e. Rapid Prediction of CO_2 Movement in Aquifers, Coal Beds, and Oil and Gas Reservoirs (Professors A. R. Kovscek and F. M. Orr, Jr., Petroleum Engineering) – develop efficient reservoir simulation tools to calculate how injected CO_2 will flow in oil and gas reservoirs, coalbeds, and saline aquifers.

5. CO_2 Capture and Separation

a. Advanced Membrane Reactors in Energy Systems: A Carbon-Free Conversion of Fossil Fuels (Dr. D. Jansen, ECN Netherlands, Professor J. Schoonman, Technical University of Delft) – develop hydrogen and CO_2 membranes to allow combination of natural gas reforming with H_2 or CO_2 separation enhanced reactors, membrane reactors for carbon-free hydrogen production or electricity generation.

b. Development of Innovative Gas Separation Membranes Through Sub-Nanoscale Materials Control (Dr. Eng. Yamada, RITE Japan) - develop a variety of efficient, low-cost polymeric and inorganic membranes that separate CO_2.

6. Advanced Combustion

a. Development of Low-Irreversibility Engines (Professor C. F. Edwards, Mechanical Engineering) – investigate the potential to design and implement engines with significantly reduced irreversibility.

b. Development of Low-Exergy-Loss, High-Efficiency Chemical Engines (Professor C. F. Edwards, Mechanical Engineering) – design and fabricate a low-irreversibility engine based on theoretical results from the earlier study on the development of low-irreversibility engines.

c. Smart Sensors for Advanced Combustion Systems (Professor R. K. Hanson, Mechanical Engineering) – develop advanced sensors for use in energy systems that minimize environmental impact via control of combustion-generated pollutants such as NO, CO and unburned hydrocarbons, reduce CO_2 emissions by improving combustion efficiency and monitor the fugitive emissions from greenhouse gas sequestration efforts.

d. Characterization of Coal and Biomass Conversion Behaviors in Advanced Energy Systems (Professor R. E. Mitchell, Mechanical Engineering) – develop experimentally validated models that predict coal and biomass gasification and combustion behaviors.

e. Optimization of Synthetic Oxygenated Fuels for Diesel Engines (Professor C. T. Bowman, Mechanical Engineering) – investigate oxygenated fuels for compression-ignition engines which would react along a pathway that minimizes soot formation.

*****f. Controlled Combustion: An Approach for Reducing Irreversibilities in Energy Conversion (Professor C. T. Bowman, Mechanical Engineering) – develop and experimentally validate detailed models of combustion chemistry for use in modeling low-irreversibility combustion engines.

*****g. Process Informatics Model: A Systematic Approach to Building Combustion Chemistry Models (Professor D. M. Golden, Mechanical Engineering) – convert the process of combustion chemistry model building into science, automate the methodology and make the information available in a prompt and convenient form on the Internet for researchers and designers of combustion equipment.

7. Advanced Materials and Catalysts

a. Efficient Interconversion of Chemical and Electrical Energy: Electrocatalysis with Discrete Metal Transition Complexes (Professor C. E. Chidsey, Chemistry) - develop efficient catalysts for direct-hydrocarbon fuel cells by investigating various configurations of late-metal multi-metallic catalyst complexes as electrooxidation catalysts, and examining biologically inspired mono- and multi-metallic copper complexes electroreduction catalysts.

8. Integrated Assessment of Technology Options

   a. Integrated Assessment of Energy Technologies (Prof. J. Sweeney, J. Weyant, Engineering and Management Science) - develop a comprehensive analysis system that can be used to estimate probable significance of technologies, to explore options to speed up diffusion of technologies, and to determine the magnitude of potential reductions in greenhouse gas emissions.