

Introduction

This report summarizes research progress during 2004-2005 for projects being conducted as part of the Global Climate and Energy Project (GCEP) at Stanford University. The current GCEP portfolio includes research in the following areas:

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

Each of these areas has potentially important roles to play in future systems that supply, transform, and use energy in a way that allows for substantially lower emissions of greenhouse gases than the systems in use today. Combustion, for example, is the primary means by which stored chemical energy in fossil fuels or biomass is made available for conversion into work. If more efficient means of conversion of chemical energy into work can be found, the emissions of CO₂, nitrogen oxides, and black carbon can be reduced.

Renewable technologies, like wind, biomass and solar generation of electricity, for example, have the potential to reduce greenhouse gas emissions by offsetting the use of fossil fuels, if the costs of providing those technologies can be reduced so that they are competitive with other methods of generation. Biomass has additional value as a resource for transportation fuels or carbon storage.

Molecular hydrogen is another carrier of chemical energy, one that must be manufactured using some other energy resource. Hydrogen has appeared attractive as an energy carrier, because the conversion of its chemical energy into work emits no CO₂. Nevertheless, current methods of manufacturing and storing molecular hydrogen require significant energy inputs that emit CO₂. Techniques that allow hydrogen production without CO₂ emission are needed if substantial use of hydrogen is to be accompanied by reductions in greenhouse gas emissions.

The capture of CO₂ generated by combustion of fossil fuels or biomass or manufacture of hydrogen, along with subsequent storage of that CO₂ in a location other than the atmosphere may also contribute to reductions in carbon emissions. The magnitude of greenhouse gas emissions from anthropogenic activity provides a compelling need for CO₂ capture, separation, and sequestration.

Research on advanced materials is connected to many of the areas and is an overarching topic, including renewables, and hydrogen storage and use.

The chapters that follow describe research activities, report results, and outline future plans for projects being led by thirty-one principal investigators in twelve departments at Stanford. Chapter 2 provides details for the following projects:

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. Nanoscale Electrochemical Probes for Monitoring Bioconversion of Hydrogen (Professor F. B. Prinz, Mechanical Engineering) – develop nanoscale 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.
- c. 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 localized measurements of electrochemical properties.
- d. 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 H₂ reversible-storage applications.
- e. 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.
- f. 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.

- g. Modeling, Simulation and Characterization of Atomic Force Microscopy Measurements for Ionic Transport and Impedance 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.
2. Renewable Energy - Solar
 - a. Nanostructured Photovoltaic Cells (Professor M. D. McGehee, Materials Science and Engineering) – develop efficient photovoltaic cells with semiconducting polymers 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.
 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. CO₂ Sequestration
 - a. Assessing Seal Capacity of Exploited Oil and Gas Reservoirs, Aquifers and Coal Beds for Potential Use in CO₂ 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 CO₂ injection affect the ability of those formations to retain the CO₂.
 - b. Rapid Prediction of CO₂ 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 CO₂ will flow in oil and gas reservoirs, coalbeds, and saline aquifers.

- c. Subsurface Monitoring of CO₂ Storage (Professor J. M. Harris, Geophysics) – develop an appropriate suite of monitoring tools to detect movement of injected CO₂ in the subsurface.
 - d. A Numerical Simulation Framework for the Design, Management and Optimization of CO₂ 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 CO₂ sequestration operations.
5. CO₂ 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 CO₂ membranes to allow combination of natural gas reforming with H₂ or CO₂ separation enhanced reactors, membrane reactors for carbon-free hydrogen production or electricity generation.
6. Advanced Combustion
- a. 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.
 - b. Development of Low-Irreversibility Engines (Professor C. F. Edwards, Mechanical Engineering) – investigate the potential to design and implement engines with significantly reduced irreversibility.
 - 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 CO₂ 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. 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.

Chapter 3 reports progress in technical analysis activities that support the overall project. The first is an Energy Systems Analysis project, led by A.J. Simon of the GCEP staff. This effort is intended to provide a capability for tracing of mass and energy flows for energy systems, so that quantitative comparisons of energy technologies can be made, and to make that capability available for general use via web-based tools. The second is a project entitled Integrated Assessment of Energy Technologies, led by Professors John Weyant and James Sweeney in the Management Science and Engineering Department. The Integrated Assessment project is aimed at developing 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.

The current GCEP portfolio is not complete. There are additional areas that will need to be addressed in a balanced portfolio of research on energy technologies with low greenhouse gas emissions. Thus, the current research portfolio should be viewed as a work in progress, which will develop and grow as more projects are added in the next years.