Hydrogen Energy Coordinating Committee Annual Report-Summary of DOE Hydrogen Programs for FY 1991-1992

May 1993

U.S. Department of Energy
Assistant Secretary, Energy Efficiency and Renewable Energy
Office of Energy Management
Washington, DC 20585

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INTRODUCTION

Technologies to use hydrogen as an energy carrier and fuel have been under development since the oil embargo of the early 1970s sent price shocks through the U.S. energy economy. Hydrogen's long-term potential value lies primarily in serving as an energy carrier whose consumption at the point of use can be achieved with little or no pollution and in some applications, with high efficiency. Hydrogen is not a primary energy source, but must be produced using renewable energy, natural gas, coal or other energy sources.

Late in 1990, Public Law 101-566, the Spark M. Matsunaga, Hydrogen Research Development and Demonstration Act of 1990 was passed. The Matsunaga Act required that a comprehensive five-year hydrogen program management plan for research and development be prepared. The plan, entitled *Hydrogen Program Plan, FY 1993 - FY 1997* (U. S. Department of Energy Report No. DOE/CH10093-147) was issued in June 1992.

The HECC was established over 14 years ago to ensure that the many varied aspects of hydrogen technology research and development within the Department are coordinated. Each year the committee brings together technical representatives within the Department to coordinate activities, share research results and discuss future priorities and directions. An annual report is published summarizing the work in progress. The last report issued was "Hydrogen Energy Coordinating Committee Summary of DOE Hydrogen Programs for FY 1991," U.S. Department of Energy Report No. DOE/CE-0341, July 1991.

This summary is the fourteenth consecutive report. It provides an overview of the hydrogen-related programs of the DOE offices represented in the HECC. For the purposes of this report, the research projects within each division have been organized into two categories:

- 1) **Fuels-related Research:**
Includes research on projects or issues directly related to hydrogen as a potential fuel, and

2) Non-fuels related Research:

A variety of projects which contribute to the understanding of the physics and chemistry of hydrogen.

A historical summary of the hydrogen budgets of the several divisions is given in Table 1. Tables 2a and 2b provide a detailed distribution of the projects by fuels and non-fuels related program elements for FY 1992. Total DOE funding in FY 1992 was \$4.6 million for fuels-related research and \$27.8 million for non-fuels related research. The individual program elements are described in the body of this report, and more specific program information can be found in the Technology Summary Forms in Appendix A. It may be noted that in Tables 1 and 2, and in the Appendix, the activities under the Assistant Secretary, Energy Efficiency and Renewable Energy (EE), and presented under Conservation and Renewable Energy (CE), the designation used during the period covered by this report.

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Table 1. DOE Hydrogen Research Funding Summary
(dollars in millions)

Research Area	FY 1976-88	FY 1989		FY 1990		FY 1991		FY 1992	
		Fuels Related	Non-Fuels Related	Fuels Related	Non-Fuels Related	Fuels Related	Non-Fuels Related	Fuels Related	Non-Fuels Related
DOE HYDROGEN	417.2	5.2	31.7	6.8	36.2	5.7	29.4	4.6	27.8
R&D TOTALS									
Energy Research/ Basic Energy Sciences (BES)	245.4	0.3	16.2	0.3	16.7	0.4	16.4	0.4	16.7
Conservation & Renewable Energy (CE)	70.3	3.0	0.0	2.2	0.0	2.6	0.0	2.1	0.0
Fossil Energy (FE)	22.9	1.9	0.0	3.3	3.3	1.7	0.0	1.1	0.0
Energy Research/ Fusion Energy (OFE)	16.4	0.0	5.3	0.0	0.5	0.0	0.0	0.0	0.0
Defense Programs/Research & Advanced Technology	62.2	0.0	10.2	1.0	15.7	1.0	13.0	1.0	11.1

Table 2a. FY 1992 Fuels Related
Hydrogen Energy Research and Development by DOE Program Element
(dollars in millions)

Divisions/Projects	Page #	Total	Production	Storage	Transport/ Materials	End Use
DOE HYDROGEN R&D TOTALS		4.597	1.807	1.149	1.000	0.641
Energy Research/Basic Energy Sciences		0.400		0.400		
Hydride Research	A2	0.400		0.400		
Fossil Energy		1.149	1.149			
Gas Separation using Ion Exchange	A3	0.006	0.006			
Production of Hydrogen & By-Product from Coal	A4					
Hydrogen Separation by Ceramic Membranes in Coal Gasification	A5	0.019	0.019			
Novel Hydrogen Separation Device	A6	0.095	0.095			
Fundamentals of Catalytic Gasification	A7	0.108	0.108			
Production of Low Cost Hydrogen	A8	0.099	0.099			
Rapid Pressure Swing Absorption Cleanup	A9					
Silica Membranes for Hydrogen Separation in Coal Gas Processing	A10					
Process for Bulk Separation of Carbon Dioxide using CaO	A11	0.094	0.094			
Process for Bulk Separation of Carbon Dioxide using MgO	A12	0.022	0.022			
Biological Conversion of Synthesis-Gas to Hydrogen	A13	0.200	0.200			
Biological Production of Hydrogen	A14					
Catalytic Membrane Reactor for Water-Gas-Shift	A15	0.500	0.500			
Conservation & Renewable Energy/Industrial Technology		0.400		0.400		
Magnetic Refrigerator (MR) for Hydrogen Liquefaction	A16	0.400		0.400		

Table 2a. FY 1992 Fuels Related (continued)
Hydrogen Energy Research and Development by DOE Program Element
(dollars in millions)

Divisions/Projects	Page #	Total	Production	Storage	Transport/ Materials	End Use
Conservation and Renewable Energy/Utility Technology		1.176	0.684	0.349		0.163
Hydrogen from Renewables Research	A17	0.166	0.083	0.083		
Hydrogen Safety & Storage and Photobiological Production	A18	0.164		0.066		0.098
Program Support and Photoconversion Processes for Hydrogen Production	A19	0.250	0.250			
Hydrogen Production from Renewable Energy	A20	0.152	0.152			
Hydrogen Hydride Storage, Photo-Electrical Hydrogen Production and Supercritical Water	A21	0.252	0.179	0.073		
Hydrogen Energy Systems Studies	A22	0.005				0.005
Activated Carbon-Based Storage System	A23	0.127		0.127		
Engineering Evolution of Hydrogen Uses and Production	A24	0.010				0.010
Hydrogen Technology Assessment and Information Transfer Program	A25	0.050				0.050
Conservation and Renewable Energy/Transportation Technologies		0.478				0.478
Advanced Hydrogen/Methane Utilization Technology Demonstration	A26	0.200				0.200
A Direct-Injected, Hydrogen-Fueled Engine Technology Demonstration	A27	0.224				0.224
Elimination of Abnormal Combustion in a Hydrogen-Fueled Engine	A28	0.054				0.054
Defense Programs Research & Advanced Technology		1.000			1.000	
Materials for Solid Storage	A29	1.000			1.000	

Table 2b. FY 1992 Non-Fuels Related
Hydrogen Energy Research and Development by DOE Program Element
(dollars in millions)

Division/Projects	Page #	Total	Basic Studies	Long-Range Hydrogen Energy			
				Production	Storage	Transport/ Materials	End Use
DOE HYDROGEN R&D TOTALS		27.810	23.500		1.040	2.830	0.440
<i>Energy Research/Basic Energy Sciences</i>		<i>18.700</i>	<i>18.700</i>				
Photochemical Generation of Hydrogen	A30	13.500	13.500				
Hydrogen Effects on Solids & Properties of Hydrides	A31	1.800	1.800				
Biological Mechanisms of Hydrogen Generation	A32	1.100	1.100				
Kinetics	A33	0.300	0.300				
<i>Defense Programs/Research and Advanced Technology</i>		<i>11.110</i>	<i>5.800</i>		<i>1.040</i>	<i>2.830</i>	<i>0.440</i>
Computer Modeling of Hydrogen and Helium in Metals	A34	0.200	0.200				
Hydrogen Transport and Trapping in Metals	A35	0.200				0.200	
Hydrogen Transport and Trapping in Metal Hydrides	A36	0.200				0.200	
Mechanical & Fracture Properties of Materials Containing Hydrogen Isotopes & Helium	A37	1.500	1.500				
Physics of Aging in Metal Tritides	A38	2.000				2.000	
Operation and Maintenance of the Tritium Research Laboratory	A39	5.100	5.100				
Studies of Hydrogen Isotopes in Metals	A40	0.430				0.430	
Metal Hydride Research	A41	1.040			1.040		
X-Ray Diffraction Studies	A43	0.200					0.200
Heat of Formation	A44						
Stoichiometry Changes and Helium Retention	A45	0.240					0.240
<i>Defense Programs/Research and Testing and Acquisition</i>							
Hydrogen Interaction With Materials	A46						
Metal-Hydrogen Reactions	A47						
<i>Domestic and International Energy Policy</i>							
Monitoring Policy	A48						

DOE PROGRAM DESCRIPTIONS

Energy Research/Basic Energy Sciences (ER/BES)

The BES research relevant to the DOE hydrogen program is supported by three divisions: Chemical Sciences, Energy Biosciences and Materials Sciences. The broad objectives of the research are to understand those chemical, physical and biological problems that are related to such topics as photochemical, electrolytic and chemical relations in which hydrogen plays an important role.

In the Division of Chemical Sciences, a variety of photochemical hydrogen research efforts are directed toward understanding the photosynthetic and biological processes which may lead to the utilization of solar energy. The photochemical research includes picosecond and femtosecond spectroscopy, porphyrin chemistry, photochemical mechanisms and kinetics, photoelectrochemistry, photoinduced electron transfer in mixed organic-inorganic systems, etc. Although very few of these projects are specifically and strictly focused on hydrogen production, the photochemistry is relevant to hydrogen production as well as to the production of electricity or other fuels. Chemical research on hydrides related to the storage of hydrogen includes synthesis, characterization and property studies of various hydride systems.

The Energy Biosciences program explores hydrogen production in a variety of organisms (algae, bacteria etc.). In this program, the emphasis is to define the mechanisms by which hydrogen is evolved and quantitatively establish the parameters governing hydrogen production.

Materials Sciences research efforts focus primarily on the effects of hydrogen on the properties of materials, the structure and behavior of minority phase hydrides and hydrogen embrittlement studies. Topics include thermodynamics, hydrogen solubility in solids, hydrogen occupancy sites within the crystal structure, diffusion, hydrogen trapping sites at lattice defects, internal reactions such as hydrogen or methane bubble formation, hydrogen dislocation reactions, electrical conductivity of hydrides (super-conductivity), surface-induced phenomena, use of ion accelerators for proton implantation or bombardment for simulation of irradiation creep, and development of neutron scattering/diffraction methods.

Conservation and Renewable Energy (CE)

In FY 1991-1992 the hydrogen program was administered by the Conservation and Renewable Energy through the Office of Utility Technologies (CE/OUT). Field management of the hydrogen program is conducted by the National Renewable Energy Laboratory (NREL). The program includes research and development focused on technologies in the areas of hydrogen storage, production, and systems.

Several different hydrogen storage concepts are being investigated. No one technology is expected to be universally used when hydrogen enters the energy infrastructure, since various applications are anticipated within the next ten years, hydrogen will probably begin to be demonstrated in both mobile and stationary applications. For mobile (transportation) applications, storage modules are needed which have minimal volume and are light-weight. For stationary applications, modules with high efficiency and low cost are preferred, while volume and weight are of less concern. Storage concepts which are of interest include metal hydrides, cryogenic adsorption and high pressure containers.

Hydrogen production R&D focuses on the need for the direct conversion of photon energy and water to hydrogen. Several photoconversion processes are candidates to meet this need. Photoconversion processes are classified into three categories: 1) Photobiological: 2) Photoelectrochemical: and 3) Photochemical. Each of these have potential, but are in very early stages of technical development.

Renewable hydrogen production research must be continuously evaluated within a context of an overall energy system (production, storage, distribution, and use) to ensure that the research goals and selected approaches are consistent with technologies in those areas. Where there is a conflict or a need for technical advances in other areas, these must be identified and considered when recommending specific production processes for further development. The goal of the supporting research is to provide a framework for the ongoing research and to look for new opportunities.

Fossil Energy (FE)

Hydrogen R&D under the Surface Gasification Program is directed toward developing a hydrogen-rich gas product from coal that can be used to upgrade other coal-derived products or as feedstock for fuel-consuming devices. The process to produce the hydrogen-rich gas stream would be an integral part of the design of the end-use application.

Types of end-use applications which could use hydrogen include the upgrading of liquid products that are produced by direct liquefaction and mild gasification, and as feed to fuel cells, turbines, or diesels. The current areas of investigation are catalytic gasification of coal, improved shift catalysts, and improved gas separation techniques.

Hydrogen R&D under the Fuel Cell Program is concerned with fuel processors which will convert natural gas to fuel cell quality feed. The areas of investigation include low-pressure drop catalysts and improvement of tube material for high temperature/pressure conversion at a low cost. Possible end-use applications which are under evaluation include fuel cells.

Defense Programs/Research and Advanced Technology (RA)

The primary objective of the hydrogen-related project within this program has been the evaluation of the potential application of fusion energy for production of chemical synfuels. The program activities are focused on the preliminary conceptualization of fusion blanket systems and the assessment of high temperature electrolytic and/or chemical processes for the production of hydrogen. Preliminary cycle flow sheets and engineering analysis of blanket configurations have been developed. Current efforts address hydrogen recycling, transport, release and erosion properties of materials relevant to fusion reactors, and tritium extraction processing and handling associated with the fusion fuel reactors, and tritium extraction processing and handling associated with the fusion fuel cycle.

In the inertial fusion process, energy is produced through the fusion of deuterium and tritium fuel contained in a tiny glass or metal spheres referred to as pellets. The hydrogen-related research within the program consists of: (1) developing fabrication techniques for inertial confinement fusion pellets containing the hydrogen isotopes deuterium and tritium; (2) studying the physical

and chemical properties of cryogenic deuterium and tritium; (3) determining the effects of deuterium and tritium on the strength of inertial confinement fusion pellet materials; (4) studying the permeation of deuterium and tritium through various fuel pellet shells at both elevated and room temperatures; and (5) determining the potential for using inertial confinement fusion to produce hydrogen.

Research on hydrogen for military applications is ongoing and will remain an important effort in the foreseeable future. Information developed in the unclassified research projects may be of interest to other users of hydrogen. Research areas include compatibility and interaction of hydrogen with various materials, hydrogen-induced crack growth experiments, and computer modeling studies.

R&D projects related to hydrogen fuel for transportation are in progress. Accurate, dependable cylinder-to-cylinder air-fuel ratio control is necessary for internal combustion engines, but it is very difficult to achieve with hydrogen. Research is underway to identify a workable fuel injection system. A prototype system for a multi-cylinder engine is being developed for future prototype demonstration.

Other Offices

Other DOE offices which have interest in hydrogen programs, but do not presently fund research, include Nuclear Energy, the Energy Information Administration (EIA), Health and Environmental Research (HER), Operational Safety (OS), and Policy Planning and Analysis (PE). A joint program between DOD and NASA deals with the modeling of the reaction kinetics of hydrogen/oxygen for the National Aerospace Plane.

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APPENDIX A
DOE Hydrogen Research Technology Summary Forms

DOE Hydrogen Research and Technology Summary

Office Energy Research (OER)/Basic Energy Sciences

Topic Hydride Research

Type of Project (check one) Fuels-Related X Non-Fuels-Related _____

Cognizant

Division Chemical Sciences

Principal

Contact J. L. Burnett **Phone** (301) 353-5804

Other Sponsoring

Organization(s) _____ **Contractor(s)** Brookhaven National Laboratory

Summary

Date June 1992

Start

Date 1986

Scheduled

Completion Open

Status _____

Funding (\$10⁶) FY 1990 0.3 FY 1991 0.4 FY 1992 0.4 To Completion _____

Objective (or goal):

To discover new hydrogen-storing compounds, to understand the chemistry of hydrogen interactions and transport in hydride systems.

Purpose (background and reason for work):

The purpose is twofold: (1) enlarge our understanding of the chemical interactions of hydrogen with matter, and (2) provide the understanding important to the economical and safe storage of hydrogen. Reversible hydrogen reactions with metallic and inorganic substances constitute a chemical approach to energy storage. Understanding the chemistry, thermodynamics, and transport of hydrogen as it interacts with storage materials strengthens our capability to improve such energy storage systems.

Summary:

The research includes synthesis, characterization, and property studies of hydride systems relevant to the storage of hydrogen. The hydrogen chemistry of pure metals, alloys, and metal-nonmetal compounds is studied to characterize important thermodynamic, structural, electronic, and transport properties which aid in the design of materials with potential for hydrogen absorption. Recent studies seek to determine the thermodynamic properties of substituted AB₃H_x alloys which are of interest for use as battery electrodes.

Next Phase:

Continuing long-range research as described above.

DOE Hydrogen Research and Technology Summary

Office Fossil Energy (FE)

Topic Gas Separation Using Ion Exchange Membranes for Producing Hydrogen from Synthesis Gas

Type of Project (check one) Fuels-Related X Non-Fuels-Related

Cognizant METC Technology Base Principal

Division Proj. Management Div. Contact V.K. Venkataraman Phone (304) 291-4105

Other Sponsoring Organization(s) U.S. Department of Commerce
Contractor(s) National Inst. of Standards & Tech.

Summary Start Scheduled
Date July 1992 Date May 1986 Completion September 1992 Status Ongoing

Funding (\$10⁶) FY 1990 0.125 FY 1991 0.102 FY 1992 0.006 To Completion 0.097

Objective (or goal):

To determine the selective separation desired for the production of hydrogen from coal gasification using carrier-impregnated ion exchange membranes. The purpose of this work is to develop a novel process which will reduce the cost associated with gas separation.

Purpose (background and reason for work):

Conventional processes for gas separation require adsorption at feed stream pressure and subsequent regeneration at reduced pressure and elevated temperatures. The separation process may consume 30 to 80 percent of the capital costs of gas processing and approximately 50 percent of the energy. Novel separation techniques, such as membrane separation, could substantially reduce the high costs of separation processes and make hydrogen production from coal economically attractive.

Summary:

The separation problems associated with the production of H₂ via coal gasification are the removal of CO₂ and H₂S and the separation of CO₂ and H₂. This project will evaluate the feasibility of using facilitated transport liquid membranes for these separations. The effect of pressure, temperature, feed gas concentration, carrier chemistry, and membrane configuration on the performance of the membranes will be determined. Mathematical models for the predictions of experimental results, scale-up, process design, and optimization of a membrane-based separation scheme for hydrogen production will be developed. Initial results on cationic type ion exchange films resulted in more extensive membrane testing on one type of membrane. Recent work has been co-funded by the Fuels Resources Management Division and the work has emphasized the separation of methane from nitrogen and carbon dioxide.

Next Phase:

Future work will depend on the successful completion of the present project and the projected economics of the process in comparison to conventional methods of separation.

Office Fossil Energy (FE)

Topic Production of Hydrogen and Byproduct from Coal

Type of Project (check one) Fuels-Related x Non-Fuels-Related

Cognizant Division METC Coal Conversion and Cleanup Branch

Principal
Contact Justin Beeson **Phone** (304) 291-4671

Other Sponsoring Organization(s) (UNDEERC) Univ. of North Dakota
Contractor(s) Energy & Environmental Res. Center

Summary	Start	Scheduled	
Date July 1992	Date April 1986	Completion Sept. 1992	Status Ongoing

Funding (\$10 ⁶)	FY 1990	0.500	FY 1991	0.620	FY 1992	0.000	To Completion
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To: 1) develop kinetics for hydrogen production; 2) develop a process for producing activated carbon from coal; 3) combine the quench system with liquid separation; and 4) evaluate the use of hydrogen from steam gasification of coal to fuel molten carbonate fuel cells.

Low-rank coals may be an ideal feedstock for producing low cost hydrogen because these coals are inexpensive (\$.75 to \$1.00 per million Btu), highly reactive to steam, and have ash components which may serve as catalysts. Bench-scale steam-char gasification tests have produced a product gas stream containing over 60 percent hydrogen and carbon conversion rates that are 10 times higher than that obtained with bituminous coal. The addition of disposable catalysts such as trona or nacholite (naturally occurring alkali carbonate minerals) also significantly increase the rate of carbon conversion.

An experimental program has been conducted in a pilot plant size 6-inch diameter fluid-bed gasification unit to confirm the laboratory findings on the effects of coal source, catalyst selection, catalyst concentration and other operating parameters on rate of carbon conversion and gas composition. Data collected have been used to make an economic assessment.

The program direction has been changed from the development of hydrogen production by catalytic steam gasification to the production of hydrogen and coproducts from coal.

Office Fossil Energy (FE)

Topic Hydrogen Separation by Ceramic Membranes in Coal Gasification

Type of Project (check one) Fuels-Related x Non-Fuels-Related

**Cognizant METC Coal Conversion and
Division Cleanup Branch**

Principal Contact R. Johnson **Phone** (301) 291-4564

Other Sponsoring Organization(s)

Contractor(s) California Institute of Technology

Summary	Start	Scheduled	
Date July 1992	Date October 1987	Completion September 1992	Status Ongoing

Funding (\$10⁶)	FY 1990	0.269	FY 1991	0.105	FY 1992	0.019	To Completion	0.120
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Improve the efficiency of hydrogen production from coal by integrating hydrogen separation and shift reaction within the gasification process. Develop hydrogen permselective silica membranes suitable for integration with the shift reactor.

Although both synthesis gas and hydrogen production require the use of the shift reaction and CO₂ removal, there is an important difference between the two flowsheets. In synthesis gas production, stage of shift reaction and CO₂ removal is adequate. In hydrogen production, CO must be eliminated completely from the product stream. Consequently, at least two stages of shift reaction and CO₂ removal are necessary. In addition, the remaining traces of CO must usually be eliminated by a final methanation step. These repeated operations and associated cooling and heating add to process complexity and cost. The combination of shift reaction and hydrogen separation by a semipermeable silica membrane will eliminate the process inefficiencies associated with these multiple process steps.

Hydrogen permselective ceramic membranes suitable for integration with the coal gas shift reactor will be developed. Membranes will be prepared by chemical vapor deposition of silica films within the walls of porous Vycor tubes. Factors which control membrane thickness, structure, and stability will be investigated. A model for the integrated shift membrane reactor will be developed. A comparative economic analysis of the integrated shift reactor-membrane hydrogen separator will be conducted.

Future work will depend on the results of this laboratory-scale experimental program.

DOE Hydrogen Research and Technology Summary

Office Fossil Energy (FE)

Topic Fundamentals of Catalytic Gasification

Type of Project (check one) Fuels-Related X Non-Fuels-Related _____

Cognizant METC Fuel Resources
Division Management Division

Principal
Contact R. Malone Phone (304) 291-4723

Other Sponsoring
Organization(s) _____ Contractor(s) Lawrence Berkeley Lab

Summary
Date July 1992 Start Date October 1, 1984 Scheduled Completion September 1992 Status Ongoing

Funding (\$10⁶) FY 1990 0.200 FY 1991 0.199 FY 1992 0.108 To Completion 0.0

Objective (or goal):

To study the basic chemistry of the reaction of carbonaceous materials with steam in the presence of catalysts to produce hydrogen and synthesis gas.

Purpose (background and reason for work):

Most coal char is not very reactive under gasification conditions. Gasification of the char remaining after devolatilization is the slowest part of the overall gasification process. Catalyzed steam gasification has been studied extensively in the past. In this project, gasification in the presence of alkali based catalysts at 600 to 800°F and atmospheric pressure has been examined. Much of the work has been done with graphite as a carbon source to insure that the observed hydrocarbon products are derived from water. The work focus has recently shifted to oxidative coupling of methane using similar catalysts.

Summary:

The steam gasification of coal char reaction can be made truly catalytic by adding cocatalytic amounts of nickel oxide to the potassium hydroxide. The CO₂/CO ratio can be varied, making it possible to produce hydrogen (H₂ + CO₂) or syngas (H₂ + CO). However, nickel is easily poisoned by ash components and sulfur. The focus of the program has been changed to the use of K-Ca catalysts which are not deactivated. The studies are being extended to examine the effects of mineral matter in the char on catalyst poisoning and on the use of K-Ca catalysts to avoid poisoning by sulfur and components in the ash. Parent coals, oxidized chars, and cheaper catalyst materials have been studied to determine the process implications. Catalyst poisoning studies have been extended to nitrogen compounds in the char. Similar catalysts have been found to catalyze the oxidative coupling methane to ethane and ethylene at low yield but 100 percent selectivity.

Next Phase:

Significant industrial interest exists for both applications. It is expected that the patented catalyst systems will be commercialized with industry cooperation.

DOE Hydrogen Research and Technology Summary

Office Fossil Energy (FE)

Topic Rapid Pressure Swing Absorption Cleanup of Post-Shift Reactor Synthesis Gas

Type of Project (check one) Fuels-Related ☒ Non-Fuels-Related ☐

Cognizant METC Technology Base Projects

Division Management Division

Other Sponsoring

Organization(s) _____

Principal

Contact V.K. Venkataraman Phone (304) 291-4105

Contractor(s) Stevens Inst. of Technology

Summary

Date July 1992

Start

Date August 1990

Scheduled

Completion Aug. 1993

Status Ongoing

Funding (\$10⁶) FY 1990 0.291 FY 1991 0 FY 1992 0 To Completion X

Objective (or goal):

Investigate the separation of gas mixtures using the novel concept of rapid pressure swing absorption (RAPSAB) of gas in a stationary absorbent liquid and combine the best features of pressure swing absorption, gas-liquid scrubbing and membrane processes in studying the cleanup of post-shift reactor synthesis gas.

Purpose (background and reason for work):

Large scale separations of gas mixtures in coal conversion processes are usually carried out by processes such as absorption in a reactive liquid, pressure swing adsorption (PSA) on solid adsorbents, cryogenic processes, selective permeation through membranes, etc. Each such technique has a specific advantage/disadvantage profile. The membrane-based Rapid Pressure Swing Absorption Process (RAPSAB) integrates locally within the gas separator device the major strengths of a number of different separation techniques to create a compact, energy-efficient, and modular process with high flux, separation factors, and purification capabilities useful in coal conversion processes.

Summary:

The novel gas separation concept of rapid pressure swing absorption (RAPSAB) will be studied using a hydrophobic microporous hollow fiber module for carbon dioxide-nitrogen mixtures with water as absorbent. The observed separation will be modeled. Next, the purification of post-shift reactor synthesis gas containing hydrogen, nitrogen, carbon dioxide, carbon monoxide, hydrogen sulfide, and methane will be studied.

Next Phase:

Future work will depend on the results of this laboratory-scale experimental program.

DOE Hydrogen Research and Technology Summary

Office Fossil Energy (FE)

Topic Silica Membranes for Hydrogen Separation in Coal Gas Processing

Type of Project (check one) Fuels-Related ☒ Non-Fuels-Related ☐

Cognizant METC Coal
Division Conversion and Cleanup Branch

Principal
Contact R. Johnson Phone (304) 291-4564

Other Sponsoring
Organization(s) _____ Contractor(s) California Inst. of Technology

Summary Start Scheduled
Date July 1992 Date September 1989 Completion September 1992 Status Ongoing

Funding (\$10⁶) FY 1990 0.283 FY 1991 0 FY 1992 0 To Completion _____

Objective (or goal):

Improve the efficiency of hydrogen production from coal by integrating hydrogen separation and shift reaction within the gasification process. Develop silica and other permselective membranes suitable for integration with the shift reactor.

Purpose (background and reason for work):

Although both synthesis gas and hydrogen production require the use of the shift reaction and CO₂ removal, there is an important difference between the two flowsheets. In synthesis gas production, one stage of shift reaction and CO₂ removal is adequate. In hydrogen production, CO must be eliminated completely from the product stream. Consequently, at least two stages of shift reaction and CO₂ removal are necessary. In addition, the remaining traces of CO must usually be eliminated by a final methanation step. These repeated operations and associated cooling and heating add to process complexity and cost. The combination of shift reaction and hydrogen separation by a semipermeable silica or other membranes will eliminate the process inefficiencies associated with these multiple process steps.

Summary:

Hydrogen permselective ceramic membranes suitable for integration with the coal gas shift reactor have been developed. Membranes have been prepared by chemical vapor deposition of SiO₂ and other oxides within the walls of porous Vycor tubes. A mathematical model for the chemical vapor deposition has been developed. A comparative economic analysis of the integrated shift reactor - membrane hydrogen separator will be conducted.

Next Phase:

Future work will depend on the results of this laboratory-scale experimental program.

DOE Hydrogen Research and Technology Summary

Office Fossil Energy (FE)

Topic Biological Production of Hydrogen

Type of Project (check one) Fuels-Related ☒ Non-Fuels-Related ☐

Cognizant METC Coal Conversion and Cleanup Branch Principal
Division Management Division Contact R. A. Johnson Phone (304) 291-4564

Other Sponsoring
Organization(s) Contractor(s) Engineering Resources

Summary Start Scheduled
Date July 1992 Date July 1990 Completion June 1992 Status Ongoing

Funding (\$10⁶) FY 1990 0.25 FY 1991 0.25 FY 1992 0.00 To Completion 0.00

Objective (or goal):

Develop bioconversion of synthesis gas to hydrogen by defining the optimal culture and bioreactor.

Purpose (background and reason for work):

In phase I of this study it was demonstrated that hydrogen gas can be produced biologically with a photosynthetic anaerobic bacterium from carbon monoxide and steam present in synthesis gas with a reaction time of about two minutes. This technology has potential commercial applications for hydrogen production.

Summary:

Engineering Resources is screening candidate cultures for enzyme activity and optimizing carbon monoxide conversion. Two types of bioreactors, immobilized cell reactors and trickle bed reactors, which can achieve high cell concentrations and mass transfer rates, will be used in this study. Advanced bioreactor concepts such as solid state fermentation, non-aqueous fermentation, and high pressure fermentation will be evaluated to enhance mass transport so that equivalent retention times of seconds can be realized. Process designs and economic evaluations of the various alternative systems will be compared.

Next Phase:

The next phase would be scale-up studies of the bioconversion process.

DOE Hydrogen Research and Technology Summary

Office Fossil Energy (FE)

Topic Catalytic Membrane Reactor for Water-Gas-Shift

Type of Project (check one) Fuels-Related ☒ Non-Fuels-Related ☐

Cognizant

Division METC Coal Conversion and Cleanup Branch

Principal

Contact J.R. Longanbach Phone 303-291-4659

Other Sponsoring
Organization(s) _____

Contractor(s) Bend Research

Summary
Date July 1992 Start
Date Sept 1991 Scheduled
Completion Sept 1994 Status Ongoing

Funding (\$10⁶) FY 1990 0 FY 1991 .050 FY 1992 0.500 To Completion 0

Objective (or goal):

To demonstrate a composite metal membrane to separate hydrogen and catalyze the water gas shift reaction to increase hydrogen yields and to develop and test a membrane module on coal derived synthesis gas at elevated temperature and pressure.

Purpose (background and reason for work):

To improve the economics of hydrogen production from coal via gasification, a membrane is needed to simplify water gas shift and hydrogen separation at elevated temperature and pressure. The membrane should produce pure hydrogen regardless of starting synthesis gas composition.

Summary:

A membrane has been developed and shown to separate hydrogen at elevated temperature and pressure in the presence of H₂S.

Next Phase:

Additional work will depend on the results on module tests using actual coal derived synthesis gas which will be conducted as part of this project.

DOE Hydrogen Research and Technology Summary

Office Conservation & Renewable Energy/Industrial Technology

Topic Magnetic Refrigerator (MR) for H₂ Liquefaction

Type of Project (check one) Fuels-Related ☒ Non-Fuels-Related ☐

Cognizant

Division Industrial Energy Efficiency

Principal

Contact Paul Scheihing **Phone** (202) 586-7234

Other Sponsoring

Organization(s) Air Products

Contractor(s) Astronautics/Air Products (Sub)

Summary

Date 4/92

Start

Date 6/90

Scheduled

Completion 1994 **Status** Complete Phase I

Funding (\$10⁶) FY 1990 0.6 FY 1991 0 FY 1992 0.4 **To Completion** 1.0

Objective (or goal):

Build and lab test a prototype 0.10 ton per day magnetic liquifier. Liquefy 1 ton per day with magnetic refrigerator.

Purpose (background and reason for work):

Propose LH₂ more cheaply, especially less than 10 tons per day.

Summary:

Phase 1 prototype design done. About to enter Phase 2 depending on negotiations.

Next Phase:

Phase II — prototype MR design, fab., and test.

DOE Hydrogen Research and Technology Summary

Office Conservation and Renewable Energy/Utility Technology

Topic Hydrogen from Renewables Research

Type of Project (check one) Fuels-Related X Non-Fuels-Related _____

Cognizant

Division Advanced Utility Concepts

Principal

Contact R. Eaton

Phone (202) 586-1506

Sponsoring

Organization(s) _____

Contractor(s) Florida Solar Energy Center

Summary

Date 6/92

Start

Date 9/86

Scheduled

Completion Open

Status Ongoing

Funding (\$10⁶) FY 1990 .400 FY 1991 .400 FY 1992 .166 To Completion TBD

Objective (or goal):

To identify, characterize and develop practical processes for hydrogen production, storage, distribution and end-use.

Purpose (background and reason for work):

The primary purpose of this work is to satisfy the need for an economic, non-polluting fuel that is inexhaustible. Large-scale fuel use of hydrogen will necessarily be produced from water splitting using renewable energy based processes. Several photoconversion processes are candidates to meet this need. Photoconversion processes are classified into three categories: 1) Photobiological; 2) Photoelectrochemical; and 3) Photochemical. Each of these have potential, but are in the very early stages of technical development.

Summary:

Continuous processes for solar-driven, water-splitting systems are under investigation at the Florida Solar Energy Center (FSEC). They are investigating the interaction between charge separation, reaction kinetics, and diffusion. This work will serve as a valuable tool for the development of new semiconductor, catalyst systems and superior photoconversion systems for producing hydrogen from water and solar energy. FSEC also is investigating hydrogen and methane integrated systems to assess such mixtures in a transition period to hydrogen power. Finally, they are exploring new processes suitable for the development of superior reversible physical and chemical carriers of hydrogen.

Next Phase:

Research will continue to develop hydrogen storage materials and processes for photoproduction of hydrogen.

DOE Hydrogen Research and Technology Summary

Office Conservation and Renewable Energy/Utility Technology

Topic Hydrogen Safety, Storage and Photobiological Production

Type of Project (check one) Fuels-Related ☒ Non-Fuels-Related ☐

Cognizant **Principal**
Division Advanced Utility Concepts **Contact** R. Eaton **Phone** (202) 586-1506

Other Sponsoring
Organization(s) **Contractor(s)** University of Miami

Summary **Start** **Scheduled**
Date 6/92 **Date** 9/86 **Completion** Open **Status** Ongoing

Funding (\$10⁶) **FY 1990** .400 **FY 1991** .400 **FY 1992** .164 **To Completion** TBD
Objective (or goal):

To identify, characterize and develop practical processes for hydrogen production, storage, distribution and end-use.

Purpose (background and reason for work):

The primary purpose of this work is to satisfy the need for an economic, non-polluting fuel that is inexhaustible. Large-scale fuel use of hydrogen will necessarily be produced from water splitting using renewable energy based processes. Several photoconversion processes are candidates to meet this need. Photoconversion processes are classified into three categories: 1) Photobiological; 2) Photoelectrochemical; and 3) Photochemical. Each of these have potential, but are in the very early stages of technical development.

Summary:

As part of a multi-faceted research program, the Clean Energy Research Institute (CERI) at the University of Miami is evaluating the safety of future large-scale hydrogen systems. Results to date have shown that the hazard of leakage and explosion for hydrogen is not significantly greater than that of natural gas or propane. CERI is also investigating advanced liquefaction processes to evaluate their potential for low cost hydrogen storage. Finally, a comprehensive screening of marine bacteria is seeking to identify active hydrogen producers for subsequent testing.

Next Phase:

Work on photoconversion will continue as well as integrated systems analysis to characterize the non-technical (economic, environmental, etc.) issue that will affect the research goals.

DOE Hydrogen Research and Technology Summary

Office Conservation and Renewable Energy/Utility Technology

Topic Program Support and Photoconversion Processes for Hydrogen Production

Type of Project (check one) Fuels-Related x Non-Fuels-Related _____

Cognizant

Principal

Division Advanced Utility Concepts

Contact R. Eaton

Phone (202) 586-1506

Other Sponsoring

Organization(s) _____ Contractor(s) National Renewable Energy Laboratory

Summary

Start

Scheduled

Date 6/92

Date 9/86

Completion Open

Status Ongoing

Funding (\$10⁶) FY 1990 .560 FY 1991 .560 FY 1992 .250 To Completion TBD
Objective (or goal):

To identify, characterize and develop practical processes for hydrogen production, storage, distribution and end-use.

Purpose (background and reason for work):

The primary purpose of this work is to satisfy the need for an economic, non-polluting fuel that is inexhaustible. Large-scale fuel use of hydrogen will necessarily be produced from water splitting using renewable energy based processes. Several photoconversion processes are candidates to meet this need. Photoconversion processes are classified into three categories: 1) Photobiological; 2) Photoelectrochemical; and 3) Photochemical. Each of these have potential, but are in the very early stages of technical development.

Summary:

Scientists at NREL have demonstrated the scientific feasibility of a new conceptual design for hydrogen production based on the immobilization of biological components on a conductive polymer substrate. Attempts are being made, in collaboration with researchers in England and Switzerland, to stabilize these materials.

Next Phase:

Work will continue on basic research to better understand the water splitting mechanisms. There will be increased emphasis on basic research of materials for hydrogen storage.

DOE Hydrogen Research and Technology Summary

Office Conservation and Renewable Energy/Utility Technology

Topic Hydrogen Production from Renewable Energy

Type of Project (check one) Fuels-Related X Non-Fuels-Related _____

Cognizant

Division Advanced Utility Concepts

Principal

Contact R. Eaton

Phone (202) 586-1506

Other Sponsoring

Organization(s) _____ **Contractor(s)** Texas A&M University

Summary

Date 6/92

Start

Date 9/86

Scheduled

Completion Open

Status Ongoing

Funding (\$10⁶) FY 1990 .400 FY 1991 .400 FY 1992 .152 To Completion TBD

Objective (or goal):

To identify, characterize and develop practical processes for hydrogen production, storage, distribution and end-use.

Purpose (background and reason for work):

The primary purpose of this work is to satisfy the need for an economic, non-polluting fuel that is inexhaustible. Large-scale fuel use of hydrogen will necessarily be produced from water splitting using renewable energy based processes. Several photoconversion processes are candidates to meet this need. Photoconversion processes are classified into three categories: 1) Photobiological; 2) Photoelectrochemical; and 3) Photochemical. Each of these have potential, but are in the very early stages of technical development.

Summary:

The Center for Electrochemical and Hydrogen Research at Texas A&M University is developing practical triple stacked photocell units that are capable of efficiently splitting water into hydrogen and oxygen, with provision for separation of the two gases and storage of hydrogen, and to incorporate these cells, in a membrane to allow hydrogen production and storage underneath. They are also examining systems that incorporate active, organic layers which contain photosensitive dyes similar to those used in color photography. The long-term goal is to develop a light-stable, triple-layer structure that is again sensitive to successively blue, green and red photons. They are also testing bacteria from the rumen environment to identify high hydrogen producers.

Next Phase:

Basic and Applied R&D in photoconversion processes will continue with an objective to achieve high efficiency, low cost production systems.

DOE Hydrogen Research and Technology Summary

Office Conservation and Renewable Energy/Utility Technology

Topic Hydrogen Hydride Storage, Photoelectrical Production and Supercritical Water

Type of Project (check one) Fuels-Related X Non-Fuels-Related _____

Cognizant

Division Advanced Utility Concepts

Principal

Contact R. Eaton

Phone (202) 586-1506

Other Sponsoring
Organization(s) _____

Contractor(s) Hawaii Natural Energy Institute

Summary

Date 6/92

Start

Date 9/86

Scheduled

Completion Open

Status Ongoing

Funding (\$10⁶) FY 1990 .400 FY 1991 .400 FY 1992 .252 To Completion TBD

Objective (or goal):

To identify, characterize and develop practical processes for hydrogen production, storage, distribution and end-use.

Purpose (background and reason for work):

The primary purpose of this work is to satisfy the need for an economic, non-polluting fuel that is inexhaustible. Large-scale fuel use of hydrogen will necessarily be produced from water splitting using renewable energy based processes. Several photoconversion processes are candidates to meet this need. Photoconversion processes are classified into three categories: 1) Photobiological; 2) Photoelectrochemical; and 3) Photochemical. Each of these have potential, but are in the very early stages of technical development.

Summary:

A new class of hydride materials for hydrogen storage is being synthesized at the Hawaii Natural Energy Institute (HNEI) at the University of Hawaii. The research is using cobalt complexes to achieve increased capacity for storing hydrogen. Current research is focused on determining the hydriding/dehydriding behaviors of such materials. This research is also yielding new information about the interaction of molecular hydrogen with metals, an issue that is important for hydrogen containment. In addition, HNEI is investigating the use of supercritical water to produce hydrogen from biomass that is too wet for other processes. Two other research projects at HNEI are attempting to develop improved electrode materials for photoelectrolysis cells and to develop genetically improved bacteria for water splitting.

Next Phase:

Work in all areas will continue through FY 1990. As new projects are defined, they will be considered for funding.

DOE Hydrogen Research and Technology Summary

Office Conservation and Renewable Energy/Utility Technology

Topic Hydrogen Energy Systems Studies

Type of Project (check one) Fuels-Related ☒ Non-Fuels-Related ☐

Cognizant Principal
Division Advanced Utility Concepts Contact R. Eaton Phone 202-586-1506
Other Sponsoring
Organization(s) _____ Contractor(s) Princeton University

Summary Start Scheduled
Date 6/92 Date 2/92 Completion 2/93 Status On-going

Funding (\$10⁶) FY 1990 _____ FY 1991 _____ FY 1992 .005 To Completion _____

Objective (or goal):

Identify the most promising paths toward the use of renewable hydrogen as an energy carrier, highlighting key technologies for research and development. System studies shall be conducted from generation through end-use.

Purpose (background and reason for work):

Studies of alternative strategies for developing renewable hydrogen energy systems.

Summary:

Reports that assess alternatives for hydrogen production, hydrogen storage, transmission, and distribution, hydrogen end-use technologies, and evaluate overall systems issues.

Next Phase:

DOE Hydrogen Research and Technology Summary

Office Conservation & Energy/Utility Technology

Topic Activated Carbon-based Storage System

Type of Project (check one) Fuels-Related ☒ Non-Fuels-Related ☐

Cognizant

Division Advanced Utility Concepts

Principal

Contact R. Eaton Phone (202) 586-6104

Other Sponsoring

Organization(s) Contractor(s) Syracuse University

Summary

Date 06/12/92

Start

Date 10/01/90

Scheduled

Completion 09/30/91

Status Ongoing

Funding (\$10⁶) FY 1990 0 FY 1991 0 FY 1992 0.127 To Completion TBD

Objective (or goal):

A major barrier to the widespread utilization of hydrogen would be lifted, if a viable and cost effective storage system for hydrogen could be demonstrated. The objectives of this study are to correlate the micropore filling of carbon by hydrogen with carbon's pore size distributions and surface functionalities.

Purpose (background and reason for work):

Hydrogen usage is limited by production and storage-cycle costs. Technological advances are needed on these issues before hydrogen can impact the energy infrastructure. Hydrogen/carbon storage systems compare favorably with liquid and compressed gas storage systems on an energy-per-unit weight basis. Therefore, many near term applications that require hydrogen storage could be satisfied with improvements in carbon/hydrogen storage systems. The purpose of this work is to investigate the adsorption physics/chemistry of activated carbon for means of optimizing its capacity for hydrogen storage.

Summary:

Different carbons, which may possess the same internal surface area, adsorb gases to different levels. Reasons for this range in adsorption capacity are not fully understood, but it is known that the carbon's pore sizes, surface functionalities and roughness all play a role in the adsorption process. Experiments on activated carbons are being conducted at Brookhaven National Laboratory to determine their pore structure by using Small Angle X-ray Scattering techniques and their chemical surface function groups by using Electron Spectroscopy for Chemical Analysis. Data from these measurements are correlated with the carbon's BET adsorption isotherms.

Next Phase:

Follow up activities would be directed at establishing a comprehensive data base on the physical/chemical features of activated carbons in order to isolate the characteristics which best promote hydrogen uptake.

DOE Hydrogen Research and Technology Summary

Office Conservation and Renewable Energy/Utility Technology

Topic Engineering Evolution of Hydrogen Uses & Production

Type of Project (check one) Fuels-Related ☒ Non-Fuels-Related ☐

Cognizant

Division Advanced Utility Concepts

Principal

Contact R. Eaton

Phone (202) 586-1506

Other Sponsoring

Organization(s) _____ Contractor(s) TDA Research, Inc.

Summary

Date 6/92

Start

Date 9/01/91

Scheduled

Completion _____

Status _____

Funding (\$10⁶) FY 1990 _____ FY 1991 _____ FY 1992 .01 To Completion TBD

Objective (or goal):

Determine which hydrogen generation, transport, and conversion applications have the highest value.

Purpose (background and reason for work):

The primary purpose of this work is to conduct a preliminary assessment of the use of hydrogen in electric utility applications as a storage and transmission medium, carry out a preliminary analysis of the use of hydrogen as a transportation fuel, and conduct more detailed analyses of the best electric utility application identified in the preliminary assessment.

Summary:

Next Phase:

Not planned.

DOE Hydrogen Research and Technology Summary

Office Conservation and Renewable Energy/Utility Technology

Topic Hydrogen Technology Assessment & Information Transfer Program

Type of Project (check one) Fuels-Related X Non-Fuels-Related _____

Cognizant

Division Advanced Utility Concepts

Principal

Contact R. Eaton

Phone 202-586-1506

Other Sponsoring

Organization(s) _____ Contractor(s) National Hydrogen Association

Summary

Date 6/92

Start

Date 8/91

Scheduled

Completion 6/92

Status TBD

Funding (\$10⁶) FY 1990 0 FY 1991 0 FY 1992 .05 To Completion _____

Objective (or goal):

Identify preliminary interest in cooperative government/industry research projects. Identify technically possible and economically promising options for hydrogen vehicles and utility hydrogen generation and storage, and determine the technology development steps necessary to achieve the technical goals for both applications.

Purpose (background and reason for work):

Assess industry's hydrogen technology interest and R&D capabilities through targeted meetings and discussions. Develop detailed energy and economic paths to technology development of hydrogen vehicles and utility hydrogen generation and storage.

Summary:

A report indentifying promising areas of joint industry/government research and potential industrial interest in NREL's research projects will be produced. It will include descriptions of alternative energy and economic paths to technology development, and the steps necessary for hydrogen vehicle, generation, and storage development.

Next Phase:

Not planned.

DOE Hydrogen Research and Technology Summary

Office Conservation and Renewable Energy/Transportation Technologies

Topic Advanced Hydrogen/Methane Utilization Technology Demonstration

Type of Project (check one) Fuels-Related ☒ Non-Fuels-Related ☐

Cognizant

Division Advanced Utility Concepts

Principal

Contact R. Eaton

Phone 303-231-1288

Other Sponsoring

Organization(s) _____ **Contractor(s)** Hydrogen Consultants, Inc.

Summary

Date 6/92

Start

Date 3/92

Scheduled

Completion 3/93

Status Ongoing

Funding (\$10⁶) FY 1990 _____ FY 1991 0.2 FY 1992 TBD **To Completion** TBD

Objective (or goal):

The objective of this project is to provide an engine and vehicle demonstration of optimized hydrogen / methane blends in terms of emissions, fuel economy, and power performance.

Purpose (background and reason for work):

Hydrogen added to methane extends the lean carburetor limit in a synergistic manner and provides reduced emission benefits. This method of using hydrogen is viewed as a bridge to moving neat hydrogen into the transportation arena on a broad scale.

Summary:

A system for blending hydrogen and methane will be designed. Blends of hydrogen in methane will be evaluated on an engine dynamometer at several power ranges, speeds, and equivalences. Optimum blends (stoichiometric and lean burn) will be selected for a vehicle demonstration where Federal Test Procedure emissions and fuel economy will be measured. Vehicle driveability will also be demonstrated.

Next Phase:

Not Planned

DOE Hydrogen Research and Technology Summary

Office Conservation and Renewable Energy/Transportation Technologies

Topic A Direct-Injected, Hydrogen-Fueled Engine Technology Demonstration

Type of Project (check one) Fuels-Related X Non-Fuels-Related _____

Cognizant Division Advanced Utility Concepts Principal Contact R. Eaton Phone 202-586-1506

Other Sponsoring Organization(s) _____ Contractor(s) Detroit Diesel Corporation

Summary Date 7/92 Start Date 5/92 Scheduled Completion 5/93 Status Ongoing

Funding (\$10⁶) FY 1990 _____ FY 1991 .224 FY 1992 .224 To Completion _____

Objective (or goal):

The objectives of this project are to develop and demonstrate an advanced injection and combustion system for a direct-injection hydrogen-fueled engine.

Purpose (background and reason for work):

One method for controlling combustion in a hydrogen fueled engine is to inject the fuel directly into the combustion chamber. Design of the injection system is the key to successfully demonstrate this approach. Delivery of sufficient volume and providing means for adequate sealing are engineering challenges. Modification of natural gas injectors proven in use offers a high probability for success in this approach.

Summary:

A high pressure hydrogen injector will be designed based on the design of a natural gas injector that is now in use. Following necessary hardware construction, performance of the hydrogen injector fuel system will be measured, auto-ignition versus surface ignition of hydrogen will be characterized, and the effect of hydrogen injection pressure, timing, and duration on engine performance and emissions will be determined in engine dynamometer tests.

Next Phase:

Not planned at this time.

DOE Hydrogen Research and Technology Summary

Office Conservation and Renewable Energy/Transportation Technologies

Topic Elimination of Abnormal Combustion in a Hydrogen-Fueled Engine

Type of Project (check one) Fuels-Related X Non-Fuels-Related _____

Cognizant

Division Advanced Utility Concepts

Principal

Contact R. Eaton

Phone 303-231-1288

Other Sponsoring

Organization(s) _____ Contractor(s) University of Miami

Summary

Date 7/92

Start

Date 4/92

Scheduled

Completion 4/93

Status Ongoing

Funding (\$10⁶) FY 1990 _____ FY 1991 .054 FY 1992 _____ To Completion TBD

Objective (or goal):

The objective of this project is to eliminate abnormal combustion in a hydrogen-fueled engine by implementing proper design of the combustion chamber and inlet port geometry together with adequate cooling of the combustion chamber.

Purpose (background and reason for work):

One of the primary drawbacks of using hydrogen in a conventional spark ignition engine application is propensity for preignition of the fuel-air mixture causing backfire and poor carburetor control. Modification of the mechanical design of the fuel induction system and the cooling system in the engine may alleviate the carburetor control problem.

Summary:

A redesigned cylinder head with additional cooling will be prepared and sodium-filled exhaust valves will be used to reduce surface ignition. The intake air port in the head will also be modified to reduce surface ignition in the spark ignition test engine. The test engine will be mapped over a range of loads and speeds and characterized as to knocking and surface ignition tendencies.

Next Phase:

Not planned at this time.

DOE Hydrogen Research and Technology Summary

Office Defense Programs/Research and Advanced Technology

Topic Materials for Solid Storage

Type of Project (check one) **Fuels-Related** x **Non-Fuels-Related**

Cognizant
Division Research & Technology Development

Principal
Contact G. J. D'Alessio **Phone** (301) 903-6688

Other Sponsoring Organization(s) _____ **Contractor(s)** Sandia National Laboratories
Livermore, CA 94551-0989

Summary	Start	Scheduled	
Date	Date	Completion	Status
July 1991	1989		Ongoing

Funding (\$10⁶)	FY 1990	1.0	FY 1991	1.0	FY 1992	1.0	To Completion
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Objective (or goal):

To characterize and understand materials in relation to solid storage applications.

Purpose (background and reason for work):

Solid storage systems could be used in weapons systems. In order to assure safety, inventory control, and operational surety, a thorough understanding and characterization of material properties are required for material selection and design.

Summary:

This work includes: (1) selection and characterization of candidate materials, and (2) measurement and modeling of material properties changes as a result of tritium exposure with time. Selection and characterization has focused on defining specifications for the current-generation material to provide consistent, predictable performance. In addition, next-generation materials and morphologies are being explored. Measurement and modeling of materials after tritium exposure has focused on determining helium accumulation and release, and thermodynamic changes with time.

Next Phase:

The selection and characterization of next-generation materials will continue, and processing techniques for the current- and next-generation materials will be explored. Processing techniques that improve the material performance and/or lower cost will be emphasized. Material properties changes with ritium exposure will continue to be measured, and the understanding gained through measurements will be incorporated into the model to allow predictions to longer time.

DOE Hydrogen Research and Technology Summary

Office Energy Research/Basic Energy Sciences (BES)

Topic Photochemical Generation of Hydrogen

Type of Project (check one) Fuels-Related _____ Non-Fuels-Related X*

Cognizant

Division Chemical Sciences

Principal

Contact M. E. Gress

Phone (301) 903-5820

Other Sponsoring

Organization(s) _____ Contractor(s) See Summary below

Summary

Date July 1992

Start

Date _____

Scheduled

Completion _____

Status Ongoing

Funding (\$10⁶) FY 1990 13.2 FY 1991 13.1 FY 1992 13.5 To Completion _____

Objective (or goal):

To provide basic understanding in photochemistry and of electron transfer processes relevant to solar photochemical energy conversion.

Purpose (background and reason for work):

Research in this area is aimed at the conversion of solar energy into a chemically usable form (as distinct from heat).

Summary:

The research involves investigation of model systems, artificial photosynthesis and photoelectrochemical and photochemical cycles and reactions. Much of the work is at so fundamental a state that we do not differentiate systems which might deliver hydrogen from H₂O, from others that might deliver methane or alcohols from CO₂, ammonia from atmospheric nitrogen, or other needed chemicals at lower cost by using sunlight. The research projects in this program, which individually are relatively small, are located at ANL, BNL, LBL, NREL, the Notre Dame Radiation Laboratory, the National Institute of Standards and Technology, and a number of universities.

Next Phase:

*Clearly related to the energy conversion mission of DOE, while only tenuously related to the narrow area of hydrogen technology.

DOE Hydrogen Research and Technology Summary

Office Energy Research/Basic Energy Sciences (BES)

Topic Hydrogen Effects on Solids and Properties of Minority Phase Hydrides

Type of Project (check one) Fuels-Related _____ Non-Fuels-Related X

Cognizant

Division Materials Sciences

Principal

Contact I. Thomas **Phone** (301) 903-3427

**Other Sponsoring
Organization(s)** _____

Contractor(s) Universities, DOE Laboratories

Summary

Date June 1992

Start

Date _____

Scheduled

Completion _____ **Status** Ongoing

Funding (\$10⁶) FY 1990 1.8 FY 1991 1.8 FY 1992 1.8 **To Completion** _____

Objective (or goal):

This is basic materials research aimed at increasing the understanding of hydrogen effects such as hydrogen interactions on solid surfaces, diffusion and embrittlement of solids, and the properties of hydrides as a class of materials.

Purpose (background and reason for work):

To increase the understanding of hydrogen-related phenomena in and on solids—an important subject underlying many DOE technologies, such as Fossil-Energy, Fusion Energy, Defense Programs, Conservation Technologies, and Solar Energy, as well as Hydrogen Production.

Summary:

A wide spectrum of research is conducted covering both the interaction of hydrogen with materials and the formation, properties, and behavior of hydrides. Research is underway on hydrogen embrittlement, stress corrosion cracking, diffusion of hydrogen isotopes, hydrogen attack, structure of hydrides using neutron scattering, superconducting properties of hydrides, thermodynamics of metal hydrogen systems, hydrogen solubility and hydride precipitation, hydrogen trapping at defects, catalysis, electrical, and magnetic properties of hydrides, absorption, and other surface-related phenomena. Additional information can be obtained from the publication DOE/ER 0447P "Materials Sciences Programs—Fiscal Year 1989."

Next Phase:

Continuing long-range research as described above.

DOE Hydrogen Research and Technology Summary

Office Energy Research/Basic Energy Sciences (BES)

Topic Biological Mechanisms of Hydrogen Generation

Type of Project (check one) Fuels-Related _____ Non-Fuels-Related X

Cognizant

Division Energy Biosciences

Principal

Contact R. Rabson

Phone (301) 903-2873

Other Sponsoring

Organization(s) _____

Contractor(s) _____

Summary

Date June 1992

Start

Date _____

Scheduled

Completion _____

Status Ongoing

Funding (\$10⁶) FY 1990 1.2 FY 1991 1.2 FY 1992 1.1 To Completion _____

Objective (or goal):

To generate an understanding of biological hydrogen generation and metabolism in a broad cross-section of organisms.

Purpose (background and reason for work):

To explore biological systems as a means to develop a hydrogen generating technology based on biological principles using solar energy as the driving force. Furthermore, the utility of hydrogen as a driving force for biological synthetic reactions in microorganisms as a prospective biotechnology basis is studied.

Summary:

The biological research is designed to explore the mechanisms by which hydrogen is evolved in various biological systems including algae and various heterotrophic microorganisms. The aim is to understand the mechanisms of production, transfer, and utilization of hydrogen in these forms. Thus, attention is given to the hydrogenase reactions as well as studies of the enzyme itself with a significant segment of this work relating to photosynthetic mechanisms. In addition, the way in which anaerobic microorganisms transfer hydrogen between species to drive bioconversion is also studied. Work on the molecular genetics of the hydrogenases of several microorganisms is included.

Next Phase:

Continuing long-range research as described above.

DOE Hydrogen Research and Technology Summary

Office Energy Research/Basic Energy Sciences

Topic Kinetics of Enzyme Catalyzed Processes

Type of Project (check one) Fuels-Related _____ Non-Fuels-Related X

Cognizant Division Chemical Sciences Principal Contact J. L. Burnett Phone (301) 353-5802

Other Sponsoring Organization(s) _____ Contractor(s) Oak Ridge National Laboratory

Summary Date June 1992 Start Date _____ Scheduled Completion _____ Status Ongoing

Funding (\$10⁶) FY 1990 0.3 FY 1991 0.3 FY 1992 0.3 To Completion _____

Objective (or goal):

To characterize the physiochemical mechanisms of artificial photosynthetic systems.

Purpose (background and reason for work):

The purpose of this research project is to study the fundamental physiochemical aspects of the conversion of light energy into chemical energy using artificial photosynthetic systems.

Summary:

Kinetic and mechanistic aspects of hydrogen and oxygen photoproduction will be studied using a unique experimental approach. Areas of investigation include: (1) simultaneous light driven production of hydrogen and oxygen; (2) long-term stability of each of the components of the chloroplast-ferredoxin-hydrogenase system; (3) separation of the two light reactions of photosynthesis; (4) constructions of photosynthetic photoelectrochemical cells; and (5) precipitation of metallic catalysts on photosynthetic membranes.

Next Phase:

Continuing long-range research as described above.

DOE Hydrogen Research and Technology Summary

Office Defense Programs/Research and Advanced Technology

Topic Computer Modelling of Hydrogen and Helium in Metals

Type of Project (check one) Fuels-Related _____ Non-Fuels-Related X

Cognizant

Principal

Division Research & Technology Development

Contact G. J. D'Alessio Phone (301) 903-6688

Other Sponsoring

Organization(s) _____ Contractor(s) Sandia National Laboratory, Livermore, CA

Summary

Start

Scheduled

Date July 1992

Date 1980

Completion _____ Status Ongoing

Funding (\$10⁶) FY 1990 0.6 FY 1991 0.2 FY 1992 0.2 To Completion _____

Objective (or goal):

Development of theoretical models and computer codes for the solubility, diffusion, and trapping of hydrogen isotopes and of helium in metallic materials. Determine the effects of material interfaces on the internal distribution of hydrogen isotopes and helium, and identify the processes of helium bubble formation and their impact on the mechanical and fracture properties of high-strength alloys exposed to tritium.

Develop predictive models and computer codes for radiolytic affects in gas mixtures containing tritium.

Purpose (background and reason for work):

The effects of tritium and helium on mechanical properties of structural materials and on the integrity of containment vessels is of prime concern. In addition, permeation and tritium inventory must be accurately predicted in order to satisfy environmental, health, and safety considerations. Furthermore, the distribution of hydrogen isotopes and helium through containment vessels must be known after long-term exposure in order to assess the structural integrity of containment vessels.

Summary:

Work has been performed to determine enhanced solubilities of hydrogen isotopes at interfaces. The energetics of helium cluster and bubble formation have been determined. Computer codes have been developed to evaluate the radial species concentrations in tritium-containing gas mixtures. Predictive models have been developed for helium bubble formation and growth and for the induced swelling.

Next Phase:

Theoretical models and computer codes will be developed for helium release from metal tritides and mixed metal deuterides and metal tritides.

DOE Hydrogen Research and Technology Summary

Office Defense Programs/Research and Advanced Technology

Topic Hydrogen Transport and Trapping in Metals

Type of Project (check one) **Fuels-Related** _____ **Non-Fuels-Related** X

Cognizant
Division Research & Technology Development

Principal
Contact G. J. D'Alessio **Phone** (303) 903-6688

Other Sponsoring Organization(s) _____ **Contractor(s)** Sandia National Laboratories
Livermore, CA 94551-0969

Summary	Start	Scheduled	
Date <u>July 1992</u>	Date <u>1980</u>	Completion _____	Status <u>Ongoing</u>

Funding (\$10⁶) **FY 1990** 0.2 **FY 1991** 0.2 **FY 1992** 0.2 **To Completion** _____

Objective (or goal):

To develop a database for use in understanding hydrogen isotope uptake, transport, and trapping metals and to determine the influence of surface processes on permeation.

Purpose (background and reason for work):

A number of Sandia programs require an understanding of hydrogen transport and aging effects in a variety of materials over a wide range of temperatures and pressures. In order to assure safety, inventory control, and operational surety, transport properties are required for material selection and design.

Summary:

The general scope of work involves research related to the measurement of hydrogen deuterium and tritium permeation and solubility in metals which are of technological importance in the storage purification of hydrogen isotopes. The program also involves investigating the influence of surface treatments and surface barriers on hydrogen uptake. Reduction of permeability would be of benefit in applications where embrittlement or corrosion are important. An apparatus for in-situ alteration and characterization of metal surfaces prior to hydrogen isotope permeation measurements has been constructed. A new technique based on ion beam analysis has been developed and used to measure deuterium and tritium trapping in gold.

Next Phase:

Continued measurements of permeation on in-situ characterized metals and determine the influence of surface treatment on these properties. Resume studies of surface effects on deuterium permeation through iron and continue studies of high pressure permeation through potential permeation barrier materials. Complete thermal desorption apparatus for determining He-3 and hydrogen isotope concentrations in aged samples.

DOE Hydrogen Research and Technology Summary

Office Defense Program/Research and Advanced Technology

Topic Hydrogen Transport and Trapping in Metal Hydrides

Type of Project (check one) **Fuels-Related** _____ **Non-Fuels-Related** X

Cognizant

Division Research & Technology Development

Principal

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**Other Sponsoring
Organization(s)** _____

Contractor(s) Sandia National Laboratories
Livermore, CA 94551-0969

Summary

Date July 1992

Start

Date 1989

Scheduled

Completion _____

Status Ongoing

Funding (\$10⁶) **FY 1990** 0.2 **FY 1991** 0.2 **FY 1992** 0.2 **To Completion** _____

Objective (or goal):

To develop an understanding of hydrogen migration and trapping in mixed-phase metal hydride systems and alloys. To determine the characteristics and effects of He-3 bubbles generated from tritium decay in metal tritides.

Purpose (background and reason for work):

A number of Sandia programs require an understanding of hydrogen transport and aging effects in hydride materials over a range of temperatures and pressures. In order to assure safety, inventory control, and operational surety, transport properties are required for material selection and component design.

Summary:

Pressure-composition-temperature (PCT) measurements and nuclear magnetic resonance (NMR) techniques have been used to identify hydrogen concentrations in various phases of mixed-phase metal hydrides. PCT measurements have characterized the thermodynamic properties of pure hydrides. He-3 NMR studies have produced data on the helium density within bubbles observed in aging metal tritides, and the interactions with the bubble-wall interface have been investigated for use in bubble size determinations. These techniques are major contributors to our knowledge of hydride properties and aging effects in metals.

Next Phase:

PCT measurements will be used to characterize the properties of alloy hydrides, and to determine the effects of aging on these properties in both pure and alloy materials. Thermal desorption measurements will be initiated to supplement information on helium and hydrogen isotope properties. Magic angle spinning techniques will be used with NMR to follow inter- and intra-phase hydrogen diffusion and segregation as a function of temperature and to look for trapping effects in aged materials.

DOE Hydrogen Research and Technology Summary

Office Defense Programs/Research and Advanced Technology

Topic Mechanical and Fracture Properties of Materials Containing Hydrogen Isotopes and Helium

Type of Project (check one) Fuels-Related _____ Non-Fuels-Related X

Cognizant

Principal

Division Research & Technology Development Contact G. J. D'Alessio Phone (301) 903-6688

Other Sponsoring

Organization(s) _____ Contractor(s) Sandia National Laboratory, Livermore, CA

Summary Start Scheduled
Date July 1992 Date 1988 Completion _____ Status Ongoing

Funding (\$10⁶) FY 1990 1.5 FY 1991 1.5 FY 1992 1.5 To Completion _____

Objective (or goal):

Develop physical models for dislocation pinning by helium clusters and bubbles. Determine the cohesive strength of grain boundaries and interfaces in terms of the density and size of helium and hydrogen clusters and bubbles on these interfaces.

Purpose (background and reason for work):

Gases, such as hydrogen and helium, contained in metals are known to degrade their mechanical properties significantly and to make them more prone to brittle fracture. It is the purpose of this research to develop and establish quantitative relationships between the changes in yield strength, plastic flow properties, fracture toughness, and creep rupture, and the concentrations and microscopic distributions of these gases within the materials.

Summary:

The change in the plastic deformation of austenitic stainless steels with tritium exposure has been successfully correlated with theoretical models. It is possible now to predict further changes with continued tritium exposure. The deformation and decohesion of model interfaces has been studied by finite element crystal plasticity calculations.

Next Phase:

Experimental results on helium-induced intergranular failure will be analyzed in terms of models which relate the fracture toughness to the bubble distribution on interfaces and within the grains of polycrystalline materials. This will provide a predictive capability to relate changes in fracture properties to the conditions for tritium exposure.

DOE Hydrogen Research and Technology Summary

Office Defense Programs/Research and Advanced Technology

Topic Physics of Aging in Metal Tritides

Type of Project (check one) Fuels-Related _____ Non-Fuels-Related X

Cognizant

Principal

Division Research & Technology Development

Contact G.J. D'Alessio Phone (301) 903-6688

Other Sponsoring
Organization(s) _____

Sandia National Laboratories
Contractor(s) Livermore, CA 94551-0969

Summary

Start

Scheduled

Date July 1992

Date 1989

Completion _____

Status Ongoing

Funding (\$10⁶) FY 1990 2.6 FY 1991 2.2 FY 1992 2.0 To Completion _____

Objective (or goal):

To develop a fundamental understanding of aging effects in metal tritides and to determine the influence of aging on the properties of these materials.

Purpose (background and reason for work):

Tritides are currently utilized in some weapons components and expected to be used in proposed systems. In order to assure safety, inventory control, and operational surety, a thorough understanding and characterization of aging effects are required for materials selection and design.

Summary:

We have determined that helium bubbles are formed in tritides through the tritium decay process. These highly pressurized bubbles lead to changes in materials properties and behavior, such as thermodynamic properties, mechanical properties, and volume changes (swelling). This program has utilized a number of experimental techniques, including electron microscopy, pressure-composition-temperature (PCT) measurements, length change measurements (for swelling), and nuclear magnetic measurement (NMR) techniques, in combination with theoretical modeling efforts to understand these phenomena. An active storage program is in place to supply aged materials and monitor aging effects.

Next Phase:

This work will be continued to achieve a predictive capability for aging effects. The initial PCT measurements mentioned above will be extended to study additional materials, temperature behavior, and the influence of helium concentration. Additional length change measurements will be initiated. Mechanical property measurements will begin on aged materials and will be combined with electron microscopy characterization of bubble-dislocation interactions in tritides. NMR measurements will be used to monitor swelling and to yield fundamental information on helium density within bubbles, modeling efforts will focus on understanding observed changes in PCT behavior, swelling behavior, and mechanical properties.

DOE Hydrogen Research and Technology Summary

Office Defense Programs/Research and Advanced Technology

Topic Operation and Maintenance of the Tritium Research Laboratory

Type of Project (check one) Fuels-Related _____ Non-Fuels-Related X

Cognizant _____ Principal _____
Division Research & Technology Development Contact G. J. D'Alessio Phone (301)903-6688

Other Sponsoring _____ Sandia National Laboratories
Organization(s) _____ Contractor(s) Livermore, CA 94551-0969

Summary _____ Start _____ Scheduled _____
Date July 1991 Date 1975 Completion _____ Status Ongoing

Funding (\$10⁶) FY 1990 4.1 FY 1991 4.1 FY 1992 5.1 To Completion _____

Objective (or goal):

The objective of this activity is the safe, environmentally benign, and efficient operation of the Tritium Research Laboratory.

Purpose (background and reason for work):

The Tritium Research Laboratory is operated to provide an applied research capability for developing a sound, fundamental understanding of the interaction between tritium and materials.

Summary:

The Tritium Research Laboratory is a multi-user facility designed for safe experimentation using tritium. This facility uses glovebox containment and tritium recovery systems to reduce worker exposure and release of tritium to the environment to levels as low as reasonably achievable. The Tritium Research Laboratory is being used for research applied primarily to the weapons program. Topics being investigated include: the effect of tritium on structural properties of materials, radiation effects caused by tritium, storage and transport phenomena, and safe handling techniques. Capabilities of the laboratory include: analysis and assay, transmission and scanning electron microscopes, x-ray diffraction, and technical support.

Next Phase:

In January, 1992, Sandia National Laboratories announced its intent to cease tritium operations at the TRL. Experimental activities should be concluded by April, 1993, and tritium inventory removed from the TRL by July, 1993. By the current planning schedule, with the necessary DOE and other approvals, decontamination and decommissioning of the TRL should be complete by the end of FY96.

DOE Hydrogen Research and Technology Summary

Office Defense Program/Research and Advanced Technology

Topic Studies of Hydrogen Isotopes in Metals

Type of Project (check one) Fuels-Related _____ Non-Fuels-Related X

Cognizant

Division Research & Technology Development

Principal

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**Other Sponsoring
Organization(s)** _____

Contractor(s) Westinghouse Savannah River Company

Summary

Date July 1992

Start

Date _____

Scheduled

Completion _____

Status Ongoing

Funding (\$10⁶) FY 1990 0.39 FY 1991 0.41 FY 1992 0.43 **To Completion** TBD

Objective (or goal):

To investigate tritium and helium effects on room temperature fracture toughness and slow crack growth properties of austenitic stainless steels. To gain a fundamental understanding of the mechanisms of hydrogen and helium embrittlement.

Purpose (background and reason for work):

Austenitic stainless steels are known to be susceptible to hydrogen-assisted cracking; slow crack growth properties are also affected by the presence of helium in the materials from tritium decay. The purpose is to define the conditions under which cracking initiates and thus establish safe limits on service lifetimes of tritium-containing vessels.

Summary:

During this past year, mechanical property and fracture toughness continued on various tritium-exposed metal alloys. Fracture toughness measurements continued on Type 21-6-9 steel tritium-exposed samples containing 500 ppm. Mechanical property and fracture toughness measurements were initiated on tritium-exposed Incoloy 903 samples prepared with a variety of microstructures. The successful development and calibration of the electric-potential system greatly improved the accuracy of crack length measurements during fracture toughness testing. Transmission Electron Microscopy (TEM) of the mechanical test samples continue to show test differences in helium bubble distribution as the reason why High-Energy-Rate-Forged 21-6-9 has improved ductility and fracture toughness than annealed 21-6-9 stainless steel.

Next Phase:

Experiments will continue to quantify the effect of tritium and decay helium on the fracture toughness of metal alloys as a function of composition, mechanical properties, and microstructure. Fracture toughness measurements on tritium-exposed samples of Incoloy 903, an alloy that can be prepared with a variety of microstructures, will continue to provide an understanding on the effects of microstructure. Also, experiments will continue to determine the effect of strength and prior microstructure on the mechanical properties of tritium-exposed Type 21-6-9 stainless steel. TEM characterization of test samples will provide insight into the He bubble distribution and its influence on the mechanical properties.

DOE Hydrogen Research and Technology Summary

Office Defense Program/Research and Advanced Technology

Topic Metal Hydride Research

Type of Project (check one) Fuels-Related _____ Non-Fuels-Related X

Cognizant

Division Research & Technology Development

Principal

Contact G.J. D'Alessio **Phone** (301)903-6688

**Other Sponsoring
Organization(s)** _____

Contractor(s) Westinghouse Savannah River Company

Summary

Date July 1992

Start

Date _____

Scheduled

Completion TBD **Status** Ongoing

Funding (\$10⁶) FY 1990 0.99 FY 1991 1.04 FY 1992 1.04 **To Completion** TBD

Objective (or goal):

To investigate the thermodynamic and metallurgical properties of various metal hydrides being developed for processing applications in the Replacement Tritium Facility (RTF) at Savannah River. To understand the long-term tritium aging effects on these hydride materials.

Purpose (background and reason for work):

Metal hydrides have been selected for use in the RTF for storage, compression, purification, pumping, and isotopic separation applications. Their use enables processing equipment to be designed to a much more compact size compared to larger conventional gas storage and distillation vessels. The small size in turn allows the equipment to be housed in nitrogen-atmosphere gloveboxes to minimize personnel exposure to tritium and releases to the environment. In pumping and compression applications, equipment can be built which requires much less maintenance due to the absence of moving parts. Tritium effects on these hydrides are of interest because the build-in of helium from tritium decay will limit the useful lifetime of the hydride materials.

Summary:

Lanthanum nickel aluminum (La-Ni-Al) alloys have been investigated and selected for storage and compressor applications. Tritium affects the pressure-composition-temperature (PCT) relationship as He-3 accumulates in the metal lattice. Methods have been developed to reverse the aging effects involving absorption/desorption cycling and heating when loaded with deuterium. Cycling alone can mitigate some of the aging effects compared to dormant storage. Palladium has also been studied because it is deposited on kieselguhr (a diatomaceous earth) and zeolite for use in a number of other processing applications. Effort on these latter materials has concentrated on determination of metallurgical properties and the effects of processing conditions on the materials. Another material, NdCo₃, has been identified as the preferred candidate to develop an advanced hydrogen isotope purification process to replace palladium diffusers currently used in the tritium facility.

(continued next page)

Tritium exposure and cycling tests on La-Ni-Al alloys will continue to extend the current data base. The goal for the coming year is to complete an analysis of 5-year-tritium exposure on these materials. New alloys will be introduced into the tritium storage program; these include NdCo₃ and Zr-Fe for tritium stripping applications and La-Ni-Al(C.05 and 0.10) for compression applications.

DOE Hydrogen Research and Technology Summary

Office Defense Programs/Research and Advanced Technology

Topic X-ray Diffraction Studies

Type of Project (check one) Fuels-Related _____ Non-Fuels-Related X

Cognizant Principal
Division Research & Technology Development Contact G. J. D'Alessio Phone (301) 903-6688

Other Sponsoring EG&G Mound Applied Technologies
Organization(s) _____ Contractor(s) Miamisburg, OH 45343-3000

Summary Start Scheduled
Date July 1991 Date 1987 Completion _____ Status Ongoing

Funding (\$10⁶) FY 1990 0.17 FY 1991 0.17 FY 1992 0.20 To Completion _____

Objective (or goal):

Palladium is widely used in hydrogen pumps and other processing equipment. The goal is to measure X-Ray Diffraction (XRD) line broadening on aged palladium tritides in order to determine the affect of helium retention on crystallite size, non-uniform strain, inhomogeneity due to solid solution, and lattice parameter changes.

Purpose (background and reason for work):

Summary:

Theory developed by Wolfer at Sandia National laboratories predicts the Pressure-Composition-Temperature (PCT) curve shifts observed in aged palladium tritides to be directly related to the strains in Pd can be measured by X-ray line broadening techniques after two months of aging. Special low background cells were purchased and received in 1991. The test facility was set up and approved in 1992. The cells were tested by x-ray diffraction for expected pressure dependent variations in lattice spacings at pressures of 0 psi and 21 psi. No verifiable variations were seen. It was discovered that the cells were already in a highly strained condition, due to the manufacturer drasing process. New cells have been requisitioned which incorporate fully annealed beryllium walls.

Next Phase:

After the new cells are received, samples will be prepared and analyzed to calibrate the test system. Aged samples will be remeasured and determinations will be made to see if the theory is supported. The various measurement parameters, such as crystallite size, non-uniform strain, etc., will be compared with helium retention to further test the theory.

DOE Hydrogen Research and Technology Summary

Office Defense Programs/Research and Advanced Technology

Topic Heat of Formation

Type of Project (check one) Fuels-Related _____ Non-Fuels-Related X

Cognizant

Division Research & Technology Development

Principal

Contact G. J. D'Alessio Phone (301) 903-6688

Other Sponsoring

Organization(s) _____

EG&G Mound Applied Technologies

Contractor(s) Miamisburg, OH 45343-3000

Summary

Date July 1992

Start

Date 1989

Scheduled

Completion _____

Status Ongoing

Funding (\$10⁶) FY 1990 0.04 FY 1991 0.04 FY 1992 0.0 To Completion _____

Objective (or goal):

Determine the heat of formation for hydriding and dehydriding several metal tritides. This will allow the determination of parameters to operate storage beds in laboratory systems.

Purpose (background and reason for work):

Summary:

Heats of formation for a number of metal hydride systems have been estimated from Pressure-Temperature-Composition (PCT) curves. A better estimate of these heats of formation are needed as well as information about the stability of these materials in the presence of tritium. Differential Scanning Calorimetry (DSC) will now determine exact values of these materials.

Next Phase:

Heat of formation work has been curtailed in order to put more effort into x-ray diffraction studies.

DOE Hydrogen Research and Technology Summary

Office Defense Programs/Research and Advanced Technology

Topic Stoichiometry Changes and He Retention

Type of Project (check one) **Fuels-Related** _____ **Non-Fuels-Related** X

Cognizant

Division Research & Technology Development

Principal

Contact G. J. D'Alessio

Phone (301) 903-6688

Other Sponsoring

Organization(s) _____

EG&G Mound Applied Technologies

Contractor(s) Miamisburg, OH 45343-3000

Summary

Date July 1991

Start

Date 1987

Scheduled

Completion _____

Status Ongoing

Funding (\$10⁶) **FY 1990** 0.23 **FY 1991** 0.24 **FY 1992** 0.24 **To Completion** _____

Objective (or goal):

To provide an understanding of aging effects in palladium-based materials, especially as they impact on helium retention and hydrogen stoichiometry, so that their use in hydrogen pumps and other processing equipment may be modeled.

Purpose (background and reason for work):

Summary:

It has been demonstrated that the Pressure-Composition-Temperature (PCT) curves vary for palladium alloys with age when exposed to tritium. Other fundamental properties, such as physical volume, have also been shown to change under these conditions. Nuclear Magnetic Resonance Spectrometry (NMR) has been applied to gain an understanding of these phenomena.

Due to stricter requirements in the ES&H area, it is necessary to develop new procedures, since NMR samples are normally handled in glass tubes and this is no longer permissible for significant quantities of tritium. Procedures were developed and approved, and an aged (approx. 10 years) sample of Pd-Rh tritide was examined after detritiding under vacuum. A very weak He-3 NMR signal was observed and was too weak to be useful.

Next Phase:

After detritiding, the resulting Pd powder is electronically conductive. It is believed that the small particle size of the Pd powder results in a surface pathway for conduction of the electromagnetic rf pulse which prevents its penetration into the depth of the sample, thus losing all sensitivity to detection of helium-3. It is planned to dilute the sample with an electrically inert material (Al₂O₃) to break the contact between the conducting palladium particles. This could increase the signal by a factor of 10 based on previous observations of diluted and undiluted PdTx samples. This work will be conducted to study the nature of helium gas retention in other metal tritide systems as well.

DOE Hydrogen Research and Technology Summary

Office Defense Programs/Research and Advanced Technology

Topic Hydrogen Interactions with Materials

Type of Project (check one) Fuels-Related _____ Non-Fuels-Related X

Cognizant

Division Research & Technology Development

Principal

Contact G. J. D'Alessio

Phone (301)903-6688

Other Sponsoring

Organization(s) _____

Contractor(s) Los Alamos National Laboratory

Summary

Date July 1991

Start

Date _____

Scheduled

Completion Indef.

Status Ongoing

Funding (\$10⁶) FY 1990 1.8 FY 1991 2.3 FY 1992 _____ To Completion _____

Objective (or goal):

To study and characterize the interaction of hydrogen with various materials.

Purpose (background and reason for work):

To improve the understanding of materials applications in nuclear weapons.

Summary:

Research and development is continuing with satisfactory progress.

Next Phase:

DOE Hydrogen Research and Technology Summary

Office Defense Programs/Research and Advanced Technology

Topic Metal-Hydrogen Reactions

Type of Project (check one) Fuels-Related _____ Non-Fuels-Related X

Cognizant

Division Research & Technology Development

Principal

Contact G. J. D'Alessio Phone (301) 903-5593

Other Sponsoring

Organization(s) _____ Contractor(s) Los Alamos National Laboratory

Summary

Date July 1991

Start

Date _____

Scheduled

Completion _____ Status Ongoing

Funding (\$10⁶) FY 1990 0.4 FY 1991 0.4 FY 1992 _____ To Completion _____

Objective (or goal):

To characterize and understand the interaction of hydrogen with metals and study the influence of other materials on this interaction.

Purpose (background and reason for work):

To improve the understanding of materials compatibility in nuclear weapons.

Summary:

Research is continuing with satisfactory progress.

Next Phase:

DOE Hydrogen Research and Technology Summary

Office Domestic and International Energy Policy

Topic Monitoring for Policy

Type of Project (check one) Fuels-Related _____ Non-Fuels-Related _____

Cognizant

Division _____

Principal

Contact Dick Holt

Phone 202-586-4449

Other Sponsoring

Organization(s) _____ Contractor(s) _____

Summary

Date _____

Start

Date _____

Scheduled

Completion _____

Status _____

Funding (\$10⁶) FY 1990 0 FY 1991 0 FY 1992 0 To Completion 0

Objective (or goal):

PE monitor hydrogen activity to keep abreast of developments in this field.

Purpose (background and reason for work):

Routine information gathering

Summary:

Next Phase:

**DATE
FILMED**

10/12/93