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IEA Agreement on the Production and Utilization of Hydrogen

1999 Annual Report

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Overview: International Energy Agency Hydrogen Implementing Agreement

The International Energy Agency

The International Energy Agency (IEA) was established in 1974, following the first oil crisis and is managed within the framework of the Organization for Economic Cooperation and Development (OECD). The mission of the IEA is to facilitate collaborations for the economic development, energy security, environmental protection and well-being of its members and of the world as a whole. The IEA is currently comprised of twenty-four member countries, ten of which are participants in the program focused on the Utilization and Production of Hydrogen.

The Hydrogen Program, or Implementing Agreement, has been in existence for more than twenty years for the purpose of advancing hydrogen technologies and accelerating hydrogen's acceptance and widespread utilization. Past collaborations have been in the areas of Thermochemical Production, High Temperature Reactors, Electroloysis, Storage, Safety, and Markets.

The following countries/organizations participate in the Hydrogen Implementing Agreement: Canada, European Commission, Japan, Lithuania, the Netherlands, Norway, Spain, Sweden, Switzerland, United States.

GUIDING PRINCIPLES OF THE HYDROGEN AGREEMENT

Today, hydrogen is primarily used as a chemical feedstock in the petrochemical, food, electronics, and metallurgical processing industries, but is rapidly emerging as a major component of clean sustainable energy systems. It is relevant to all of the energy sectors - transportation, buildings, utilities, and industry. Hydrogen can provide storage options for intermittent renewable technologies such as solar and wind, and, when combined with emerging decarbonization technologies, can reduce the climate impacts of continued fossil fuel utilization. The members of the IEA Hydrogen Program agree that energy related hydrogen technologies, thus, merit serious attention. The following are the guiding principles on which the scope of the Agreement is based:

- Hydrogen--now mainly used as a chemical for up-grading fossil-based energy carriers--will in the future increasingly become an energy carrier itself. It is necessary to carry out the analysis, studies, research, development and dissemination that will facilitate a significant role for hydrogen in the future.

- Significant use of hydrogen will contribute to the reduction of energy-linked environmental impacts, including global warming due to anthropogenic carbon emissions, mobile source emissions such as CO, NOx, SOx, and NMHC (non-methane hydrocarbons), and particulates.

- Hydrogen is currently used to up-grade lower-quality, solid and liquid fossil fuels, such as coal and heavy oils. The use of hydrogen in such applications reduces harmful emissions through more efficient end-use conversion processes and extends the range of applicability. Ultimately, with the addition of hydrogen, carbon dioxide emissions can be used to produce useful chemicals and fuels.

Hydrogen has the potential for short, medium and long-term applications and the steps to realize the potential for applications in appropriate time frames must be understood and implemented.

All sustainable energy sources require conversion from their original form. Conversion to electricity and/or hydrogen will constitute two prominent, complimentary options in the future.

Hydrogen can assist in the development of renewable and sustainable energy sources by providing an effective means of storage, distribution and conversion; moreover, hydrogen can broaden the role of renewables in the supply of clean fuels for transportation and heating.

Hydrogen can be produced as a storable, clean fuel from the world's sustainable non-fossil primary energy sources - solar energy, wind energy, hydropower, biomass, geothermal, nuclear, or tidal. Hydrogen also has the unique feature that it can upgrade biomass to common liquid and gaseous hydrocarbons, thus providing a flexible, sustainable fuel.

Hydrogen can be used as a fuel for a wide variety of end-use applications including important uses in the transportation and utility sectors.

All countries possess some form of sustainable primary energy sources; hence, hydrogen energy technologies offer an important potential alternative to fossil fuel energy supply (in many instances to imported fuels). Utilization of hydrogen technologies can contribute to energy security, diversity and flexibility.

Barriers, both technical and non-technical, to the introduction of hydrogen are being reduced through advances in renewable energy technologies and hydrogen systems including progress in addressing hydrogen storage and safety concerns.

Hydrogen energy systems have potential value for locations where a conventional energy supply infrastructure does not exist. The development of hydrogen technologies in niche applications will result in improvements and cost reductions that will lead to broader application in the future.

The members of the IEA Hydrogen Agreement recognize that a long-term research and development effort is required to realize the significant technological potential of hydrogen energy. This effort can help create competitive hydrogen energy production and end-use technologies, and supports development of the infrastructure required for its use. Attention is to be given to the entire system, in particular all of the key elements should be covered either with new research or based on common knowledge.

If the technological potential of hydrogen is realized, it will contribute to the sustainable growth of the world economy by facilitating a stable supply of energy and by helping to reduce future emissions of carbon dioxide. Cooperative efforts among nations can help speed effective progress towards these goals. Inasmuch as hydrogen is in a pre-commercial phase, it is particularly suited to collaboration as there are fewer proprietary issues than in many energy technologies.

IEA Hydrogen Vision: Our vision for a hydrogen future is one based on clean sustainable energy supply of global proportions that plays a key role in all sectors of the economy.

IEA Hydrogen Mission: The mission of the IEA Hydrogen Program is to accelerate hydrogen implementation and widespread utilization.

IEA Hydrogen Strategy: Our strategy is to facilitate, coordinate and maintain innovative research, development and demonstration activities, through international cooperation and information exchange.

We will achieve this strategy by meeting the below listed objectives:

Technology Objective:

To promote acceptance of hydrogen as an energy carrier.

Actions:

- Conduct research and development activities to address important barriers to hydrogen's acceptance.
- Foster and maintain a balanced portfolio of hydrogen technologies.
- Develop safe, efficient, and cost-effective hydrogen storage systems.
- Demonstrate integrated hydrogen systems.
- Collect, disseminate, and analyze information on hydrogen technologies.
- Develop direct hydrogen production technologies.

Economic Objective:

Develop cost-effective hydrogen energy systems that can compete in global markets.

Actions:

- Encourage industry participation to obtain market oriented input for the prioritization of research, development and demonstration activities.
- Develop and utilize analysis tools to evaluate and optimize hydrogen systems.
- Increase involvement of industry in the Agreement's activities.
- Foster clean system incentive policies.
- Identify secondary benefits of hydrogen energy systems, such as demilitarization.

Energy Security Objective:

Contribute to global energy security.

Actions:

- Facilitate the transition from fossil fuel energy systems to sustainable hydrogen-based energy systems.
- Provide resources for the conversion of intermittent and seasonal renewables to base-load, load following or peak-load power supplies, and to transportation fuels.
- Assist developing countries in evaluating sustainable, indigenous resources for hydrogen production.

Environmental Objective:

Exploit the environmental benefits of hydrogen.

Actions:

- Carry out research and development on renewable hydrogen production techniques.
- Promote hydrogen as a "clean" fuel.
- Perform life cycle assessments of hydrogen technologies and energy systems.
- Conduct research and development on technologies that lead to the decarbonization of fossil fuels.

Deployment Objective:

Promote deployment of hydrogen technologies with important local and global energy benefits.

Actions:

- Provide design support for hydrogen demonstrations.
- Conduct cost-shared and task-shared deployment activities for hydrogen energy systems.
- Act as an information resource for on-going and proposed hydrogen demonstration activities, including performance analyses.
- Conduct case studies for hydrogen systems in developing countries.

Outreach Objective:

Advertise the benefits of hydrogen.

Actions:

- Increase involvement of private and public organizations in the Hydrogen Program.
- Utilize media tools to promote hydrogen education.
- Establish collaborative research and development projects that promote international networks.
- Collaborate with other IEA Agreements to increase the effectiveness of cross-cutting research and development activities.
- Increase cooperation to reach “critical mass” in research and development activities.

Market Objective:

Identify and overcome barriers for hydrogen’s penetration into the energy and fuel markets.

Actions:

- Contribute to the scientific and technical basis for approved codes and standards.
- Promote hydrogen infrastructure for supply, maintenance and operation.
- Pursue technologies that will lead to Increased market penetration for hydrogen.
- Initiate safety-related educational and technology assessment activities.

Summary

As we enter the new millennium, concerns about global climate change and energy security create the forum for mainstream market penetration of hydrogen. Ultimately, hydrogen and electricity, our two major energy carriers, will come from sustainable energy sources, although, fossil fuel will likely remain a significant and transitional resource for many decades. Our vision for a hydrogen future is one of clean sustainable energy supply of global proportions that plays a key role in all sectors of the economy. We will implement our vision with advanced technologies including direct solar production systems and low-temperature metal hydrides and room-temperature carbon nanostructures for storage.

Current and Completed Annexes of the IEA Hydrogen Implementing Agreement

Annex 1	Thermochemical Production	1977-1988
Annex 2	High Temperature Reactors	1977-1979
Annex 3	Assessment of Potential Future Markets	1977-1980
Annex 4	Electrolytic Production	1979-1988
Annex 5	Solid Oxide Water Electrolysis	1979-1983
Annex 6	Photocatalytic Water Electrolysis	1979-1988
Annex 7	Storage, Conversion and Safety	1983-1992
Annex 8	Technical and Economic Assessment of Hydrogen	1986-1990
Annex 9	Hydrogen Production	1988-1993
Annex 10	Photoproduction of Hydrogen	1995-1998
Annex 11	Integrated Systems	1995-1998
Annex 12	Metal Hydrides for Hydrogen Storage	1995-
Annex 13	Design and Optimization of Integrated Systems	1999-
Annex 14	Photoelectrolytic Production of Hydrogen	1999-
Annex 15	Photobiological Production of Hydrogen	1999-

REPORT OF THE CHAIRMAN

Mr. Neil P. Rossmeissl

U.S. Department of Energy

INTRODUCTION

Although another extremely productive year for the Hydrogen Agreement, this was also a very sad year for our Executive Committee and Experts. We lost three dear friends and colleagues with the passing of Dr. Abraham Bahbout, former Executive Committee Member from the European Commission, Dr. David Hall, former Executive Committee Member and Annex 10 expert from the United Kingdom, and Dr. Steven Guthrie, Annex 12 expert from the United States.

Dr. Abraham Bahbout: From 1994-1998, Dr. Abraham Bahbout represented the European Commission on the Hydrogen Agreement Executive Committee through his position at the Joint Research Centre in Ispra, Italy. Dr. Bahbout was a man of great vision and insight. His many years of technical leadership, including as Coordinator for the Euro Quebec Hydro Hydrogen Pilot Project, lead to significant contributions to the international community in several fields, including the advancement of hydrogen technologies. Dr. Bahbout’s unique perspective on the path to achieve a hydrogen future challenged all of us to see outside of our respective program objectives to hydrogen's true potential in the international arena. We are all better leaders, and individuals, for having the benefit of Dr. Bahbout's intelligence, perspective, guidance and companionship.

Dr. David Hall: Dr. Hall touched many lives in his years as a professor of Biology at the King’s College London. The students who passed through his classrooms and laboratories all benefitted greatly from a true expert in renewable energy. A recognized world leader in bioreactor development, hydrogen research and biomass innovation, Dr. Hall contributed greatly to a number of international collaborations, including our own Annex 10, Photoproduction of Hydrogen. His expertise and insight were essential to the progress made by our Annex 10 experts and for laying the groundwork for our new Annex 15. He was a great man whose influence was felt by all of us. The number of technical leaders who traveled from around the globe to attend Dr. Hall’s memorial service gives testament to the kindness and warmth that he exhibited in his daily interactions and the great void his passing leaves in the scientific community.

Dr. Steven Guthrie: The metal hydride community lost one of its most productive and respected members with the passing Dr. Steven Guthrie. Dr. Guthrie’s work at Sandia National Laboratory, Livermore, California, was a valuable contribution to our Annex 12 activities and to the overall advancement of metal hydride materials for hydrogen storage. An active participant from the start of Annex 12, Dr. Guthrie leaves a great base of work for the experts to carry forward. His legacy of hard work, dedication, contribution and companionship set a standard by which our future task efforts can only hope to come close to achieving.

Our deepest sympathies go to the families, friends and colleagues of Drs. Bahbout, Hall and Guthrie. Their loss is felt by all of our members and by the technical communities of which they were a part.

STATUS OF IMPLEMENTING AGREEMENT

June 1999 marked the conclusion of our five year term for the Hydrogen Agreement. Based on the interest of our members and approval by the Governing Board, we requested and were granted another five year extension that will take us through to June 2004. The past five years have been very productive. We launched four highly-effective, task-shared annexes that resulted in a number of advances for hydrogen technologies. We published ten reports, with seven more in the draft stage. Our experts presented their results at numerous international conferences and published in world-class journals. Special thanks go to our Executive Secretary, Ms. Carolyn Elam, for her outstanding work, leadership and guidance. Her contributions to our Agreement are too numerous to list, but I would like to take special note of her efforts in completing all of our end-of-term requirements, including the presentation to the Renewable Energy Working Party.

MEMBERSHIP

I am very pleased to announce that Lithuania has joined our Agreement’s activities. They will begin their official participation in 2000, but have already been making valuable contributions to our Task 13, Design and Optimization of Integrated Systems. Lithuania will be represented on the Executive Committee by Dr. Jurgis Vilemas, Director of the Lithuanian Energy Institute. Mr. Algis Vasys, Cambridge Associates, will act as the alternate. We welcome both Dr. Vilemas and Mr. Vasys and look forward to working with them and the Lithuanian experts for many years to come.

Our membership now includes Canada, the European Commission, Japan, Lithuania, the Netherlands, Norway, Spain, Sweden, Switzerland and the United States. The United Kingdom has expressed a renewed interest via the Defence Evaluations Research Agency (DERA). Dr. Richard Jones from DERA participated in our Spring ‘99 meeting in Stockholm as an observer and is now working towards initiating the procedures to become a Member. We hope that Dr. Jones and DERA are successful in reestablishing the United Kingdom’s participation in the Hydrogen Agreement.

We continue to seek out new members. There are a number of countries in which we have identified complimentary research activities where there would be a mutual benefit by including them in our task activities. We are currently involved in discussions with the government officials in several of these countries and hope that during 2000 we will be able to announce additional new members to our Agreement.

STATUS OF TASKS

This year marked the official start for three new tasks: Task 13, Design and Optimization of Integrated Systems, Task 14, Photoelectrolytic Production of Hydrogen, and Task 15, Photobiological Production of Hydrogen. Additionally, Task 12, Hydrogen Storage in Metal Hydrides and Carbon, continues to make great progress in advancing hydrogen storage technology.

Task 12 - Hydrogen Storage in Metal Hydrides and Carbon

Since its inception, there have been 20 projects (16 metal hydride and 4 carbon) included in the scope of work for Task 12. Of these, 13 remained active during 1999. A great deal of progress has been made in this task thanks to the dedication of our experts and the exceptional leadership of our Operating Agent, Dr. Gary Sandrock. Most notable is the work with the catalyzed sodium aluminum hydrides. These materials have already shown reversible hydrogen storage capacities of 5 weight percent at 150°C. They are now coming close to meeting the new task target of 5 weight percent at temperatures at or below 100°C.

Task 13 - Design and Optimization of Integrated Systems

Task 13 officially started on 1 January 1999. Our experts are off to a great start, having converted all of the component models developed under Task 11 so that they are compatible with the new version of the modeling software. Three integrated systems have also been selected for evaluation. The incorporation of Life Cycle Analysis into the overall system evaluations will prove extremely important in demonstrating the environmental benefits of hydrogen energy systems. Mrs. Catherine Grégoire Padró and her task experts continue to make exceptional strides in increasing the visibility of hydrogen and in providing tools for designing and optimizing energy systems with hydrogen as a key component.

Task 14 - Photoelectrolytic Production of Hydrogen

This new task continues the work conducted in Subtask A of the completed Task 10, Photoproduction of Hydrogen. Task 14 officially started on 1 July 1999 and will continue through June 2002. We welcome Dr. Andreas Luzzi as the Operating Agent, representing Switzerland. As an expert in the Solar Chemistry Task of the SolarPACES Agreement, Dr. Luzzi provides a key bridge between the two Implementing Agreements. We are looking forward to expanded collaborations between our Agreements, including joint experts meeting starting in early 2000.

Task 15 - Photobiological Production of Hydrogen

This new task continues the other half of the work from the completed Task 10. The Task officially began on 1 June 1999 and will run for three years with a possible two year extension. We welcome Dr. Peter Lindblad, previously an expert for Task 10, as the Operating Agent, representing Sweden. Dr. Lindblad’s involvement in the European Photobiological Network, as well as his demonstrated leadership and expertise, will be very beneficial for the advancement of our Task 15 activities.

NEW INITIATIVES

In addition to our ongoing tasks, we have three initiatives for future tasks:

Industrial Uses of Hydrogen

Hydrogen use in non-energy processes, such as the chemical, metallurgical, and ceramics industries was identified as an area where a concentrated research effort could facilitate the increased utilization of hydrogen. Annually, these industries account for nearly 50 percent of the world's 500 billion Nm^3 hydrogen consumption. Process improvements and novel synthesis approaches could lead to overall efficiency improvements and reduced environmental impacts. Likewise, increased market share for hydrogen in these arenas should lead to expedited infrastructure development, a necessity for facilitating the advancement of the energy-related and renewable-based applications. During 1998, two workshops were held with industry representatives to identify research needs. A large scope of activities was identified. During

1999, a questionnaire was sent out to a number of industries world-wide to better refine of the scope of work. Based on the input from the industry representatives a number of research areas were identified as potential opportunities for collaborative research. However, the degree of interest in participating was not sufficient enough to warrant initiating a new task at this time. We thank Dr. Gerhard Schriber and the Swiss Federal Office of Energy for sponsoring this activity and Mr. Karsten Wurr for all of his efforts in leading the task development work and compiling all of the related information. I expect that interest in the activity will grow and that in the coming years, the timing will be ripe to launch a new IEA task dedicated to this topic.

Hydrogen from Carbon Containing Materials

The questionnaire sent out as part of the task development for the Industrial Uses of Hydrogen activity also included topics related to hydrogen production technologies from carbon-containing raw materials. There was a great deal of industrial interest in this topic, which is not surprising since approximately 95% of the hydrogen produced today comes from carbon-containing raw material, primarily fossil in origin. Most of the conventional processes convert the carbon to carbon dioxide, which is discharged to the atmosphere. With the growing awareness of the impact of greenhouse gas emissions on global climate change, there is a need to reassess the conventional approaches. There is a great deal of international interest in integrating carbon dioxide sequestration with conventional steam reforming of fossil fuels to achieve "clean" hydrogen production. Improved robustness of pyrolytic cracking technologies for the conversion of hydrocarbons to hydrogen and solid carbon is another area where there is a great deal of interest, both from the standpoint of improved economics and the applicability to a variety of feeds. Finally, the thermal processing of biomass is expected to yield an economic and carbon-neutral source of renewable hydrogen.

Norsk Hydro and the Research Council of Norway are leading the task development efforts. Workshops will be held during 2000 to further the task development efforts and define the scope of work. I would like to thank Mr. Bjorn Gaudernack and Mr. Trygve Riis for all of their efforts in coordinating the development of this activity. We look forward to working with the new Task Development Leader and proposed Operating Agent Mrs. Elisabet Fjermestad Hagen of Norsk Hydro in the coming year to launch this new IEA task.

Hydrogen Storage in Metal Hydrides and Carbon

Task 12 will be coming to an end in September 2000. As previously mentioned, great strides have been made, particularly with the catalyzed sodium aluminum hydrides. However, this work is still in the early development stage. Safety, durability and cost still require a significant investigative effort. Likewise, some formulation improvements still need to be made to achieve the current storage target of 5 weight percent at temperatures below 100^{o}C in order to be suitable for vehicle applications. Carbon adsorbents, such as carbon nanotubes, are being touted as having the greatest potential for meeting the hydrogen storage requirements. However, work in this area is still at the very fundamental stage. During 2000, our Operating Agent and experts will define a new task to carry forward the efforts of Task 12 and address some of the needs discussed above. The task will likely include an extensive modeling effort on hydrogen storage mechanisms in carbon absorbent materials.

HIGHLIGHTS FROM THE 1999 EXECUTIVE COMMITTEE MEETINGS

41st Meeting, Stockholm, Sweden, 18-21 May 1999

- Dr. Jurgis Vilemas, Lithuania, and Dr. Richard Jones, United Kingdom participated in the meeting as Observers. Both Lithuania and the United Kingdom were invited to pursue participation in the Hydrogen Agreement. Each have projects that fit in well with the ongoing tasks:
  Lithuania - Modeling activities are underway to study the physical and chemical processes during the anearobic digestion of swine manure to produce hydrogen-rich biogas and for the subsequent use of the biogas in a fuel cell power plant. This project will be included in Task 13.
  United Kingdom - A number of projects are underway in the storage area, including the use of fullerenes and graphite nanostacks. This includes a great deal of modeling work that would compliment the current Task 12 work, as well as the proposed new hydrogen storage task.
- Both Task 14, Photoelectrolytic Production of Hydrogen, and Task 15, Photobiological Production of Hydrogen, were approved to begin work.
- A Visiting Scientist Fund was established to provide support for task activities. The fund will provide travel expenses to selected experts to either attend experts meetings or for visits to a specific laboratory for collaboration. The Operating Agents will periodically present proposals for consideration by the Executive Committee.

42nd Meeting, Toronto, Ontario, Canada, 26-29 October 1999

- The Executive Committee drafted a new Strategy Plan.
- Plans were initiated for IEA Hydrogen Day at the Hyforum 2000 Meeting in Munich, Germany, 11-14 September 2000. The IEA Hydrogen Agreement will sponsor one day of the meeting and will develop a booth for the Exposition. A Round Table Discussion with representatives from the Hydrogen Agreement member countries will be included.
- A new effort to track international projects related to hydrogen was launched. The Secretary will begin compiling a list of projects, including brief descriptions where available.

SUMMARY

I am very excited about the opportunities for hydrogen technologies. Industrial interest in hydrogen energy systems continues to grow. Royal Dutch Shell's recent establishment of Shell Hydrogen is a clear example of industry taking an active role in planning for our energy future. Ballard fuel cells are finding their way into an increasing number of applications throughout the world. Stuart Energy System's fuel appliances are already delivering fuel to vehicle fleets and will soon be providing hydrogen for the personal automobile. Norsk Hydro is rapidly becoming a world leader in "clean" hydrogen production from fossil fuels. Iceland, in partnership with Ballard, Daimler and Norsk Hydro, will host one of the largest hydrogen demonstration projects to date and the WE-NET program is well on track for establishing a hydrogen-based clean energy network in Japan. These are but a few examples of industry's leadership in hydrogen energy system development.

Our international research organizations continue to achieve significant advances of their own. Hydrogen-producing algal mutants have been developed. Combined with the recent advances in bioreactors, these organisms could likely provide us with renewable hydrogen within the next twenty years. The advances that have already been discussed for metal hydrides and carbon have important implications for on-board applications, namely providing a safe storage option for hydrogen fuel. Photoelectrochemical water-splitting devices are producing hydrogen at efficiencies of more than 12 percent and biomass is proving a viable and economical feedstock for carbon-neutral hydrogen production.

Our Hydrogen Agreement is in a key position to help facilitate a growing number of hydrogen projects. Our integrated system tools provide a mechanism by which hydrogen energy systems can be designed, optimized and compared with conventional technologies. The collaborative mechanism has led to a rapid advancement in storage options. Furthermore, world leaders in bioreactor development will be brought together with genetic experts to accelerate the application of the photobiological production routes. We continue to benefit through involvement with industry, in particular our Agreement signatories Stuart Energy Systems (formerly the Electrolyser Corporation). Now Norsk Hydro joins our leadership group as Operating Agent for the new Hydrogen from Carbon Containing Materials task. In addition to this direct industry involvement, many of our experts have ongoing collaborations with industrial partners, which is essential for rapid introduction of our technologies into the commercial market.

Again, I would like to welcome Dr. Vilemas and Mr. Vasys to our Executive Committee as the representatives from Lithuania. We are very excited about this new member to our Agreement. Special thanks go to Mr. Bjorn Gaudernack for all of his excellent work and for his leadership of Annex 10. We welcome Drs. Luzzi and Lindblad and thank them for the exceptional jobs they have done in launching our new photoproduction activities. Our task experts deserve special recognition for all of their contributions over the last five years. They have made our task-shared activities a true success. Finally, I would like to thank all of my colleagues on the Executive Committee for their hard work in supporting the development of our new activities, redefining our strategic plan, researching international hydrogen projects, and identifying potential new members.

TASK 11 - INTEGRATED SYSTEMS

Catherine E. Grégoire Padró
National Renewable Energy Laboratory
Operating Agent for the
U.S. Department of Energy

Introduction

The final reports for Task 11 were completed this year, chronicling the efforts of the participants in the development and application of tools for design and analysis of hydrogen energy systems. The highly-successful task efforts included the development of over two dozen component models, the evaluation of the technical aspects of a number of integrated systems, the analysis of over a dozen hydrogen demonstration projects throughout the world, and the development of a systematic design procedure for evaluating and comparing hydrogen energy systems.

Task Description

A structured approach was developed to minimize the perceived and real risks associated with the introduction of hydrogen as an energy carrier. Within the framework of the International Energy Agency Hydrogen Implementing Agreement, Task 11 was undertaken to develop tools to assist in the design and evaluation of existing and potential hydrogen demonstration projects. Emphasis was placed on integrated systems, from input energy to hydrogen end use. The activities were focused on near- and mid-term applications, with consideration of the transition from fossil-based systems to sustainable hydrogen energy systems.

In order for hydrogen to become a competitive energy carrier, experience and operating data need to be generated and collected through demonstration projects. A framework of scientific principles, technical expertise, and analytical evaluation and assessment needed to be developed to aid in the design and optimization of hydrogen demonstration projects to promote implementation. The task participants undertook research within the framework of three highly coordinated subtasks that focused on the collection and critical evaluation of data from existing demonstration projects around the world, the development and testing of computer models of hydrogen components and integrated systems, and the evaluation and comparison of hydrogen systems.

Systems considered included stand-alone and grid-connected hydrogen production and hydrogenation systems; hydrogen and oxygen transport and storage systems; conversion devices including fuel cells, turbines, combustors, and hydrogenation units; electric load leveling systems; and general characteristics of mobile applications.

This work was carried out in cooperation with other IEA Implementing Agreements, where appropriate.

Subtask A: Case Studies

Hydrogen energy systems were critically evaluated and compared, with system performance measurement as the central focus. Project descriptions of existing hydrogen demonstration projects were collected and assembled including the project goals, a description of the main components, a representative set of experimental results, and discussion of lessons learned.

The projects described in the Subtask A report were selected according to the following criteria:

- The projects were required to be integrated systems, with two or more of subsystems (production, storage, transport/distribution and end use) included in a relevant connection.
- The selection was primarily restricted to projects located in one of the countries participating in the IEA Hydrogen Implementing Agreement (to ensure access to data and other relevant information).
- Active cooperation of the project leaders was required.

A comparative overview of the selected integrated systems indicated that the sun is the primary source of energy for many of the hydrogen demonstration projects. Accordingly, the operation of electrolysers with intermittent sources of power (solar and wind) and the various possibilities for matching photovoltaic current with the characteristics of the electrolyser was one of the recurrent design issues in all such projects. Most of the electrolysers were of the alkaline type and operated at low pressure. Two projects used solid polymer electrolysers, and three projects operated the electroyser at higher pressures. While the storage technologies were restricted to the use of compressed gas and metal hydrides, a great variety of utilisation technologies and applications were included. In most of the projects, hydrogen is used in a fuel cell, with a wide variety of fuel cell types included. Transportation applications included two projects in which vehicles were fitted with polymer exchange fuel cells, and one in which trucks were fueled with compressed hydrogen generated from a PV-electrolysis system, fed to a modified internal combustion engine.

Ten projects were analysed and evaluated in detail. As appropriate, each project report includes sections on project goals, a general description of the project, descriptions of the components, simulation and system integration, performance and operational experience, data acquisition, a discussion of public acceptance and safety issues, environmental aspects, future plans, and conclusions. The detailed project descriptions included in the Subtask A report are:

Project
Solar hydrogen demonstration at Neunburg vorm Wald
Markus Friedl solar hydrogen plant on residential house
Photovoltaic hydrogen production - Alexander T. Stuart renewable energy test site
Phoebus Jülich demonstration plant
Schatz solar hydrogen plant
INTA solar hydrogen plant
Clean Air Now: solar hydrogen fueled trucks
SAPHYS: stand-alone small size PV hydrogen energy system
Hydrogen generation from stand-alone wind-powered electrolysis systems
Palm Desert renewable hydrogen transportation project

Additionally, short reports are included for several other hydrogen demonstration projects for which detailed information was not available.

Subtask B: Analysis Tools

As part of the effort to design and optimize hydrogen energy systems, computer models were developed and validated for hydrogen production, storage, transport/distribution, and end use components. The modeling platform selected for Task 11 was the process simulation package ASPEN Plus^{TM}. The models are available to interested users and the Task 11 experts can assist in the use of the models and in the interpretation of results.

The component models developed were:

- Production (8 component models)
- Storage (5)
- Transport/Distribution (5)
- End Use/Refueling (9)

The component models available are:

Technology	Team Lead
Production	
PV-Electrolysis	Spain
Wind-Electrolysis	USA
Grid-Electrolysis	USA
Steam Methane Reforming	USA
Biomass Gasification	USA
Biomass Pyrolysis	USA
Coal Gasification	Netherlands
Storage	
Pressurized Gas	Canada
Metal Hydrides	USA
Liquefaction	Japan
Chemical Storage	Netherlands
Chemical Hydrides	Switzerland

Distribution	
Transport Tanker	Japan
Pipeline (trunk & distribution)	USA
Tank Truck	Japan
Methanol Transport	Netherlands
Utilization	
PEM Fuel Cell	Canada
Phosphoric Acid Fuel Cell	Spain
Solid Oxide Fuel Cell	USA
Molten Carbonate Fuel Cell	USA
Gas Turbine	USA
Internal Combustion Engine	USA
Refueling Station	USA

Standardization of the component models was essential, since individual component models were to be used in combination with other component models to form integrated hydrogen energy systems. Documentation for each component model was developed to provide important information on the model series, flow sheet number, authors, date created, ASPEN Plus^{TM} version, and a technical abstract of the model. (Major changes were made in the new release of ASPEN Plus^{TM}, rendering many of the original models virtually unuseable by most potential users. In order to permit use of the component models in the new version, all component models were converted to ASPEN Plus^{TM} Version 10.1, although this version was released after the end date of Task 11).

The documentation also provides a detailed summary of the model including both a description and its implementation. In the description section, the flow sheet is described along with system inputs and outputs. The physical property set selected, along with descriptions of important design specifications and Fortran blocks, are provided in the implementation section. Each component model report concludes with a listing of the input and output streams (material, work and heat).

Subtask C: Design Evaluation and System Comparison Guidelines

Guidelines for the evaluation and comparison of system designs were developed to aid in the optimization and selection of hydrogen systems. A design methodology was instituted to ensure unambiguous and optimal use of these guidelines. For this purpose, five design steps were defined. The guidelines consist of information that has been collected and formatted according to the data structure defined by the design methodology, and include indications for the use of data in the subsequent design steps. Systems can be compared to each other and to non-hydrogen systems and/or conventional systems using the measures of performance.

Distinguishing five different steps in the design of hydrogen energy systems is useful. These steps are:

- ***Generation of process routes:*** In the first step, the possible process routes or ‘energy chains’ that can fulfil the function that has been defined for the energy chain are generated;
- ***Preselection of process routes:*** The second step consists of selecting those process routes that seem most attractive, with the objective of reducing the number of systems that are to be studied in more detail;
- ***Process integration:*** This setup includes modeling an integrated system for the selected process routes, making use of or making available, respectively, the output streams (heat, work, mass) and the required input streams;
- ***Determination of the measures of performance (MOP)*****:** In this step, predefined system characteristics (MOP) are calculated and used to compare different integrated systems. These characteristics are indicated as the measures of performance of the system;
- ***System selection*****:** In the final step, a system is selected, for example, by comparing different systems that have been selected in the first phase or by comparing an integrated hydrogen system to conventional energy systems.

Using the guidelines, the experience acquired in existing and future integrated systems is made accessible for use in designing integrated systems. Guidelines for the design and optimization of future demonstration projects were based on data collection, demonstration case studies, component simulation, and integrated systems modeling. The guidelines have been formulated using the experience of the experts participating in Task 11, experiences from existing demonstration projects and other experiences of the participating experts.

The guidelines assist in making choices for the system configuration of future demonstration plants that meet operating and user requirements. Ultimately, the guidelines will facilitate the systematic integration of hydrogen into the world’s energy system.

Integrated System Design and Optimization

In order to demonstrate the use of the tools developed in Task 11, several integrated hydrogen energy systems were designed and analyzed. The systems were designed following the guidelines established in Subtask C, and were modeled using the component models developed in Subtask B (using the data collected in Subtask A).

Four biomass-to-hydrogen thermal processing routes, in combination with gaseous and liquid hydrogen transport and storage, were examined to determine the most efficient method of decentralized renewable-based hydrogen production for a vehicle refueling operation. The tool was used to reduce the number of options to a manageable number, and simulations were conducted. Based on the results, it appears that gasification and pyrolysis production processes are essentially equivalent on an efficiency basis, although purity and storage issues can have a large effect on the overall efficiency (and cost-effectiveness) of the processes.

Intermittent renewable resources such as photovoltaics (PV) and wind were evaluated as elements of stand-alone renewable power systems for remote communities. In two case studies, the electricity produced by the PV or wind farm was first routed to the community to fulfill its power requirements, with any remaining power routed to the electrolysers to produce hydrogen. The hydrogen was then stored as a compressed gas or in metal hydrides. If the resource was insufficient to meet demand, the stored hydrogen was used to produce electricity in a fuel cell or generator set. The results of the case studies showed that intermittent renewables could provide reliable power to a remote community if the hydrogen generation and storage units are properly sized.

Detailed papers on these two studies were presented at the World Hydrogen Energy Conference in Argentina in June, 1998 and can be found in the proceedings.

Duration

The Task was formally begun on 1 August 1995 and ended on 15 November 1998. This represents an extension of 3.5 months from the original schedule, and was authorized by the Executive Committee on 12 November 1997.

Results

The collaborative efforts of Task 11 resulted in the following outputs:

- Case study report to document hydrogen energy system demonstrations;

- Report describing the component models, including the required inputs and the expected outputs, and limitations and capabilities of the models, with a library of component models for use in the common integrating platform; and

- Report of recommendations for optimizing existing hydrogen energy systems and the set of design guidelines for planning future integrated hydrogen energy systems.

Participation

Seven countries participated in Task 11: Canada (Subtasks A and B); Italy (Sub-tasks A and C); Japan (Subtasks A, B, and C); the Netherlands (Subtasks B and C); Spain (Subtasks A and C); Switzerland (Subtasks A and B); and the USA (Subtasks A, B, and C).

The Lead Countries for Subtasks A, B, and C are Switzerland, the USA, and the Netherlands, respectively.

Publications in 1999

The Task produced three reports that cover the work completed in the three Subtasks. These reports are available from the Secretariat:

- Subtask A: “Case Studies of Integrated Hydrogen Energy Systems” - a critical evaluation and comparison of ten international hydrogen based energy system demonstration projects
- Subtask B: “Analysis Tools” - documentation for the 27 component models developed for this Task
- Subtask C: “Design Evaluation and System Comparison Guidelines” - guidelines for selecting components and optimizing hydrogen system designs, so that performance comparisons can be made between different hydrogen system designs and between hydrogen-based and conventional systems

TASK 12 - Metal Hydrides and Carbon for Hydrogen Storage

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Task Description

There is rapidly growing interest in hydrogen vehicles, especially those that incorporate fuel cells for motive power. The challenge of on-board fuel storage stands as a serious impediment to that concept. The use of hydrogen as a vehicle fuel requires a storage means that has inherent safety and both volumetric and gravimetric efficiency. Metal hydrides and carbon offer alternatives to the storage of hydrogen in gaseous and liquid form. They store hydrogen in an essentially solid form and offer the potential for volume efficiency, high safety, low pressure containment and ambient temperature operation. Unfortunately, all known hydrides are either heavy in comparison to the hydrogen they carry or require high temperature for hydrogen release. Special forms of carbon may have potential as new hydrogen storage media, but that concept is new and not yet clearly defined. The purpose of this Task is to attempt development of hydrides and carbons for on-board hydrogen storage using nonconventional materials and synthesis techniques. In addition, the option of reversible electrochemical hydrogen storage is included, although that was a minor component of Task 12 activity in 1999. Task 12 is also the source of the on-line IEA/DOE/SNL hydride databases used widely around the world.

The specific targets of the Task are as follows:

- The identification of a formulation technique for a metal hydride or carbon material that is capable of 5 wt.% hydrogen capacity with a desorption temperature of less than 100°C and a desorption pressure of at least 1 atmosphere absolute.
- The development of a metal hydride surface treatment such that high-efficiency, reversible electrochemical reactions can be accomplished over thousands of cycles.
- The establishment and maintenance of a series of on-line hydride databases, openly and freely available to the public via the Internet.

Except for the retrospective hydride databases, the Task is highly experimental in nature and is centered around two general efforts: (1) the synthesis of new and different materials and (2) the characterization of those new materials relative to their ability to store hydrogen.

Project Descriptions

There were thirteen distinct hydride projects active in 1999, nine on metal hydrides and four on carbon. Each project was led by one or two of the Task 12 Experts and usually involved experimental contributions by other Experts on an international basis. Brief descriptions and national participations of the 1999 projects are as follows:

- **Project 1: Destabilized magnesium nickel hydride [Leader: D. Noréus (Sweden); co-participants: USA, Japan]**

Mg_2NiH_4 formed above 240°C develops a microtwinned structure upon cooling, but is twin-free if formed below 240°C. The purpose of this project is to experimentally determine if the twin-free microstructure results in a destabilization effect that is manifested in decreased hydrogen desorption temperatures. This project also tries to improve the electrochemical properties of Mg_2NiH_4.

- **Project 6: Structural investigations of intermediates and end products in the synthesis of Ti-doped alkali metal - aluminum hydrides [Leader (acting): D. Noréus (Sweden); co-participants: Japan, Norway, Sweden, USA, Germany (unofficial)]**

Ti-doping renders the normally nonreversible $NaAlH_4$ and Na_3AlH_6 hydrides reversible. Although the kinetics are low, along with possible cyclic stability problems, Ti-catalyzed alkali metal - aluminum hydrides are close to meeting the capacity-temperature target of Task 12. This project aims at developing a clear understanding of the chemistry of the system so that reasonable judgments can be made toward the design of improved catalysts.

- **Project 7: Comprehensive Hydride Review and Associated IEA Databases [Leaders: G. Sandrock and G. Thomas (USA), co-participants: Switzerland, Japan]**

This project is aimed at cataloging past work on hydriding materials and applications in support of IEA Task 12 and its search for new and innovative hydriding materials. It is also aimed at encouraging hydride R&D throughout the world by making past results widely and easily accessible via the Internet in the form of on-line IEA databases. The databases can be reached at the Sandia National Laboratories' Hydride Information Center (**http://hydpark.ca.sandia.gov**).

- **Project 11: High pressure synthesis of new hydrogen storage materials [Leader: K. Yvon (Switzerland); contributor to Swiss effort: Russia]**

The University of Geneva has long been a center for the discovery of new saline and complex metal hydrides. Some have hydrogen storage capacities greater than 5 wt.%, but decompose only above 300°C; others decompose below 100°C, but are too heavy or expensive for H-storage applications. The goal of this new project is to synthesize new lightweight metal hydrides based on inexpensive 3d-elements, such as Mn and Fe, by using high-pressure techniques. The ultra-high-pressure (several kbar) facilities of Lomonosov Moscow State University (V. Verbetsky) will be used to help achieve experimental conditions hitherto unexplored.

- **Project 12: Ball milling effects during fluorination of the eutectic alloy Mg-Mg_2Ni [Leader: S. Suda (Japan), co-participants: Sweden, Switzerland, USA]**

Kogakuin University has developed the application of fluorination (F-treatment) to enhance the surface properties of hydriding alloys. This project combines ball milling (shown in other IEA 12 projects to increase hydriding/dehydriding kinetics) with F-treatment (shown by KU to provide surface protection, increased kinetics and improved activation). The alloy chosen (Mg-23.5 wt.% Ni) for the study is a two-phase mixture of Mg and Mg_2Ni that is capable of meeting the wt.% target of Task 12.

- **Project 13: Ca-based ternary alloys [Leader: N. Kuriyama (Japan); co-participants: Sweden, Switzerland]**

The objective of this new project is to search for reversible hydrides based on ternary alloys consisting of cheap and light metals, e.g., Ca, Mg, Al and transition metals. Sample materials will be prepared by sintering methods and evaluated for hydrogenation characteristics and metallurgical structures.

- **Project 14: Catalytically-enhanced sodium aluminum hydride [Leader: C. Jensen (USA); co-participant: G. Thomas (USA)]**

This project is an extension of Project 10, completed in 1998. It continues the work on Ti/Zr (and other) catalyzed $NaAlH_4$ with the following two objectives: (1) Determine the mechanism of the catalytic action and (2) Demonstrate the feasibility of a moderate scale hydrogen storage system.

- **Project 15: Metal hydride safety testing [Leader: Lynch (USA); co-participants: Thomas and Jensen (USA)]**

It is necessary to know how catalyzed sodium-aluminum-hydrogen compounds behave in credible accident scenarios. Catalyzed hydride specimens will be subjected to U.S. Department of Defense standard tests for shock, impact and friction. Other standardized tests will be applied to determine the explosibility of hydride dust clouds. *(New Project started in 1999)*

- **Project 16: Synthesis and crystal structural analysis of new ternary hydrides based on hydride-fluoride similarity [Leader: Akiba (Japan)]**

Gingl and Yvon (University of Geneva) reported the similarity of hydrides and fluorides, especially in crystal structure and developed a Hydride Fluoride Crystal Structure Database (HFD). This project will do experimental work on the synthesis of novel ternary hydrides effectively using the HFD as a guide. The overall objective of the project is to synthesize novel hydrides that have a large hydrogen capacity and a potential to reach the Task target. *(New Project started in 1999)*

- **Project C-1: Optimization of single-wall nanotube synthesis for H_2 storage [Leaders: M. Heben (USA) and P. Bernier (European Union)]**

Carbon has received considerable recent attention as a possible storage medium for hydrogen (physical and chemical). The purpose of this carbon-project is to optimize the production and purification techniques of single-wall nanotubes (SWNTs) for physical hydrogen storage in the vicinity of room temperature. It will carefully survey both arc and laser ablation processes for SWNT production, as well as purification, techniques.

- **Project C-2: Hydrogen storage in fullerene-related materials [Leaders: R. Murphy and R. Loutfy (USA)]**

Although fullerenes (C_{60} and C_{70}, for example) have the potential for high gravimetric and volumetric hydrogen storage densities, the high activation energies associated with chemical adsorption and desorption processes pose potential difficulties in the realization of such attractive storage performance at desired conditions. The main objective of this project will be to reduce the activation energies and associated process temperatures for reversible hydrogen storage, especially via the use of catalysts. *(Project terminated in 1999)*

- **Project C-3: Assessment of Hydrogen Storage on Different Carbons [Leaders: Chahine (Canada) and Loutfy (USA)]**

Several carbon structures have been proposed as adsorbents for hydrogen. Results are sometimes contradictory, and in many cases experimental techniques are not clear. The main objective of this project is to carry out a comparative study of hydrogen adsorption properties on the different carbons under the same experimental conditions of pressure and temperatures and using the same experimental setup. In-house samples, as well as samples from other sources, will be tested. *(New Project started in 1999)*

- **Project C-4: Hydrogen-Carbon, Hydrogen-Metals [Leader: Schlapbach (Switzerland)]**

The University of Fribourg has extensive experience in both metal-hydrogen and carbon-hydrogen systems. A new project has been funded by the Swiss BEW to involve the following R&D areas: (1) hydrogen in metals, (2) hydrogen in carbon, (3) hydrogen-driven optical displays and (4) hydrogen in diamond synthesis. Most of the IEA activities will probably center around electrolytic storage of hydrogen in nanotubes and other forms of carbon, but some metal hydride R&D may also be included. *(New Project started in 1999)*

Duration

Task 12 was officially initiated September, 1995, for a duration of three years. In late 1997, the Task was extended for two years and it is now scheduled to end in September, 2000.

Participation

The countries that participated during 1999 were Canada, Japan, Sweden, Switzerland and the USA. The European Commission did not confirm its planned participation in 1999 and was therefore dropped from from the Task. The official Experts, past and present, are as follows:

Canada: R. Chahine, University of Quebec
A. Zaluska*, McGill University

(European Union)*: (P. Bernier*, University of Montpellier)

Japan: E. Akiba, National Institute of Materials & Chemical Research
S. Suda, Kogakuin University
I. Uehara*, Osaka National Research Institute
N. Kuriyama, Osaka National Research Institute

Norway*: A. Maeland*, Institute for Energy Technology

Sweden: D. Noréus, Stockholms University
(B. Bogdanovic’, Max-Planck-Institute für Kohlenforschung)

Switzerland: L. Schlapbach, University of Fribourg
K. Yvon, University of Geneva
(V. Verbetsky, Moscow State University)

United States: M. Heben, National Renewable Energy Laboratory
C. Jensen, University of Hawaii
R. Loutfy, MER Corporation
F. Lynch, Hydrogen Components, Inc.
R. Murphy*, Oak Ridge National Laboratory
G. Sandrock, SunaTech, Inc. (Operating Agent)
G. Thomas, Sandia National Laboratories

* indicates no longer active; ( ) indicates unofficial

Activities and Progress During 1999

Task activity was good during 1999 with measurable progress in most of the active projects. The majority of the Task Experts participated in the Gordon Research Conference, held in Henniker, USA, during July. Visiting Scientists Bogdanovic' (Germany) and Mitrokhin (Russia) were funded by the IEA Hydrogen Task 12 member countries to visit the USA and participate in the Task Workshop held in conjunction to the Gordon Conference.

An overview presentation of the Task 12 was given at the Canadian Hydrogen Association Annual Meeting (February, Vancouver). There were numerous other specific Task 12 publications and presentations during 1999. Proceedings of the papers given during MH98 (Hangzhou, Zhejiang, China) appeared in the Journal of Alloys and Compounds (Elsevier Science) during 1999. IEA Hydrogen was a sponsor of that historic hydride symposium and its published Proceedings. A list of the Task 12 1999 presentations and publications is given below.

The IEA/DOE/SNL Hydride Databases

The purpose of the IEA/DOE/SNL hydride databases is to provide a continually-updated inventory of hydride technology and other information to Task 12 Experts, as well as the entire hydride R&D community, via the Internet. The information is presented in the form of specific searchable databases accessible at the URL **http://hydpark.ca.sandia.gov**. The data is tabulated from the open literature and presented under the auspices of the IEA with financial support from the US Department of Energy. Sandia National Laboratories supplies the Internet Server and associated Web site. This effort was active during 1999 with the addition of new databases (Hydride Complexes and Applications) and the updating of established ones. Late in 1999, the entire Web site architecture was changed to allow more convenient use and searching. The planned addition of the Hydride/Fluoride Database (HFD) has been delayed because of personnel limitations at Sandia. Following are a list of records on-line at the end of 1999:

Database	Records
Hydride Alloy Listings	1942
AB_5 Intermetallic Compounds	330
AB_2 Intermetallic Compounds	509
AB Intermetallic Compounds	156
A_2B Intermetallic Compounds	103
Misc. Intermetallic Compounds	287
Solid Solution Alloys	171
Mg Alloys	213
Complex Hydrides	173

Database	Records
Hydride Properties	47
References	1180
M-H Organizations	22
M-H Meetings Calendar	Varies
IEA 12 Profile	Text
Hydride Applications	271
Hydride & Fluoride Structures	Planned

It is estimated that the hydride databases are accessed about 20 times per day, from points around the world.

Work Planned for 2000

Next year will be the last for Task 12, which will expire September, 2000. No new projects will be started. All presently active projects will be winding down toward the Task expiration date. A Final Report for Task 12 is planned for completion by the end of calendar year 2000. That report will consist of the following components:

- Introduction and Overview by the Operating Agent
- List of Task Publications (compiled by the Operating Agent)
- Publication Quality Summaries of Each of the 20 Projects [2-6 pages each] (by the Experts)

Work on the Hydride Databases will be very limited during 2000 due to limited availability of personnel.

The need for improved means of practical hydrogen storage (especially vehicular) will certainly remain after the end of Task 12. Although the storage problem continues, the general success of Task 12 has resulted in interest by both the IEA Hydrogen Executive Committee Members and current Experts that another IEA hydrogen-storage activity be considered. During 2000, a Task proposal will be developed. Assuming continued interest, the new Task would begin work in early 2001.

Publications and Presentations during 1999

Code: [PU] = Publication; [PR] = Presentation; [PA] = Patent

Akiba, E. and P. Tessier, "Catalyzed reactive milling," J. Alloys and Compounds **293-295** (1999) 400-402 [PU] (Proj. 9)

Bénard, P. and R. Chahine, "Modeling of Hydrogen Adsorption on Activated Carbon and SWNT Nanotubes," Proc. 9th Canadian Hydrogen Conference, Canadian Hydrogen Association, 1999, pp.554-559 [PR+PU] (Proj. C-3)

Bertheville, B. and K. Yvon, "High-pressure synthesis and crystal structure of Sr_2MgH_6," J. Alloys and Compounds **288** (1999), 197-199 [PU] (Proj. 11)

Bertheville, B. and K. Yvon, "$Ca_{19}Mg_8H_{54}$, a new salt-like ternary hydride," J. Alloys and Compounds, **290** (1999) L8-L10 [PU] (Proj. 11)

Bogdanovic', B., "Introduction to Catalyzed Alanates," Oral Presentation, Gordon Research Conference on Hydrogen Metal Systems, July 22, 1999 [PR]

Bortz, M., M. Gutmann and K. Yvon, "Synthesis and Structure Determination of the First Ternary Cadmium Hydride, Cs_3CdH_5," J. Alloys and Compounds **285** (1999), L19-L21 [PU] (Proj. 11)

Bortz, M., B. Bertheville, G. Böttger and K. Yvon, “Structure of the High Pressure Phase gamma-MgH_2 by Neutron Powder Diffraction,” J. Alloys and Compounds **287** (1999), L4-L6 [PU] (Proj. 11)

Chahine, R., P. Bénard, A. Tessier, H. Benaddi and T. Bose, “Hydrogen Adsorption Storage Systems,” Proc. 9th Canadian Hydrogen Conference, Canadian Hydrogen Association, 1999, pp.374-382 [PR+PU] (Proj.C-3)

Dillon, A.C., T. Gennett, J.A. Alleman, P.A. Parilla, K.M. Jones and M.J. Heben, “A Renaissance in Carbon Materials for Hydrogen Storage,” 10th Annual U.S. Hydrogen Meeting of the National Hydrogen Association, April 7-9, 1999 [PR] (Proj. C-1)

Dillon, A.C., T. Gennett, J. L. Alleman, K.M. Jones, P.A. Parilla and M.J. Heben, “Carbon Nanotube Materials for Hydrogen Storage,” Proceedings of the 1999 DOE Hydrogen Program Review, May 4-6, 1999, Rept. NREL/CP-570-26938, pp. 422-438 [PU] (Proj. C-1)

Dillon, A.C., T. Gennett, K.M. Jones, J.L. Alleman, P.A. Parilla and M.J. Heben "Simple and Complete Purification of Carbon Single-Wall Nanotubes," Advanced Materials, **11** (1999) 1354-1358 [PU] (Proj. C-1)

Gingl, F., T. Vogt, E. Akiba and K. Yvon, “Structure Refinement of $Rb_4Mg_3D_{10}$ on Neutron Powder Diffraction Data,” J. Alloys and Compounds **284** (1999), L4-L6 [PU] (Proj. 11)

Gingl, F., T. Vogt, E. Akiba and K. Yvon, “Cubic $CsCaH_3$ and Hexagonal $RbMgH_3$: New Examples of Fluoride-Related Perovskite-Type Hydrides,” J. Alloys and Compounds **282** (1999), 125-129 [PU] (Proj. 11)

Gingl, F. and A. Akiba, “The Hydride Fluoride Crystal Structure Database, HFD - An Update,” Poster Presentation, Gordon Research Conference on Hydrogen Metal Systems, July 19, 1999 [PR] (Proj. 7 & 16)

Gross, K.J., S. Guthrie, S. Takara and G. Thomas, “In Situ X-ray Diffraction Study of the Decomposition of $NaAlH_4$,” Poster Presentation, Gordon Research Conference on Hydrogen Metal Systems, July 21, 1999 [PR] (Proj. 14)

Gross, K.J., “Intermetallic Materials for Hydrogen Storage,” Doctor’s Thesis, Faculté des Sciences, Universeté de Fribourg (Suisse), 1998 [PU] (Proj. 3)

Gross, K.J., S. Guthrie, S. Takara and G. Thomas, “In-situ X-ray diffraction study of the decomposition of $NaAlH_4$,” J. Alloys and Compounds, **297** (2000) 270-281 [PU] (Proj. 14)

Heben, M., “Carbon Nanotubes for the Storage of Hydrogen,” Small Fuel Cells, Knowledge Foundation, New Orleans USA, April 27, 2000 [PR] (Proj. C-1)

Hollmuller, P., J.-M. Joubert, B. Lachal and K. Yvon, “Evaluation of a 5 kW_p Photovoltaic Hydrogen Production and Storage Installation for a Residential Home in Switzerland,” Int. J. Hydrogen Energy, **25** (2000) 97-109 [PU] (Proj. 11)

Jensen, C.M., R. Zidan, N. Mariels, A. Hee, and C. Hagen, "Advanced Titanium Doping of Sodium Aluminum Hydride: Segue to a Practical Hydrogen Storage Material?," International Journal of Hydrogen Energy **24** (1999) 461-465 [PU] (Proj. 14)

Jensen, C.M., S. Takara and R.A. Zidan, “Hydrogen Storage via Catalytically Enhanced Metal Hydrides,” Proceedings fo the 1999 DOE Hydrogen Program Review, May 4-6, 1999, Rept. NREL/CP-570-26938, pp. 472-477 [PU] (Proj. 14)

Kadir, K., T. Sakai and I. Uehara, “Structural investigation and hydrogen capacity of YMg_2Ni_9 and $(Y_{0.5}Ca_{0.5})(MgCa)Ni_9$: new phases in the AB_2C_9 system isostructural with $LaMg_2Ni_9$,” J. Alloys Comp., **287** (1999), 264 [PU] (Proj. 13)

Kadir, K., N. Kuriyama, T. Sakai, I. Uehara, L. Eriksson, “Structural investigation and hydrogen capacity of $CaMg_2Ni_9$: a new phase in the AB_2C_9 system isostructural with $LaMg_2Ni_9$,” J. Alloys Comp., **284** (1999), 145 [PU] (Proj. 13)

Kadir, K., I. Uehara, T. Sakai and H. Tanaka, “Ternary hydrogen storage alloys and process for production thereof,” EU Patent No. 99119299.8 (Dec. 1999) [PA] (Proj. 13)

Kind, H., J.-M. Bonard, Ch. Emmenegger, L.-O. Nilsson, K. Hernadi, E. Maillard-Schaller, L. Schlapbach, L. Forro and K.Kern, “Patterned Films of Nanotubes using Microcontact Printing of Catalysts,” Advanced Mat., **11** (1999) 1285 [PU] (Proj. C-4)

Kohlmann, H., F. Gingl, T. Hansen and K. Yvon, “The First Determination of Eu-H Distances by Neutron Diffraction on the Novel Hydrides $EuMg_2H_6$ and $EuMgH_4$,” Angew. Chem. Int. Ed., **38** (1999), 2145-2147 [PU] (Proj. 11)

Mitrokhin, S., “Metal hydrides - properties and practical applications. Review of the work in Russia,” Oral Presentation, Gordon Research Conference on Hydrogen Metal Systems, July 20, 1999 [PR]

Noréus, D., “Hydrogen - a stabilizing ligand in formal low valent transition metal complexes,” Oral Presentation, Gordon Research Conference on Hydrogen Metal Systems, July 22, 1999 [PR] (Proj. 1)

Nützenadel, C., A. Züttel, D. Chartouni and L. Schlapbach, “Electrochemical Storage of Hydrogen in Nanotube Materials,” Electrochemical and Solid-State Letters, **2** (1999) 30-32 [PU] (Proj. C-4)

Nützenadel, C., A. Züttel, D. Chartouni, G. Schmid and L. Schlapbach, “Critical size and surface effects of the hydrogen interaction of palladium clusters,” European Phys. J. D., **8** (2000) 245 [PU] (Proj. C-4)

Nützenadel, C., A. Züttel, Ch. Emmenegger, P. Sudan and L. Schlapbach, “Electrochemical Storage of Hydrogen in Carbon Single Wall Nanotubes,” Science and Application of Nanotubes, Kluwer Academic Publishing/Plenum Press, Fundamental Research Series, (1999) p. 205 [PU] (Proj. C-4)

Nützenadel, C., A. Züttel and L. Schlapbach, “Electrochemical Storage of Hydrogen in Carbon Single Wall Nanotubes,” in Electronic Properties of Novel Materials- Science and Technology of Molecular Nanostructures, AIP Proc. IWEPMN 99, Ed. H. Kuzmany et al., (1999) p. 462 [PU] (Proj. C-4)

Olofsson-Mårtensson, M., M. Kritikos and D. Noréus,, “A Novel Tetrahedral Formally Zerovalent-Palladium Hydrido Complex Stabilized by Divalent Alkaline Earth Counterions,” J. American Chem. Soc., 121 (1999) 10908-10912 [PU] (Proj. 1)

Orimo, S., G. Maijer, T. Fukunaga, A. Züttel, L. Schlapbach and H. Fujii, “Hydrogen in mechanically prepared nanostructured graphite,” Appl. Phys. Lett., **75** (1999) 3093 [PU] (Proj. C-4)

Rönnebro, E., “Structural Investigations of Some Ternary Metal Hydrides,” Doctoral Dissertation, Dept. of Structural Chemistry, Stockholm University, 1999 [PU] (Proj. 1 & 6)

Rönnebro, E., D. Noréus, K. Kadir, A. Reiser and B. Bogdanovic’, “Investigation of the perovskite related structures $NaMgH_3$, $NaMgF_3$ and Na_3AlH_6,” J. Alloys and Compounds, **299** (2000) 101-106 [PU] (Proj. 6)

Rönnebro, E., J.O. Jensen, D. Noréus and N. Bjerrum, “Distorted Mg_2NiH_4 formed by mechanical grinding,” J. Alloys and Compounds **293-295** (1999) 146-149 [PU] (Proj. 1)

Sandrock, G. and G. Thomas, “Metal Hydrides and Carbon for Hydrogen Storage: International R&D Activities under Task 12 of the IEA Hydrogen Implementing Agreement,” Proc. 9th Canadian Hydrogen Conference, Canadian Hydrogen Association, 1999, pp.94-103 [PR+PU] (Proj. 7)

Sandrock, G., “A panoramic overview of hydrogen storage alloys from a gas reaction point of view,” J. Alloys and Compounds **293-295** (1999) 877-888 [PU] (Proj. 7)

Schlapbach, L., “Carbon Nanostructures for Electrochemical and Gas Phase Hydrogen Storage, Supercaps and as Electron Emitters,” Carbon Nanotubes, Knowledge Foundation, Miami USA, April 10, 2000 [PR] (Proj. C-4]

Tanaka, H., H. Miyamura, D. Noreus, N. Kuriyama, H. T. Takeshita, T. Sakai and I. Uehara, Structure and hydrogen storage property of $(Ca,La)(Al,Si)_2$-based system,” Rare Earths, **32** (1998), 166 [PU] (Proj. 4)

Tanaka, H., H. Miyamura, N. Kuriyama, T. Sakai and I. Uehara, “Calcium-aluminum system hydrogen absorbing alloy,” U.S. Patent 5,803,995, Sep. 8, 1998 [PA] (Proj. 4)

Tanaka, H., H. Miyamura, N. Kuriyama, T. Sakai and I. Uehara, “Hydrogen storage material consisted from Ca-Al system alloy,” Japan Patent No. 2972847 (Sep. 1999) [PA] (Proj. 4)

Tanaka, H., H. T. Takeshita, T. Sakai, I. Uehara and D. Noreus, “ABC-type hydrogen storage alloys and process for production thereof,” Japan Patent No.3000146 (Nov. 1999) [PA] (Proj. 4)

Thomas, G., S. Guthrie, and K. Gross, “Hydride Development for Hydrogen Storage,” Proceedings of the 1999 DOE Hydrogen Program Review, May 4-6, 1999, Rept. NREL/CP-570-26938, pp. 452-461 [PU] (Proj. 14)

Wang, J.C., R.W. Murphy, F.C. Chen, R.O. Loutfy, E. Veksler and A. Singh, “Hydrogen Storage in Fullerenes and Liquid Organic Hydrides,” Proceedings of the 1999 DOE Hydrogen Program Review, May 4-6, 1999, Rept. NREL/CP-570-26938, pp. 439-451 [PU] (Proj. C-2)

Zaluski, L., A. Zaluska and J.O. Ström-Olsen, “Synergy of hydrogen sorption in ball milled hydrides of Mg and Mg_2Ni,” J. Alloys Comp., **289** (1999) 197-206 [PU] (Proj. 8)

Zaluska, A., L. Zaluski and J. Ström-Olsen, “Metal Hydrides for Hydrogen Storage,” Proc. 9th Canadian Hydrogen Conference, Canadian Hydrogen Association, 1999, pp.648-655 [PR+PU] (Proj. 8)

Zidan, R.A., S. Takara, A.G. Hee, and C.M. Jensen, "Hydrogen Cycling Behavior of Zirconium and Titanium-Zirconium Doped Sodium Aluminum Hydride," Journal of Alloys and Compounds **285** (1999) 119-122 [PU] (Proj. 14)

Zidan, R., “Catalytically enhanced aluminum hydrides: practical hydrogen storage materials,” Oral Presentation, Gordon Research Conference on Hydrogen Metal Systems, July 22, 1999 [PR] (Proj. 10 & 14)

Züttel, A., D. Chartouni, Ch. Nützenadel, L. Schlapbach, V. Güther, A. Otto, M. Bürtsch and R. Kötz, “Comparison of the Electrochemical- and Gasphase Hydrogen Sorption Process,” Materials Science Forum, **315-317** (1999) 84 [PU] (Proj. C-4)

Züttel, A., V. Güther, A. Otto, M. Bärtsch, R. Kötz, D. Chartouni and Ch. Nützenadel, “About the mechanism and the rate limiting step of the metalhydride electrode reaction,” J. Alloys and Compounds **293-295** (1999) 663-669 [PU] (Proj. C-4)

Meetings Held in 1999

- Experts’ Workshop, Henniker, NH, USA, July 19-20, 1999
- Extensive Task participation in the Gordon Research Conference on Hydrogen-Metal Systems, Henniker, NH, USA, July 18-23, 1999

Meeting Schedule for 2000

- Experts’ Workshop, Davos, Switzerland, March 2-3, 2000
- Final Experts’ Workshop, Noosa, Australia, October 6-7, 2000
- Task participation (included Invited Speakers) at MH2000, Noosa, Australia, October 1-6, 2000

TASK 13 - DESIGN AND OPTIMIZATION OF INTEGRATED SYSTEMS

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Introduction

Hydrogen energy systems have been proposed as a means to increase energy independence, improve domestic economies, and reduce greenhouse gas and other harmful emissions from stationary and mobile sources. These systems, however, face technical and economic barriers that must be overcome before hydrogen can become a competitive energy carrier for the 21st century. In a recent effort supported by the International Energy Agency (Annex 11 - Integrated Systems), design guidelines were developed for a large number of hydrogen-based and non-hydrogen-based components. These guidelines provide data on individual components to assist in the design of integrated energy systems. Included in the guidelines are measures of performance, which provide relevant means to compare systems. In addition, a tool was developed to assist in the design of hydrogen energy systems. Computer models were developed for a large number of hydrogen production, storage, distribution, and end use technologies, based on data collected from hydrogen demonstration projects throughout the world. These models can be linked through the use of a common integrating platform into integrated hydrogen systems. Renewable-based and fossil-based components are included in the component model library to assist in comparative analysis between advanced systems and commercial systems.

Objective

The objective of Task 13 is to provide a means to increase energy independence, improve domestic economies, and reduce greenhouse gas and other harmful emissions from stationary and mobile sources. Emphasis will be placed on comparison of systems with respect to efficiency, environmental impact, capital and operating costs and other measures of importance.

To accomplish this objective, the participants will undertake research within the framework of two coordinated subtasks.

Task Description

Subtask A: Model Development

Subtask A will include improvement to existing component models, development of additional component models, and the development of cost models for each component model. The results of this Subtask will support the analyses that will be performed in Subtask B.

In the evaluation of existing and proposed hydrogen demonstration systems, it may become necessary to develop additional component models in order to perform technical and cost analyses. In this activity, data will be collected and ASPEN-based models will be developed and validated for an additional 3-5 components, as needed. In addition, several of the original models may require modification, based on new or improved data. For example, a more robust pressure swing adsorption model that can operate as a stand-alone model (rather than as an integral part of several of the current models) is needed. Documentation of the new or revised models will follow the standard format established in Annex 11. The existing component library will be updated as necessary.

The basis for the development of consistent cost models will be established, including the appropriate size ranges, scaling factors, installation factors, operating and maintenance costs, etc. This basis will be used throughout this activity to insure consistency and fairness. Cost models based on existing non-proprietary data and standard engineering procedures will be developed for each component. This activity will include development of ASPEN-based cost models, spreadsheet models, and/or graphical representations. A range of sizes will be identified for the components, so that the cost models will be applicable for a range of integrated system sizes. These models will include non-proprietary projections for future costs based on cost-reduction parameters (such as mass production, market size, and technological advances) that will be defined as part of this activity (based on literature values to the largest extent possible).

In addition to developing traditional engineering cost models, this activity will also address the issue of externality costs. Specifically, a set of cost parameters will be developed for important greenhouse gas emissions, so that the benefits of renewable hydrogen production systems can be compared to fossil-based production systems. Some effort will also be directed to assigning value to other intangible benefits such as job creation, energy independence, etc. A report describing the cost models will be produced. This report will also include a description of the basis used in the development of the cost models.

 # Subtask B: Systems Analysis

Subtask B activities involve the identification of candidate configurations (in cooperation with Subtask A), design of the system using the design guidelines developed in Annex 11, modeling of the integrated systems using the tool developed in Annex 11, and evaluation of the performance, costs, andenvironmental benefits of hydrogen energy systems.

Experts have canvassed potential hydrogen demonstration project leaders in participant and non-participant countries to identify candidate configurations for analysis. Using information, tools, and methodologies developed in Annex 11, comparison of different system configurations for a particular application can be made. This requires a set of criteria on which the comparison can be made, including efficiency, environmental impacts, economic impact, capital and operating costs, and other measures of importance to the analyst. In all cases, these parameters can be reduced to a comparison of costs, given that appropriate value can be assigned to the individual criteria. It is important to develop consistent cost models for the various hydrogen components so that fair assessments can be made of alternative designs. This is particularly important when comparing dissimilar systems at very different levels of development and commercialization.

Three systems have been selected for evaluation:

- **Home/Residential Systems**

The development of “greenfield” communities is an important opportunity for hydrogen energy systems. There are regulations on energy use and emissions at the national level in many countries, and integrated planning requirements at most local levels. In the Netherlands, there is an ambitious national plan to require the power generation mix to include 3% renewables (green energy) by 2010 and 10% renewables by 2020. The national energy policy includes price supports via an eco-tax of 10% on non-green energy. With current technology, wind energy is nearly competitive with conventional (taxed) fossil-based generation.

In a preliminary study, an integrated systems approach was used to design the energy system for a new community or district. Services required include heating, lighting, communications, etc. Technologies considered included PV, solar hot water, wind, heat pumps, combined heat and power (CHP), heat buffer, batteries, electric grid, natural gas grid, etc. Using Matlab, systems were designed using cost, efficiency, and environmental impacts as Measures of Performance. The results of the simulations indicated that the size of the buffer was influenced by and influenced the size of the components and the use of the grids (for storage and as an energy supplier). Networks that were considered include electric, high temperature heat, low temperature heat, natural gas, and hydrogen.

The critical element that drives the overall efficiency of the system is the reformer. Heat integration is important, as are costs. Other factors include the developmental stage of fuel cells, and the pipeline distribution of hydrogen to residential areas (distribution to industrial sites is fairly common practice in both the US and Europe). With the use of a hydrogen distribution network, renewable production systems could be integrated easily.

The objective of this proposal for consideration by Task 13 participants is to identify technical and non-technical barriers to the use of a hydrogen network in a residential district. The systems and markets will be based on the Dutch situation: new urban (= residential) districts are being developed, with housing additions of 60,000 per year (5-10% per year). Given the requirement to integrate renewables in the national power mix, the deregulation of utilities, and the desires by many communities to include “green” homes, this is a very interesting case study for the Task to examine. There is funding available from the government to support such systems, and consumers have “over-subscribed” to buy green electrons from utilities.

- **Remote Power Systems**

An island off Norway, currently connected to the mainland via undersea electrical cable, is in need of a replacement system (due to end-of-lifetime concerns for the cable and the high cost of replacement). The island has about 75 households (~300 residents) and fishing is the major industry. The wind resource is good and data are available, as are demand profiles. The choices for the island include diesel generators; wind/diesel hybrids (non- hydrogen option); wind-hydrogen (with and without battery); and PV-hydrogen. There is interest in Norway to study the design of a system to provide reliable power to the island using renewable hydrogen. A number of issues were identified, including the limitation of wind power to the grid due to frequency fluctuations (does the grid need to be stabilized with some percentage of the power demand provided by the fuel cell at all times?) and the desirability or need for multiple small turbines or one large turbine. Databases are available that include insolation data, from which insolation profiles can be generated using standard techniques. There is some additional difficulty in generating profiles for the wind resource. The load profiles for the remote community can be developed and variations introduced to reflect seasonal variability. There is a lot of support within the Norwegian island community to pursue the wind-hydrogen option. There is also interest in the Netherlands to replace existing systems (cables and diesel generators) in remote areas and in resort areas specializing in eco-tourism. Smaller units for telecommunications applications are also of interest. Replacement of the diesel fuel with hydrogen for the shipping fleet and/or the ferry may also be considered.

The objective of this proposal is to identify technical and non-technical barriers to the use of stand-alone power applications. The case study of interest is a Norwegian island of 75 households with an annual electricity consumption of about 15,000 kWh per household. Statistical generation of time series will be used unless and until real resource data are collected.

- **Transportation Applications**

Fuel cell vehicles have received a great deal of attention from automobile manufacturers recently. This attention is often directed at the use of “conventional” liquid fuels with on-board reforming to produce hydrogen for the fuel cell. This proposal will examine the various configurations that have been proposed to compare the costs, energy efficiencies, and environmental emissions. Off-board hydrogen production processes for fuel cell vehicles to be considered include large-scale steam methane reforming (SMR) with liquid or compressed gas delivery, small-scale SMR (100,000 scfd or 300 kg/day), and electrolysis. Liquid and compressed hydrogen storage on board will be considered. On-board hydrogen production processes for fuel cell vehicles to be considered include methanol and gasoline reforming. In addition, we will be considering non-fuel cell alternatives such as battery/gasoline ICE hybrids and advanced gasoline ICEs.

There is significant information available from hybrid vehicle programs in the US and elsewhere that will be used to obtain the required performance data for the various vehicles, particularly the on-board reforming processes. Using the available data, the fuel requirements and emissions for each configuration will be calculated for a specified driving range using a similar vehicle (aerodynamics will be the same; weight differences will be figured into the calculations). In this way, fair comparisons can be made for the various vehicle configurations.

The value of hydrogen energy systems is often linked to environmental improvements (greenhouse gas reductions, and CO, NO_x, and SO_x reductions, etc.) or other intangible benefits (job creation, energy independence, etc). Quantification of some of these benefits can be made using life cycle assessment (LCA) comparisons. LCA is a systematic analytical method to identify, evaluate, and help minimize the environmental impacts of a specific process or competing processes. Material and energy balances are used to quantify the emissions, resource depletion, and energy consumption of all processes between transformation of raw materials into useful products and the final disposal of all products and byproducts. The results are then used to evaluate the environmental impacts of the process so that efforts can be focused on mitigating possible effects.

The scope of an LCA for hydrogen systems will be defined, based on established (published) LCA methodologies. The measures to be considered include comparison of CO_2 and other gaseous emissions, and determination of net energy ratio (amount of energy produced per unit of fossil fuel input). In addition to studies on to comparative analysis of process efficiencies, cost and emissions analysis will be performed using the models developed in Subtask A.

Duration

The Task began on 1 January 1999 and is schedule to be completed 31 December 2001.

Participation

Seven countries participate in Task 13: Canada, Japan, Lithuania, the Netherlands, Norway, Spain, and the USA. Sweden has expressed its intent to participate.

Meetings in 1999

Spring 1999	Seville, Spain
Fall 1999	Washington, DC, USA

Upcoming Meetings

Spring 2000	Amsterdam, the Netherlands
Fall 2000	Munich, Germany*

* In conjunction with Hyforum 2000 meeting

Publications in 1999

No papers were published in the first year of this three-year task. A number of papers are planned for the remaining 2 years of the activity.

Task 14 - Photoelectrolytic Production of Hydrogen

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Introduction

Photoelectrolysis of water is the process whereby light is used to split water into hydrogen and oxygen. This can be achieved by illuminating a photocatalytic semiconductor device or system either directly or via dye sensitization. Such systems eliminate the need for separate power generation (e.g. via photovoltaic (PV) solar cells or solar thermal power station) and electrolysis (e.g. electrochemical cell), and hence offer great potential for cost reduction of electrolytically produced hydrogen using solar energy.

Task Description

The overall objective of Task 14 is to significantly advance the fundamental and applied science in the area of photoelectrolysis of water over a period of three to five years. More specifically, it is aimed at establishing performance data on practical system efficiency, device lifetime and costs. From a scientific point of view, key investigations are focusing on semiconductor materials and structures, photo-sensitive dyes, integrated PV/electrolysis systems, and novel single- and dual-bed reactor arrangements.

To accomplish the objectives, the participants are undertaking individual and collaborative research within the framework of two coordinated subtasks. These are of common interest to the current photoelectrolysis research programs worldwide and carry forward, in a more specific and targeted fashion, the preliminary work previously addressed by IEA Hydrogen Agreement Task-10, Subtask A (March 1995 - October 1998).

Some of the work under Task-14 is carried out in close collaboration with Task-2, Solar Chemistry, of the IEA SolarPACES (Solar Power And Chemical Energy Systems) Implementing Agreement.

Subtask A: Material Studies

This subtask has two main groups of activities. They concern the improvement of light absorption of wide-bandgap semiconductor materials such as titanium dioxide and gallium/arsenide by dye-sensitization and other techniques, and the development of catalytic and protective layers for photoelectrochemical (PEC) cells.

- **Activity A**: Improvement of Solar Light Absorption in Semiconductors

Semiconductors with wide bandgaps provide the necessary potential for water splitting, but because they absorb only the most energetic portion of the solar spectrum, conversion efficiencies are limited. The light absorption may be improved by modification of the semiconducting materials, or by combining them with 'photo-sensitizers,' such as dyes that absorb a larger portion of the solar spectrum.

- **Activity B**: Development of Catalytic and Protective Layers

PECs require appropriate catalysts to enhance the water splitting reactions and to provide electrolyte-resistant layers to protect the semiconducting materials from corrosion. Work is focusing on the development and characterization of such layers.

Subtask B: System Studies

This subtask has three main groups of activities. They target maximizing the efficiency of multi-junction water splitting systems and assessing reactor system design options for the photoproduction of hydrogen, including the new 'dual-bed system' concept.

- **Activity A**: Efficiency Optimization of Multi-junction Systems

Improved device conversion efficiencies can be achieved by the application of multi-junction systems. These systems have already demonstrated encouraging, but non-stable efficiencies on the order of 12-14%. Multi-junction systems are being developed and studied with the aim of reaching a stabilized target efficiency of 10%.

- **Activity B**: Investigation of Reactor Design Options

Various conceptual reactor and system designs for the photoelectrolysis of water have previously been proposed. Engineering efforts are focusing on the development of mathematical models for reactor designs, the development of methods for the measurement of key reactor performance parameters, and comparative evaluations of alternative reactor designs.

- **Activity C**: Assessment of Dual-bed Systems.

A series of particulate semiconductor photo-catalysts for hydrogen, as well as for oxygen evolution, and mediators for charge transfer are being tested for application in a new, compact and efficient dual-bed reactor system.

Duration

This Task was formally started on 1 July 1999 and is scheduled for a period of 3 years.

Participation

The following countries participated in Task 14 during 1999: Japan, Sweden, Switzerland and the United States.

Activities & Progress During 1999

During the early part of 1999, the Program of Work for Task 14 that was drafted at the last expert meeting of Task 10 in October 1998 at NREL, USA, was reviewed and revised.

The following organizations participated in Task 14 during 1999: The National Renewable Energy Laboratory (NREL) and the Florida Solar Energy Center (FSEC), United States; The University of Uppsala, Sweden; the University of Geneva, the University of Bern and the Swiss Federal

Polytechnic School of Lausanne, Switzerland; and the National Institute of Materials and Chemistry Research (NIMC), Japan.

The half-year initiation period of Task 14 has seen excellent collaboration among experts from all four member countries, notably visits of group leaders and exchange programs of researchers (CH&USA, CH&J, CH&S & USA&J). The first Task 14 experts meeting is scheduled for early 2000.

Subtask A: Material Studies

Photoelectrochemical (PEC) devices for water splitting are best designed with two cells in which oxygen evolution and hydrogen evolution occur separately. This eliminates the need for gas separation and allows for better "synchronisation" of both reactions, whereby the anodic oxidization of water to oxygen is generally the performance-limiting step. Such devices are studied under Subtask A of Task 14.

In Switzerland, a tandem PEC device based on two superimposed photosystems with complementary light absorption in the visible range has been developed. The device comprises a thin-film anode of polycrystalline tungsten trioxide (WO_3) in combination with a thin-film cathode that is based on dye-sensitized nanocrystalline titania (TiO_2) [Graetzel, 1999]. The collaboration among all three Task 14 Swiss expert groups has led to the successful demonstration of such a tandem PEC system for water splitting, achieving a net solar-to-chemical conversion efficiency of 5%. Figure 1 shows this tandem dye-cell photosystem in operation.

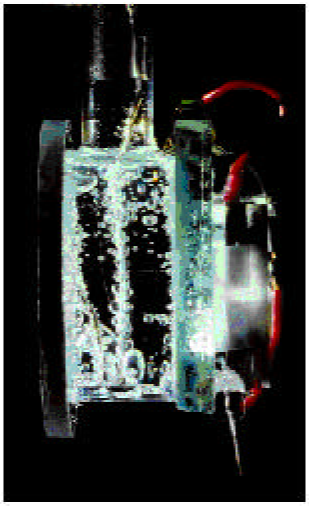

Figure 1 - Tandem dye-cell photosystem for water splitting using mesoscopic semiconductor films

Research efforts concerning light harvesting in semiconductors have followed two main routes: a) the preparation and characterization of "common" photoanodes (above all WO_3) and b) the investigation of alternative semiconductors (mainly Fe_2O_3, AgCl, and organic pigments) for the photoanode or photocathode. In this early stage of material screening, the issue of electrolyte-resistance (corrosion) has had minimal emphasis.

Tungsten trioxide (WO_3) - At the University of Geneva, a new proprietary method for preparing oriented, nanosized WO_3 films using sol-gel techniques has been developed. Similarly, the University of Uppsala has prepared colloidal suspensions with nanosized WO_3 particles for thin films, with studies of variations in film thickness (1.5 - 5.0 µm), light intensity (100 - 700 W/m^2) and temperature (5 - 50°C) in a water-based electrolyte (pH 4.68). In collaboration with NREL, characterizations of the optical, structural and photoelectrochemical properties of WO_3 films have been performed. Preliminary results confirmed that the promising new Swiss WO_3 material is n-type, but showed some variability in the measured band edge position. Regarding the Swedish WO_3, an Incident Photon-to-Current-Efficiency (IPCE) of up to 60% has been measured at 380 nm. Photocurrents increased linearly with increasing light intensity.

Hematite (α-Fe_2O_3) - At the University of Uppsala, synthetic procedures for "purpose-built materials" have been developed. This allows the controlled assembly of oxides (e.g. α-Fe_2O_3) in the nanoparticle regime into various shapes, including onto flexible substrates. Sample α-Fe_2O_3 films were found to be highly non-isotropic, forming micrometer-long crystals that are oriented mainly normal to the plane of the films. In collaboration with NREL, α-Fe_2O_3 samples have been tested in water-based electrolytes with a pH of 4, 7 and 10. The material has been confirmed to be n-type and is regarded promising as a photoanode due to its abundance. Preliminary I-V and C-V test data, however, showed strong differences from more common photoanodes.

At the Swiss Federal Polytechnic School of Lausanne, the preparation and characterization of Fe_2O_3 films (with assistance of the University of Augsburg, Germany) have also advanced. Transparent Fe_2O_3 films of a few micron thickness have been achieved via a spray pyrolysis method on conducting glass. The films were doped with ions such as Ti, Sb and Si, some of which are able to augment the number of majority carriers achievable upon illumination. These Fe_2O_3 films allowed photocurrents of up to 2 mA/cm^2 to be reached under simulated AM-1.5 sunlight using water as the electron source. This corresponds to an encouraging solar-to-chemical conversion efficiency of 3% for light-induced water cleavage. An IPEC maximum was found when applying multiple spray-layers of Fe_2O_3. A downside of the current spray-pyrolysis iron oxide layers is the nanocrystalline or fractal nature of them, which limit the I-V characteristics of the Fe_2O_3 film (Figure 2).

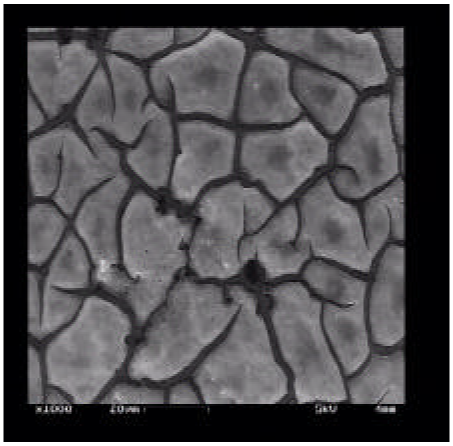

Figure 2 - SEM picture of iron oxide at 1000-X magnification, showing the unwanted fractal surfaces.

At the NIMC, research efforts focus on the development of a two-step water splitting system that uses oxide semiconductor powder photocatalysts (Bamwenda et al., 1999). The aim is to find oxides (e.g. tungsten and iron oxide, the latter one as an Fe^{3+}/Fe^{2+} redox pair) that have a comparably narrow bandgap to make use of the visible light for a water splitting process in aqueous suspension.

Silver chloride (AgCl) - At the University of Bern, thin silver chloride (AgCl) layers are being developed to act as photoanodes [Lanz et al., 1999]. The photoactivity of AgCl extends from the UV into the visible light region in a process known as self-sensitization, which is due to the formation of silver during the photoreaction. This silver can be almost quantitatively re-oxidized electrochemically, making it feasible that a thin AgCl layer deposited on a conducting substrate could be used as a photoanode for water splitting if coupled with an appropriate photocathode.

Heteroaromatic compounds - Organic pigments can be promising semiconductor photocatalysts. At FSEC, with assistance from the University of Arizona and in collaboration with the NIMC, a combination of simple screening procedures based on semi-empirical molecular orbital calculations and thin film voltammetry was developed, allowing the quick determination of whether new prospective compounds are capable of O_2 or H_2 evolution. This new assessment procedure has thus far found a number of fused heteroaromatic compounds (e.g. various perylene, indanthrone and quinacridone compounds) to evolve O_2 and various phthalocyanine compounds of H_2, both under Xenon lamp illumination. In combination with immobilized pigment films containing 1%-wt. platinum (Pt) catalyst, the perylene pigments evolved more O_2 than common TiO_2 samples tested under identical conditions.

These results on improved light harvesting pigments are in good agreement with investigations conducted at the Swiss Federal Polytechnic School of Lausanne, where phthalocyanine (zinc, aluminum and ruthernium), naphthalocyanines, merocyanines and ruthenium complexes containing novel ligands have been identified as promising near-infrared sensitizers for the tandem dye-cell photosystem [Nazeeruddin et al., 1999]. Figure 3 illustrates a typical ruthenium-naphthalocyanine sample.

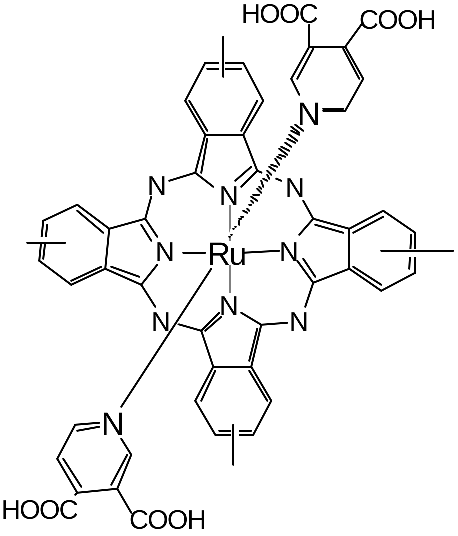

Figure 3 - Ruthenium-naphthalocyanine as promising dye for light harvesting.

Subtask B: System Studies

The main progress during 1999 concerns the further assessment of multi-junction devices by NREL and the confirmation of a combination of oxygen and hydrogen evolving photocatalyst suspensions that make two-stage and dual-bed reactor systems possible.

Multi-junction systems - Encouraged by world-record performance results in 1998 at NREL [Khaselev & Turner, 1998], efforts focusing on monolithic multi-junction PEC devices have continued. Based on a number of detailed cost evaluations of the NREL multi-junction PEC system, a risk analysis of these costs has been performed [Mann, 1999]. It was found, for example, that there is an 80% certainty for hydrogen produced with such a PEC system to cost less than $41.3 US per Gigajoule.

In order to overcome challenges of semiconductor stability and interfacial kinetics encountered with NREL's original multi-junction PEC device, integrated systems that combine a conventional PV device with an electrolyser unit into a single system are being investigated by NREL [Khaselev et al., 2000]. A GaAs/$GaInP_2$ system and an a-Si system have been constructed and tested, both integrated with an alkaline electrolysis unit with platinum electrodes. The gallium-based system demonstrated a solar-to-hydrogen efficiency over 16% whereas the system using low-cost triple-junction a-Si PV still achieved a remarkable 7.8% solar-to-hydrogen conversion efficiency.

Dual-bed system - Progress has been made at FSEC and NIMC in the development of organic pigments as semiconductor photocatalysts for two-stage water decomposition schemes. In FSEC's scheme, two photocatalysts are immobilized in separate containers, or beds (Figure 4). Using ditridecyl perylene diimide as the O_2-evolving photocatalyst and copper phthalocyanine as the H_2-evolving photocatalyst, respective oxidative and reductive water decomposition was observed using the same IO_3^-/I^- redox electrolyte, demonstrating that continuous closed cycle dual-bed photocatalytic water-splitting is feasible.

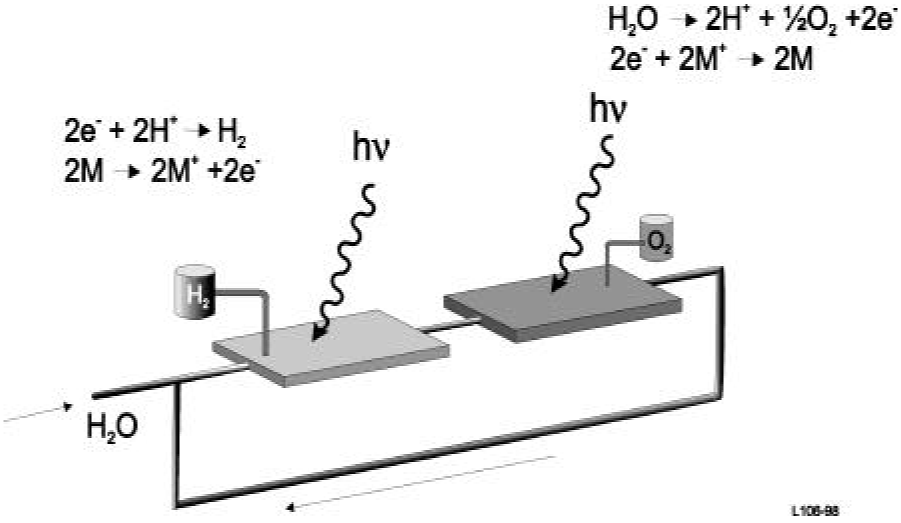

Figure 4 - Schematic of a dual-bed photocatalytic water-splitting system.

Future Activities

Future work by Task 14 experts from all four countries will aim at further improving the efficiency of tandem devices through the increase of the photon-to-current densities (aim: 6 mA cm^{-2}) and IPCE (aim: ~60% over a broad band of the visible light). This might be achievable by (a) using organic matter as the electron donor instead of water, (b) enhancing the absorption of the visible light in WO_3 film anodes via doping with light scattering particle centres or by using colloidal suspensions with nano-sized particles, and (c) using smaller band-gap oxides (i.e. current: ~2.6 eV versus ideal: ~1.6 eV) as photo-anodes. Hematite (α-Fe_2O_3 iron oxide) seems to be the alternative semiconductor of choice for option (c).

Task 14 experts also aim to increase the interfacial kinetics at the photo-anode via catalysis. NiO, CoO, SiO_2, RuS_2 and RuO_2 are among the prime catalyst candidates for investigation. Furthermore, the application of devices with solar concentrators is also being considered, since it was indicated that WO_3-based photo-anodes perform better at higher temperatures.

Encouraged by the results of NREL's a-Si-based multi-junction PEC investigations, such systems have attracted the interest of researchers from Mexico, New Zealand and Australia. Matching the PV and electrolysis devices needs success in stabilizing the bandgap and its overlap and in achieving speedy charge transfer. Since amorphous silicon cells produce unattractively low current densities (typically about 6 mA/cm^2), the use of solar concentrator devices to increase the current density to at least 120 mA/cm^2 will be pursued. This compares with the current density of commercial alkaline electrolysis, which is typically around 1000 mA/cm^2. However, a rise in current density results in an unwanted migration of the band edge positions. A suitable passivation of the semiconductor (e.g. p-type iron oxide or zinc selenide) is therefore needed to limit this migration.

Publications and References

Bamwenda G., Sayama K. and Arakawa H. (1999): "The effect of selected reaction parameters on the photoreduction of oxygen and hydrogen from a WO^2 - Fe^{2+}/Fe^{3+} aqueous suspension. *J. Photochem and Photobiol. A: Chemistry* in press.

Khaselev O. and Turner J. (1998): "A monolithic photovoltaic - photoelectrochemical device for hydrogen production via water splitting." *Science*, Vol.2, pp 425-427.

Khaselev O., Bansal A. and Turner J. (2000): "High-efficiency integrated multi-junction photovoltaic / electrolysis systems for hydrogen production." *Int. J. of Hydrogen Energy*, in press.

Graetzel M. (1999): "The artificial leaf, bio-mimetic photocatalysis." Published by Baltzer Science Publishers in *CATTECH*, the magazine of Catalysis Sciences, Technology and Innovation, Issue 5, Volume 3 (August 1999) Number 1, pp 4-17.

Lanz M., Schürch D. and Calzaferri G. (1999): "Photocatalytic oxidation of water to O_2 on AgCl-coated electrodes." *J. Photochem. Photobiol. A: Chem.* 120, pp 105-117.

Mann M. (1999): "Sensitivity study of the economics of photoelectrochemical hydrogen production". Milestone report for the US DOE Hydrogen Program Process Analysis Task, Milestone Type P, November.

Nazeeruddin M., Humphry-Baker R., Grätzel M., Wöhrle D., Schnurpfeil G., Schneider G., Hirth A. and Trombach N. (1999): "Efficient near-IR sensitization of nanocrystalline TiO_2 films by zinc and aluminum phthalocyanines”. *J. Porphyrins and Phthalocyanines*, Vol.3, pp 230-237.

TASK 15 - PHOTOBIOLOGICAL HYDROGEN PRODUCTION

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Introduction

Biological hydrogen production, the production of hydrogen by microorganisms, has been an active field of basic and applied research for over two decades, with significant applied R&D programs supported in Europe, Japan and the United States. Realization of practical processes for photobiological hydrogen production from water using solar energy would result in a major, novel biological source of sustainable and renewable energy, without greenhouse gas emissions or environmental pollution. However, development of such practical processes will require significant scientific and technological advances, and relatively long-term (>10 yr) basic and applied R&D. Photobiological hydrogen production was a component of the prior Task 10 of the IEA Hydrogen Agreement, and has evolved into the independent Task 15. This effort covers research areas and needs at the interface of basic and applied R&D that are of mutual interest to the countries and researchers participating in the IEA Hydrogen Agreement. Task 15 provides for the establishment of collaborative research projects among participating countries in a coordinated program.

Task Description

Task 15 deals specifically with "biophotolysis," i.e. the biological production of hydrogen from water and sunlight using microalgal photosynthesis. An earlier IEA Task 10 Report [Benemann 1998] concluded that, in theory, photobiological reactions could achieve close to a 10% solar energy conversion efficiency. The overall objective of Task 15 over the next five years is to advance the basic and early-stage applied science in this area. This will allow an evaluation of the potential of such a technology to become a renewable energy source for the 21st Century. Presently conceptual, the biophotolysis process to be developed under Task 15 was recently subjected to a preliminary economic assessment, published by the IEA Hydrogen Agreement [Benemann 1998]. This proposed process uses microalgae, either green algae or cyanobacteria, to fix CO_2 into carbohydrates that are used by the algae to generate H_2 gas, first in the dark by fermentations and then in the light through photosynthesis-coupled reactions. The analysis published by the IEA suggests that the goal of a 10% conversion efficiency, although ambitious, is potentially approachable in the long-term. The tentative Task 15 goal is to achieve a light conversion of 3% into hydrogen gas.

The main objective of Task 15 is to develop hydrogen production by microalgae (both green algae and cyanobacteria) emphasizing on early-stage applied research on biophotolysis processes with intermediate CO_2 fixation. This research will help to provide the advances required to achieve the practical efficiencies and cost goals of biological hydrogen production. The Task investigates microalgal hydrogen metabolism, both in the dark and in the light, as well as the mechanisms that would allow the photosynthetic processes and hydrogen evolution reactions to achieve their maximum possible efficiencies. In addition, subsidiary metabolic processes require investigation, such as the efficient accumulation of large amounts of carbohydrates, the regulation of the photosynthetic processes and the recycling of the algal cells after hydrogen evolution is completed. Complex underlying genetic mechanisms and biochemical pathways are involved in these physiological processes and require significant research efforts.

The work in Task 15 is divided into four Subtasks; (A) Light-driven Hydrogen Production by Microalgae; (B) Maximizing Photosynthetic Efficiencies; (C) Hydrogen Fermentations; and (D): Improve Photobioreactor Systems for Hydrogen Production.

Subtask A: Light-driven Hydrogen Production by Microalgae

Light-driven hydrogen evolution mediated by hydrogenase(s) was discovered in green algae over fifty years ago, and subjected to extensive investigations over the following decades. However, there are still many fundamental and applied issues that must be addressed before this type of reaction can be considered for practical applications:

- The electron transport pathways coupling stored products with hydrogenase activity and involvement of the photosynthetic system(s) directly (through light-driven electron transport) and/or indirectly (through metabolic energy generation)
- The activation of pre-existing and biosynthesis of new hydrogenase enzymes, their regulation and genetics, in selected microalgae
- The down-regulation of the oxygen-evolving component of the photosynthetic process, to avoid oxygen production and concomitant inhibition of hydrogenase function during the light-driven hydrogen production phase

These objectives requires a fundamental understanding of the genetics, biochemistry and physiology of hydrogenase functions, including the metabolism and factors affecting growth of microalgae. This research requires the application of modern and advanced tools of molecular biotechnology and microbial physiology, techniques already available at leading laboratories in the participating countries.

Subtask B: Maximizing Photosynthetic Efficiencies

Photosynthesis can achieve relatively high solar conversion efficiencies, but only at low light intensity. At full sunlight, efficiencies drastically decline. The reason is the large amounts of so-called light-harvesting pigments, which capture more photons at full sunlight than the photosynthetic apparatus can actually handle. These excess photons are thus wasted, with their energy released as heat or fluorescence, even causing damage to the photosynthetic apparatus. Reducing antenna sizes is a method for increasing photosynthetic efficiencies, and this is a central R&D need in photobiological hydrogen production. Specific activities within this Subtask are to:

- Develop green algae and cyanobacteria with considerable reduced light-gathering pigment contents in both photosystems using molecular genetic techniques
- Demonstrate that such organisms can be used in CO_2 fixation, carbohydrate storage and H_2 production with greatly enhanced overall conversion efficiencies at high light intensities
- Use photosynthetic bacteria as laboratory model systems to demonstrate increased photosynthetic efficiencies in pigment-reduced mutants of single photosystem microbes

Subtask C: Hydrogen Fermentations

After accumulation of carbohydrates and activation of their inducible hydrogenase, a fermentation process is initiated in which storage carbohydrates are converted to hydrogen and a number of fermentation products, including acetate, glycerol, and other excreted substrates. Such fermentations have been reported in both green algae and cyanobacteria, but require further study. At present, typical hydrogen yields from storage carbohydrates in the algae are less than 10%, based on a stoichiometry of 12 H_2/mole glucose. A goal of a 30% yield or higher is required and could be achieved through application of the modern methods of metabolic engineering to redirect metabolic reactions. Specific activities include:

- Investigate yields of anaerobic fermentations as a function of both genetic and environmental factors when using different green algae, cyanobacteria and photosynthetic bacteria
- Carry out fundamental research using model systems such as *Escherichia coli,* and apply the tools of metabolic engineering to demonstrate improved H_2 production from glucose and waste waters in relevant systems
- Apply the techniques developed in the fermentative studies to photosynthetic bacteria, cyanobacteria and green algae and study the utilization of excreted metabolites (e.g. acetic acid) in hydrogen production (both in the dark and in the light-driven hydrogen production stage)

Subtask D: Improve Photobioreactor Systems for Hydrogen Production

A major objective of applied R&D in photobiological hydrogen production has been the development of suitable photobioreactor systems. Development of such systems will serve as an intermediate step in the scale-up of hydrogen production from the laboratory scale to the commercial sector. A large number of different concepts and designs have been proposed and tested. However, there is a lack of engineering research for practical devices. As part of this international collaboration, R&D in photobioreactor engineering and operations is included under Subtask D:

- Development of mathematical models for photobioreactors adapted to hydrogen production, including mass transfer, hydrodynamic, and heat balance calculations
- Development of methods for measurement of the major photobioreactor performance parameters, including hydraulic (dispersion coefficients), gas transfer coefficients, sunlight interception and H_2 losses
- Comparative evaluations of alternative photobioreactor designs, including side-by-side comparisons and testing for biological hydrogen production
- Experiments in pilot plants for determination of the H_2 production capacity

Duration

Task 15 was approved in May 1999 and officially started work in July 1999. It is scheduled for a three-year period, with an option for a two-year extension.

Participation

Japan, Norway, Sweden, and the United States are the original participants in Task 15. Canada joined the activity in Fall 1999.

Activities and Progress During 1999

Experts Meeting: During 22-23 June 1999 the National Institute for Advanced Interdisciplinary Research (NIAIR) of Japan arranged BioHydrogen ’99 *An approach to Environmentally Acceptable Technology* in Tsukuba (Japan) with about forty participants. During this workshop a Task 15 Experts meeting with national experts from Japan, USA, and Sweden was held and the new Annex *Photobiological Hydrogen Production* discussed. The Operating Agent presented an overview of the IEA, the Hydrogen Agreement, and specifically Annex 15 during the workshop. About 20 contributions/chapters (several written by national experts participating in Task 15) will be edited (Editor: Miyake, Jun; national expert of Japan) and published as "BioHydrogen ’99" by Elsevier during 2000.

Encouraged by several very relevant presentations at "BioHydrogen ’99" by scientists/countries not participating in Task 15, and by the new network in Europe (COST 8.41 *Biological and Biochemical Diversity of Hydrogen Metabolism*) it was decided that the Operating Agent will work on increasing the number of participating countries in Annex 15, specifically targeting Canada, the Netherlands, and Hungary. Canada has already joined the Task. It is hoped that the Netherlands and Hungary will become official participants during 2000.

An abstract (IEA Hydrogen Agreement Task 15: *Photobiological Hydrogen Production* - An international collaboration, by Peter Lindblad; Operating Agent, IEA Hydrogen Agreement Annex 15) was submitted and accepted for the *Thirteenth World Hydrogen Energy Conference* to be held in Beijing, China, June 12-15, 2000.

Work within the different Subtasks has begun. Targeted areas include the following:
Subtask A:
- Identification of genetic information required for hydrogen production
- Transcriptional analyses of structural genes in microalgae
- Two-stage photobiological hydrogen gas production in green alga

Subtask B:
- Identify green alga transformants with reduced chlorophyll antenna size

Subtask C:
- Measure yield of hydrogen production in microbial fermentations

Subtask D:
- Analyze specific/constructed mutants in small-scale bioreactors and perform competition experiments
- Initiate development of mathematical models and drafts for pilot plants

Future Activities

The next Experts meetings are scheduled for March 20-21 (2000) at NREL, Colorado, USA, and August 10-11 (2000) in Potsdam, Germany (following "Hydrogenases 2000," 6th International Conference on the Molecular Biology of Hydrogenases).

The Operating Agent will continue to work on increasing the number of participating countries, including presenting the IEA Hydrogen Agreement Task 15 at the following international conferences:

- 10th Canadian Hydrogen Conference (Quebec; May 2000)
- 13th World Hydrogen Energy Conference (Beijing; June 2000)
- 4th Asia-Pacific Conference on Algal Biotechnology (Hongkong; July 2000)

Plans will be initiated for an international conference on BioHydrogen during 2002.

Publication

Lindblad, P, 1999, "Cyanobacterial H_2-metabolism: Knowledge and potential/strategies for a photobiotechnological production of H_2," Biotecnologia Aplicada 16: 141-144.

Reference

Benemann, J.R., 1998, "Process Analysis and Economics of Biophotolysis of Water," IEA Technical Report.

Large Scale Industrial Use of Hydrogen:
Final Task Development Report

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BACKGROUND

In the coming years the demand for hydrogen will grow in most industrialized regions of the world. It is needed for the production of base chemicals like ammonia and methanol, for hydrotreating processes in the petroleum industry and for the manufacture of numerous high-tech products like alloys for the aerospace industries or integrated circuits. Refineries, in particular, will demand more hydrogen for intense hydrotreating of crudes and fuels due to three world-wide trends:

- an increasing proportion of heavy and high-sulfur crudes;
- stricter legislation in western countries regulating sulfur content in diesel and aromatic saturation of diesel and gasoline; and
- lighter refined products with a higher hydrogen to carbon ratio needed for modern engines.

Though new uses for hydrogen are not expected to have a significant, immediate market impact, there is potential for increased market share in the longer-term.

Today more than 95% of hydrogen is produced from fossil fuels. In the near- and mid-term, no other significant sources of hydrogen are likely to be available. Only the longer-term horizon shows promise for sufficient sustainable sources for hydrogen. Thus, efficient use of hydrogen is imperative in order to minimize carbon dioxide emissions and wasted energy. Every unit of hydrogen vented, burned off or used for significantly lower value applications contributes to the net greenhouse gas emissions and increases the price of the commodities produced. This problem cannot be addressed as a “one process, one solution.” Hydrogen is used as an energy carrier or chemical commodity in a large variety of processes. Thus, a multidimensional approach is necessary. The efficiency of the overall use of hydrogen needs to be targeted, starting with the technical processes involved.

Merchant hydrogen represents less then 2% of the total hydrogen market world-wide. Seldom is merchandised hydrogen transported between different industrial regions (more than 1000 km), even though natural gas pipelines very easily cover this distance and the transport of liquid hydrogen is practically unlimited. Only a few large gas merchandising companies have the knowledge to master the difficulties in purification, storage, distribution and application of hydrogen. Thus, by-product hydrogen generators are not active in the merchant business. If not sold to a specialized gas merchandising company this hydrogen is used for lower grade applications, or simply not used at all. This fact becomes more relevant, since the amount of merchandised hydrogen will have to grow in the coming years to meet the increasing demands.

Handling costs are also quite high for hydrogen compared to more conventional gases. More cost-effective processes for distributing hydrogen are needed if hydrogen is to become a competitive commodity. An extensive long-range network of pipelines does not exist for hydrogen. In addition, there has been no concerted effort to understand the issues or to demonstrate the use of existing natural gas pipelines for hydrogen transport. Further research areas that are underserved are the development of large-scale bulk storage of hydrogen and high-efficiency hydrogen compressors. Finally, the appropriate hydrogen purity requirements for various applications are not fully understood, often resulting in the end-user paying for higher-purity hydrogen than is necessary for the application of interest, or the hydrogen being sold at below its potential value.

Detailed figures on the use of hydrogen are currently available only for the western industrialized countries. Even where figures are available, on-site use of hydrogen is not always well document, especially for its use as a fuel. If potentials in the hydrogen economy are to be defined, reliable figures for at least the key parameters are needed. This includes not only volumes and applications of use, but also environmental impacts. With modern data acquisition techniques and computing it is possible to calculate how industrial processes interact with their environment. Life cycle assessments can be employed to compare processes providing similar services. By compiling the necessary data and utilizing the available tools, the savings potential for hydrogen in bulk processes may be calculated and, ultimately, aid in making the afforded decisions on investment for research and construction.

TASK DEVELOPMENT EFFORTS

Overview

The Fall 1997 IEA Hydrogen Agreement Executive Committee Meeting in Kyoto, Japan, saw the first discussion paper for a new IEA activity dealing with other than pure energetic uses of hydrogen. The goal of such an effort would be to stimulate increased demand and more efficient use of hydrogen, resulting in improved infrastructure development, which, in turn, would facilitate the commercialization of energy-related technologies. After the initial discussions, the Swiss Federal Office of Energy sponsored a first draft Task proposal for "Hydrogen Utilization in Novel and Conventional Processes." This proposal targeted technologies where hydrogen could be substituted for conventional chemicals or fuels. Improvements to conventional technologies, as well as development of novel approaches would be applied to petrochemical processing, metallurgy, and ceramics and microelectronics manufacturing. Life cycle assessments would be used to fully understand the advantages and impacts of substituting hydrogen into the industrial processes. This initial proposal included five Subtasks:

- Evaluation of the Production of Hydrogen (data on current and expected levels of production)
- Evaluation of Transport, Storage and Safety of Hydrogen
- Evaluation of the Utilization of Hydrogen as an Energy Carrier
- Utilization of Hydrogen as a Commodity
    - Petrochemistry and Carbon Dioxide Mitigation
    - Metallurgy and Mining
    - Unconventional Processes
- Life-Cycle Analysis of Hydrogen Driven Processes

Using this proposal as a basis, two workshops were held (Washington, D.C., United States, and Winterthur, Switzerland) in May 1998. These workshops culminated in a second draft proposal, focused mainly on large scale industrial use of hydrogen. During this same period a separate development effort was underway, led by Norway, for Hydrogen Production from Carbon Containing Materials. As the two proposals had related activities and targeted similar industries, a decision was made to have the Task development leaders combine their efforts. A questionnaire was developed and sent out to industry leaders in early spring 1999. Approximately 500 companies received the questionnaire, which solicited their opinions and interests towards the two suggested topics. More then 50 replies were received by the Task development leaders, about a third of which favored the establishment of the two proposed Tasks. However, efforts to take this interest forward and secure support and participation in the Large-Scale Industrial Uses of Hydrogen Task were unsuccessful. Thus, at the Fall 1999 Executive Committee meeting in Toronto, Ontario, Canada, it was unanimously decided to discontinue the Task development effort for the time being. However, the members felt that industrial interest would continue to grow and that the topic of an IEA Task on large-scale industrial use of hydrogen should be revisited in 2-3 years.

Workshops

Washington, D.C., 3-4 May 1998

Fourteen technical representatives from the United States and Japan participated in a Task Definition Workshop on “Use of Hydrogen in Processes.” The workshop was organized by Frederick H. Morse from Morse Associates, Inc.

The animated, yet very constructive discussion first dealt with the possible objectives of the new Task. It was suggested that ecology, as well as oil and cost savings, be included in the list of motifs for the Task. Closing the methodological gap of hydrogen use in several key processes is an important factor. In order to stimulate the energetic use of hydrogen, close links between the use of hydrogen in industrial processes and as an energy carrier should be identified. This dual characteristic of hydrogen needs to be emphasized to facilitate the increased energetic use of hydrogen.

The participants agreed that the Task needed some focusing in its scope to avoid becoming too broad for the available resources and interest. However, this turned out to be a difficult undertaking as many areas could prove potentially important. Quite a number of topics were mentioned during the discussion:

- The origin of the used hydrogen (oil, field crops, electrolysis) seemed equally important as the existing, competing resources for hydrogen (methane or methanol).
- The rising use of hydrogen in the aerospace materials industry (paint shops, bright annealing, casting) needed to be addressed in the definition of new processes to reduce the carbon dioxide emissions.

It was clear that the criteria for the new Task should not be artificially divided into energetic and non-energetic uses of hydrogen. Two alternative groups of Subtasks were suggested:

- Petrochemistry, Metallurgy, Ceramics, Microelectronics and Analysis
- Current major uses (Petrochemistry, Fertilizers), Current minor uses (Metallurgy, Microelectronics), Emerging uses (Ceramics, other) and Analysis.

The participants agreed that the R&D program needed to focus on pre-competitive subjects and processes that should be validated and or demonstrated at the end of the Task. Preliminary analysis for each area of the new Task should determine further action. Analysis would be integral throughout the duration of all of the Subtasks. Life cycle assessments would provide the feedback mechanism and control the ultimate outcome of the Task. However, there were two main issues identified for this key role of analysis. First is the lack of available data on conventional processes, as much of it is proprietary. Second is the availability and cost of analysis software. Proposed work plans were also discussed at length, with emphasis on the means, the schedule and the level of effort for each of the possible Subtasks. The results were later incorporated into a modified version of the Task proposal.

Finally, a portion of the workshop was dedicated to the topic of attracting participants to the Task, particularly those from industry. Suggested approaches included informing companies of the results of the Task definition workshops through direct visits, letters of endorsement from the IEA or from the government agencies of the Member Countries, advertising on Web sites (e.g. hydrogen associations), and use of industry corporate connections. Producing a special brochure targeted at industry was also suggested. It was agreed that a broad range of industrial companies should be sought, rather than just those from the "classically" hydrogen using industries. These should include the gas industry, small users of hydrogen, hydrogen traders and their associations, producers of hydrogen and environmental associations. Companies that provide enabling technologies should also be included. It was proposed that the Task be based on a simple cost share model that requires only a small percentage of the total Task cost from each participant.

Winterthur, Switzerland, 18-19 May 1998

Two weeks after the Washington, D. C., meeting, eight technical representatives from four European Member Countries (Netherlands, Norway, Spain, Switzerland) of the IEA Hydrogen Agreement met in Winterthur to discuss the same topics in a Task Definition Workshop organized by the author of this report. There was good representation from both hydrogen producing and consuming industries at this workshop.

The discussion focused on both the draft proposal and the results of the Washington, D.C. meeting. Unlike the earlier workshop where a broad set of objectives for the new Task was preferred, the participants in Winterthur were strongly in favor of a much narrower focus. They agreed that there could be a need for a new IEA Task assuming that a precise answer to the questions “Why?” and “With which goals?” could be found. The participants stressed that the connection to existing IEA Tasks should not be overlooked and that the extension of existing Tasks was preferable to the creation of a new one. It was clear that the points of view expressed during this workshop differed significantly from those of the Washington, D.C. workshop.

The participants were not convinced that new materials and processes should be the primary focus of the proposed Task, since these do not relate to near- and mid-term societal and industrial issues. Rather, it was suggested to base the Task on the following:

- Cost and Efficiency - transport and storage at reasonable cost, efficient use of all available hydrogen, increase in the value of used hydrogen, purification and quality of hydrogen
- Market development - acceleration of existing technologies, demonstration projects, emphasis on “door opener” technologies
- Future Applications - new hydrogen related materials for storage and catalysis, new hydrogen related processes (especially in metallurgy, materials science and carbon dioxide mitigation)
- Information - diminishing of consumer distrust in hydrogen driven processes through education and public relation, better public access to actual and thorough state-of-the-art information concerning hydrogen, identification of dependencies between the commodity and the energy market for hydrogen

Summary

The recommendations from the two workshops were transformed into a revised Task proposal. This proposal had a somewhat different focus than suggested in the original discussion paper. It was strongly oriented at common practical needs with high future market relevance. New uses for hydrogen, namely use in materials science and technology, no longer formed the main body of the proposed Task. As a result, an additional Task definition phase of six months was recommended in order to more precisely define the objectives, means, etc., of the new Task. During this time, definitive participants from industry, government and/or academia had to be identified. Three main restrictions for the suggested Task were set:

- Close connection to environmental issues, in order to fit within the IEA goals
- Concentration on pre-competitive measures, such as infrastructure and guidelines
- Involvement of industrial partners

Additionally, a precise overview of the current use of hydrogen, as well as reports summarizing the perspective of industries and a list of promising validated concepts would be needed.

Questionnaire

By the Fall 1998 meeting of the IEA Hydrogen Agreement Executive Committee in Ispra, Italy, two Swiss reports dealing with hydrogen use in general and its role in materials science and technology were completed. [The latter was published as part of the 1998 IEA Hydrogen Agreement Annual Report.] However, the needed industrial involvement for the new Task had still not been secured. Additionally, the other IEA Task development effort on Hydrogen from Carbon Containing Materials had its own requirements for industrial support. To aid both development efforts, the Executive Committee decided that a common questionnaire should be prepared and sent out to potentially interested companies. The questionnaire would be accompanied by a introductory letter and examples of the two proposed Tasks. (The questionnaire and the example Tasks are documented in the appendices to this report.)

Switzerland led the development of the questionnaire with support from Norway. It was then distributed in early Spring 1999 by the Executive Committee members to industrial companies in their respective countries. Of the roughly 500 companies send the questionnaire, 53 from 7 of the IEA Member Countries responded. (A list of the responses can be found in the Appendices.) Twenty (38%) of the respondents expressed either general or specific interest in some of the proposed Tasks and Subtasks, with interest split equally between the two Tasks. Below is a summary of the questionnaire responses:

Q1: What is the role of your company in the H_2 *market?*

Most of the respondents played multiple roles in the hydrogen market. The majority (~80%) were active as producers (40) and/or consumers (39) of hydrogen. One quarter (13) were refineries. Strong minorities came from the equipment manufacturers (11) or hydrogen merchandising companies (9). Other businesses like safety were seldom mentioned.

Q2: What is your present level of H_2 *use?*

Some of the participating companies used quite large amounts of hydrogen. Three of them, all large petrochemical firms, produced as much as 25 MNm^3 per day.

Hydrogen per day	Production	Consumption
None	7	5
up to 10000 Nm3	6	13
10000 to 100000 Nm3	14	10
100000 to 1 MNm3	9	6
above 1 MNm3	10	8

Hydrogen per day	Production	Consumption
No Answer	7	11

Q3: How do you cover your H_2 consumption?

The majority (33) of the companies produced their hydrogen on-site. Most of them via steam-reforming (18) or chlorine-alkali-electrolysis (7). Some utilized electrolysis (3), chlorate production (1) and ammonia cracking (1). Others purchased merchandised hydrogen (7) or did not use hydrogen in their processes (5).

Q4: Do you have a surplus H_2 (by-)production?

About 40% (21) of the companies produced a surplus of hydrogen. The amounts of surplus ranged from under 1000 up to 720,000 Nm^3 per day. The main uses for this surplus were either venting (11) or process heat generation (10). Some companies traded (6) or upgraded and reused their hydrogen (4). The larger producers of surplus hydrogen mainly traded or burnt this valuable commodity.

Q5: How do you expect the H_2 market to develop?

The general trend for the use of hydrogen by industry was expressed as a growing demand in all fields of today's and future application areas. The classic process use is especially expected to grow - up to 50% above today's usage level. The refinery business (10) and, in part, the production of chemicals (4) and metals (3) are seen as the main areas for growth. Only a few participants expect a downward movement in some classic uses, namely chemical synthesis (2) and refining of edible oils (1).

Area of use	Up	Stable or mixed	Down	No Answer
Process use	21	12	2	18
Energy storage	10	12	0	31
Fuel	15	9	1	28
Supply	18	8	0	27

Many companies also see a high demand for novel supply systems. Mentioned were new steam reformers (5), advances in chemical decomposition (2), water electrolysis (3) and biomass decomposition (1), as well as the need for smaller supply systems (2) and advances in purification of hydrogen (1).

The majority of the respondents expressed no opinion towards the use of hydrogen in energy storage or as a fuel. This is not particularly surprising, considering the nature of the industries represented.

Q6: What do you consider to be the main problems of the technology currently used (e.g. costs, purity, efficiency) and how would you suggest to improve its efficiency and economy?

Though most respondents had difficulty foretelling the future development of hydrogen use, most (41) had quite detailed ideas on why the use of hydrogen is currently limited. Among the many reasons cited, the cost of the hydrogen and its applications was mentioned most often (28). Very often this was coupled with the efficiency of the related processes being too low (19). The other mentioned obstacles ranged from purity problems (9), lack of infrastructure (4) and adequate transport or storage methods (5), high power costs (4), issues with fuel cell technology (4), deficits in compression technology (2), the current relationship to carbon dioxide emissions (from fossil fuel production) (2), the costs of raw materials (2), and short life time of hydrogen related equipment (1). Costs were definitely the recurring theme in the answers, but the suggested solutions included some fairly specific topics:

- Increased efficiency (energy savings) through developments in technology and processes - heat recovery, lower reaction temperature with new catalysts, more efficient use of fuel seed
- New Catalysts and special materials - avoid tube failure at high temperatures
- New purification technologies to increase reuse of hydrogen - better molecular sieves and PSA-mechanics
- Cheaper and more reliable end-use technologies - fuel cells
- Lowered transportation costs through small and mid-size on-site hydrogen production
- Cheaper storage alternatives
- Reduction of power consumption for water electrolysis
- Better overall hydrogen management

Q7: How do you think eventual restrictions on CO_2 *emissions will affect the future* H_2 *market?*

More than half of the participating companies (29) saw close connections between restrictions on carbon dioxide emissions and the use of hydrogen. Nearly equal numbers saw resulting price increases for hydrogen (9) and a rise in its use (10). Some companies also expect other and better hydrogen production methods (8) to be developed. These methods included hydrogen from renewable sources and capture of carbon dioxide. Only a couple of responses suggested the use of hydrogen would decline with growing restrictions on carbon dioxide emissions (2).

Q8: How would you approach potentially arising problems caused by such restrictions?

Again many of the respondents (29) had fairly detailed ideas on how to tackle issues arising from such restrictions. Most suggested alternative hydrogen production processes (14), improvement of existing processes (7) and technologies to reduce carbon dioxide emissions (7). Some even suggested strategies like transferring production to less developed countries (2). The cursory overview reads as follows:

- Natural gas use rather than coal or oil
- Renewable electrical energy for hydrogen production via water electrolysis
- Fuel conversion for hydrogen rich gas
- Utilization of different feedstocks for hydrogen production
- Reduction in valve trade off of hydrogen
- Concentration on energy and cost saving improvements
- Adoption of new high-efficient processes (e.g., in steam reforming)
- Better Hydrogen purification and “molecule management”
- Technical gas treatment and deposition of carbon dioxide
- By-product market for carbon dioxide and a political bonus for this utilization
- Trade with carbon dioxide quotas

Q9: Would you be interested in participating in the 2 new IEA collaborative tasks in one (or more) of the areas indicated below?

While 20 companies did not answer this question and 13 gave a negative answer, a total of 20 respondents showed interest in the two suggested new Tasks. Of these, 15 could envision direct involvement in one of the two proposed Tasks. The most notable points of interest were

Subtasks 3 and 4 of the proposed Task 16 (Hydrogen from Carbon Containing Materials) and the Subtasks 1 to 3 of the proposed Task 17 (Large-scale Industrial Uses of Hydrogen).

	Country	**CAN**	**GER**	**NOR**	**ESP**	**SWE**	**SWI**	**USA**	**Total**
Task	**General**	**2**	**2**	**4**	**2**	**1**	**1**	**8**	**20**
16	**New Production methods**	1	2	3	1	1	1	6	**15**
16-1	**Advanced thermal processes**		1	1		1			3
16-2	**Biomass**		1	2				1	4
16-3	**Water electrolysis**			2			1	4	7
16-4	**Small production systems**	1		1				4	6
17	**Large scale use**	2	2	2	2	1		6	**15**
17-1	**Hydrotreating processes**	2	1					2	5
17-2	**Transport systems**	1	1	1				2	5
17-3	**Upgrading processes**	1	1	1	1			2	6
17-4	**Quality analysis**			1		1		1	3
17-5	**Intermediate energy storage**							2	2
17-6	**Recovering systems**		1					2	3

The main interest came from United States (8) and Norwegian (4) companies. However, 8 companies from 5 other IEA member countries also answered positively.

Findings

While formulating and shaping this proposed IEA Hydrogen Agreement Task, several previously neglected issues and some new ideas for overcoming existing deficiencies have been identified and discussed. The following is a brief description of some of these problems and some proposed approaches for resolution. Some general rules can be employed as guidelines:

- Hydrogen is not an abundant resource and must be produced from other resources.
- The ecological costs of hydrogen use must be reduced.
- The economic costs of hydrogen use have to be reduced and must be comparable with other fuels.
- Hydrogen must be a reliable source for energy and raw materials.
- An integrated approach must be used for assessing the economic and ecological costs of hydrogen systems.

Production of Hydrogen

Hydrogen use produces too much carbon dioxide.

World-wide more than 95% of hydrogen is produced from fossil sources, which in turn results in carbon dioxide emissions. Thus, a major Task of developing the hydrogen economy will be to reduce the use of fossil resources (both feedstocks and energy inputs) for producing hydrogen. This concerns not only the main hydrogen delivering processes (steam reforming and partial oxidation), but also those processes where hydrogen is produced as a by-product (ethylene production and chlorine-alkali-electrolysis) or as an on-site speciality product (direct electrolysis or dissociation of ammonia). All of these processes require substantial energy inputs to produce the hydrogen. Thus, the amount of emitted carbon dioxide is substantially dependant on the primary energy sources, not just the chemical process involved.

Refineries will produce less hydrogen in the future.

Refineries currently generate excess amounts of hydrogen due to the large share of light, low-sulfur crude oils being processed. As the market share for lower-grade crudes grows, the amount of excess hydrogen will, in turn, be reduced.

Regional oversupply leads to waste of hydrogen.

As mentioned earlier, the hydrogen market tends to be regionally restricted. Seldom is the hydrogen transported beyond the industrial region in which it is produced. As a result, many regions will actually suffer from oversupply of hydrogen, even though the world demand for hydrogen is rising. An example of this is the hydrogen market in Western Europe where hydrogen demand is expected to remain static during the coming years. This same market produces large amounts of by-product hydrogen, far beyond current usage requirements. In other world markets, their own by-product hydrogen supply is far below their demands, so hydrogen must be produced specifically to meet their needs. This regional disparity in hydrogen supply and demand ultimately contributes to an overall increase in carbon dioxide emissions, as well as inefficient use of energy resources.

The quality of hydrogen is difficult to guarantee.

Companies that market their hydrogen are generally required to meet a set of minimum specifications based on the purchaser's needs. In order to guarantee these specifications, the supplier must perform the necessary, certified analyses for hydrogen purity. Controlled transport is also an important factor, which reduces or eliminates opportunities for more economic shared transport. This burden often deters companies from marketing their excess hydrogen.

Enhance the production of hydrogen and reduce carbon dioxide emissions.

Processes with a neutral carbon dioxide balance are needed to meet the growing hydrogen demand. New processes have to be developed and/or existing processes have to be enhanced. Demonstration plants have to be built and their market potential must be strengthened. Target technologies include:

- Fossil fuels or biomass to produce hydrogen, with sequestration of the carbon
- Solar thermal, photoelectrolytic and photobiological production of hydrogen
- Natural hydrogen wells

A review of conventional hydrogen producing processes will identify opportunities for gains in economic efficiency and reduction of ecological impacts. Research, plant construction and market potential will require the following measures:

- Improved processes for carbon-based, large-scale plants
- More efficient small-scale, carbon-based units
- Decomposition of ammonia or methanol using sustainable resources
- Electrolysis powered by renewable energy sources

Consumption of Hydrogen

The demand for hydrogen will definitely grow.

Hydrogen demand will continue to grow with the expansion of a large number of already important industries. This will impact most world regions as hydrogen is required for the production of base chemicals, such as ammonia and methanol; for petrochemical processing; and for the production of numerous high tech products, including steel alloys and silicon wafers. In particular, existing refineries will require greater amounts of hydrogen due to the increasing proportion of heavy and high-sulfur crudes, stricter regulations concerning sulfur content and aromatic saturation in diesel, and higher hydrogen to carbon ratio requirements for modern engines.

The quality of hydrogen is often better than needed.

Merchandised hydrogen is often sold at below its potential value. Because of the high cost of analyses, the hydrogen is only tested to meet minimum requirements rather than to determine its actual purity.

Hydrogen may be more expensive than necessary.

Because of the regional nature for hydrogen supply and consumption, rising demands for hydrogen could become a serious problem in regions where hydrogen demand is already keeping pace with supply (e.g. Japan). In these areas, the cost of hydrogen will be comparatively high, which will impede opportunities for hydrogen substitution in carbon-based processes or materials.

Demand for hydrogen could grow more than expected.

Substitution of hydrogen for conventional raw materials in ore reduction and engine fuel applications could result in even greater demand for hydrogen. Though hydrogen use in these markets is not expected to have a significant impact in the near-term, the longer-term impact could be substantial.

Hydrogen must be used more efficiently.

Current bulk processes that use hydrogen require efficiency improvements. Venting, burning, or any useless degrading of hydrogen must be avoided. Furthermore, the value per unit of hydrogen needs to be increased. Key to intensifying the use of hydrogen is technological enhancement and cost-reduction of upgrading and purification techniques and on-stream analysis methods. Research, development and demonstration should be done in co-operation with the respective industries:

- Hydro-treating in refineries
- Ammonia production
- Methanol production
- Other bulk processes using hydrogen

Processes with comparatively high carbon dioxide emissions or raw material consumption should be targeted for substitution. New hydrogen-based processes for equivalent applications may present opportunities for improved efficiency and decreased emissions. Some processes may already be at the development stage for, at least, partial commercial substitution for carbon-based processes. It will be important to strengthen the market potential of the respective products:

- Small engines and generators
- Reduction of ores to metals and alloy production
- Welding
- Corrosion protection and oxygen scavenging

Transport and Storage of Hydrogen

Transport and storage of hydrogen are too expensive.

Transport and storage costs are quite high for hydrogen compared to other more conventional energy carriers. Significant reductions of these costs will be needed if hydrogen is to become a competitive fuel. Gaseous transport is currently limited to distances of less than 200 km. Seldom is merchandised hydrogen transported between different industrial regions (more than 1000 km), even though natural gas pipelines very easily cover these types of distances as can liquid tankers. Material and safety issues currently limit the use of gas pipelines, and liquefaction and storage of hydrogen can be very expensive, at least at the smaller scale. Cost reductions in liquefaction and storage units could result from increased demand and production levels.

Transport and storage of hydrogen are a kind of patchwork.

When compared with the world-wide system for natural gas, hydrogen transport and storage is a mere patchwork of systems and approaches. No special network of pipelines exists for hydrogen, nor have concerted attempts been made to utilize existing natural gas pipelines for hydrogen transport. Buffer systems, such as the low pressure spherical tanks used for natural gas, are absent for hydrogen. Large scale hydrogen compressors are not yet available, though they could be adapted from current natural gas technology, assuming sufficient demand existed. High pressure storage provides an interesting option, since the additional compressing energy requirements for gaseous hydrogen decline with higher pressures, however storage vessels are not yet available for these higher pressures. Finally, liquid storage is quite effective on an energy density basis, however evaporative losses are still on the order of 0.4 to 1%, which proves uneconomical for longer-term storage.

Know-how in hydrogen merchandising is lacking.

Merchant hydrogen shipped by pipeline or truck represents less than 2% of the total hydrogen market. The required knowledge and capabilities for hydrogen purification, storage, distribution and application keeps the number of companies involved in the merchant business very low. As a result, each industrial region forms its own closed market for hydrogen and excess amounts of produced hydrogen are generally used for very low value applications.

Search for a competitive and complete transportation system for hydrogen.

Gas handling and transport is not new to industry. It should be possible to adapt existing technologies (especially those from the natural gas industry) to the needs of hydrogen transport and storage. In the process of developing more competitive means of hydrogen transport the following elements will play important roles:

- Decentralized hydrogen production and distribution systems
- Use of existing pipeline networks
- Small hydrogen liquefaction units
- Buffer capacities

Apart from needed research, demonstration plants and strengthening of market potentials will likely be necessary.

Some requirements of hydrogen transport and storage will not be met by the simple adaptation of conventional systems. Special attention must be given to energy density requirements, gas losses, storage vessel integrity and hydrogen purification. New materials and systems will have to be developed, tested and implemented:

- Composite storage materials for pressurized gaseous hydrogen
- Insulation materials and technology for small scale liquid storage
- New materials for hydrogen storage (glass spheres, iron sponge, carbon whiskers, metal hydrides, chemical hydrides, etc.)
- Complete storage systems for small scale industrial and household uses
- Purification systems for hydrogen from multi-user pipelines

Substantial hydrogen transport and storage developments are needed.

In order to achieve a true hydrogen economy, substantial developments in hydrogen transport and storage must be made:

- Decentralized hydrogen distribution systems
- Utilization of multi-user and even multi-gas pipeline networks
- Purification and analyses systems operating at pipeline outlets
- Regional shared transport logistics under independent control
- Distribution of hydrogen transport technology and know-how

Overall Deficits of the Hydrogen Economy

Detailed figures and a complete overview are missing for hydrogen.

Detailed figures for hydrogen use throughout the different world regions are not readily available. Only the western industrialized countries tend to have governmentally managed reporting systems. Even where these systems exist, on-site use of hydrogen, particularly as a fuel, is often not well documented. For potentials in the hydrogen economy to be defined, reliable figures for, at least, key hydrogen production and utilization parameters are needed.

No validated estimates of future developments for hydrogen exist.

Although it is impossible to know for certain what the future will bring, estimates can be made based on likely scenarios. Modern data acquisition and computing provides the necessary platform for calculating these trends. However, the necessary inputs need to be made available. Likewise, a mechanism for understanding the technology potential needs to be employed. Life cycle assessment provide the necessary tool for characterizing the cradle to grave energy, cost and environmental repercussions and benefits.

Definition of a new and more coherent up-to-date strategy is necessary.

No single world-wide strategy for shaping the future hydrogen economy exists today. With the diversity of the businesses and individuals involved in the hydrogen arena, development of such a strategy remains unlikely. However, it is important that the players at least identify and agree upon a set of key elements for the strategic alignment of hydrogen with our future energy and commodity needs. The IEA Hydrogen Program and its strategic plan are a good example of compiling national viewpoints into a common theme. It will be essential to continually update the strategy and activities to reflect new ideas, concepts and developments in the hydrogen community. However, for the IEA Hydrogen Program to be effective, it must obtain buy-in and participation from the broad range of companies, organizations, universities and governments involved with hydrogen.

Organize the future hydrogen economy now.

Building of the future hydrogen economy requires a better understanding of the world situation. Only through a concerted effort to collect, organize and process realistic data on hydrogen production and utilization will the savings potential of hydrogen in bulk processes and the growth potential for new processes be understood. This requires:

- Better organized report system on hydrogen use
- Support for existing data research projects, even commercial ones
- Life cycle analyses for key processes
- Close co-operation with organizations treating related commodities
- Scenario planning to estimate future hydrogen developments

Appendix I
The questionnaire

1. What is the role of your company in the H_2 market?

O Production
O Consumption
O Equipment
O Merchandising
O Other: ___________

2. What is your present level of H_2 use?

Production: ___________
Consumption: ___________

3. How do you cover your H_2 consumption?

O On-site production: ____________ (type)
O Merchandised: ____________ (type)

4. Do you have a surplus H_2 (by-)production?

a. How much? __________

b. How is it used?
O Upgraded and reused
O Traded
O Burned for process heat
O Vented

5. How do you expect the H_2 market to develop in the areas of

a. Process use ____

b. Energy storage ____

(e.g. as intermediate) ____

c. Fuel ____

(e.g. for vehicles) ____

d. Supply ____

(e.g. equipment) ____

6. What do you consider to be the main problems of the technology currently used (e.g. costs, purity, efficiency) **and how would you suggest to improve its efficiency and economy?**

____

7. How do you think eventual restrictions on CO_2 emissions will affect the future H_2 market?

____

8. How would you approach potentially arising problems caused by such restrictions?

____

9. Would you be interested to participate in the 2 new IEA collaborative tasks in one (or more) of the areas indicated below?

Task16
O H_2 from advanced thermal processes
O H_2 from biomass
O H_2 by water electrolysis
O Small scale distributed H_2 production

Task17
O Efficiency of hydrotreating processes
O Efficiency of H_2 transport systems
O Upgrading of H_2 containing gases
O Analyses of H_2 quality
O H_2 for intermediate energy storage
O Recovering system for H_2

Company: ____________________________ **Name:**
____

Address: ____________________________ **Function:** _______________________

Telephone: ____________________________ **Fax:** _______________________

E-Mail: ____________________________

Please return questionnaire (if possible by May 15th, 1999) to:

E3M GmbH c/o Karsten Wurr ,

Spaldingstr. 160 d , D-20097 Hamburg , Germany

Fax: +49-40-659 99 820

Appendix II Sample projects

IEA Hydrogen Agreement

Sketch of sample project #1

Hydrogen Production from Biomass Using High-Temperature Plasma Reactors

Objective

Production of hydrogen from biomass has the advantage of being CO_2-neutral (not leading to increased CO_2-contents in the atmosphere), as well as having the potential to be economically competitive. The objective of the proposed project is to develop a versatile and efficient process for such hydrogen production.

Biomass may be gasified or converted to liquids bio-oil) via pyrolysis. The resulting gaseous or liquid mixtures may be processed by catalytic steam reforming or partial oxidation, followed by shift reactions, to produce hydrogen. Due to the complexity of the mixtures, problems may arise in conventional reformers caused by deposits (coking) on the catalysts. Conventional reformers are also best suited for large central plants, while biomass may be more economically suited to small local plants. Plasma reactors are very fuel-flexible and have been developed for hydrogen production from a range of hydrocarbons, including heavy fuel oil. They have also been adapted to waste gasification. Such reactors are modular and suitable for small-scale distributed hydrogen production. If the hydrogen is used for power generation in a fuel cell, a portion of the power could support the plasma generator, resulting ina completely autonomous plant.

Means

In order to achieve the above objective the Participants will carry out a collaborative research project within the proposed Task “Industrial Hydrogen Production” of the IEA Hydrogen Agreement. The project will comprise a state-of-the-art assessment (literature and patent review) and the planning and performance of experimental work to be carried out in the Participants´ laboratories (Phase 1).

If agreed by the Participants this will be followed by a Phase 2, comprising testing in one or more pilot plants. The project shall result in a Feasibility Study, including process analyses and cost estimates.

Work Plan

Phase 1 is assumed to last for three years: 0.5 year for state-of-the-art assessment and planning, 2.5 years for experimental work.

Phase 2 is assumed to last for another three years: 2.5 years for testing and 0.5 year for reporting.

Funding

Phase 1 could be carried out on a task sharing basis. The extent of the work will depend upon the number of Participants, their interests and the resources they are able to provide. A minimum of three participating countries and a total effort of at least 20 person-years should be sought. Phase 2 will be accomplished on a cost or task sharing basis.

Intellectual Property

The IEA Implementing Agreement on Hydrogen Production and Utilization has provisions for the protection of information and intellectual property of the Participants. They secure that ”Arising information regarding inventions shall be owned in all countries by the inventing Participant”. It can be assumed that this will be applicable also in the proposed new Tasks, thus providing adequate protection of the intellectual property of the Participants.

IEA Hydrogen Agreement

Sketch of sample project #2

Recovery System for Hydrogen

Objective

For many processes in which hydrogen is used (e.g. for reduction or hydrotreating), the gas leaving the reaction zone still contains substantial amounts of hydrogen. It is mixed with other gases and thus of lower technical and economical value. Common follow-on uses of this gas stream are to burn it for process energy or simple venting. Economically competitive methods to recycle and upgrade the diluted hydrogen are not yet available. If such methods could be found they would provide a valuable resource for usable hydrogen. Thus, less capital would be needed for hydrogen production and overall carbon dioxide emissions would be lowered, since less hydrogen would need to be produced.

The aim of this collaborative work will be to develop a system for several medium or large scale hydrogen applications to recover hydrogen from dilute gas mixtures. Overall energy consumption and costs of the respective processes shall be lowered by finding modifications and additions to these processes. The carbon dioxide balance and finally the overall efficiency of several hydrogen driven processes shall be improved. Methods for on-stream analysis, separation and cleaning of gases, and the search for new, better-suited materials will be a priority. Promising results should be verified in one or more demonstration plants.

Means

The above mentioned project will be organized as a Subtask within the proposed new Task “Industrial Use of Hydrogen” of the IEA Hydrogen Agreement. Phase 1 of the effort will be to conduct a state-of-the-art assessment and evaluation of known processes.

Phase 2 of the effort will consist of highly coordinated research and development activities carried out by the participants from academic and governmental institutions and industry.

The final phase (Phase 3) of this project will involve the implementation of resulting technologies through testing in one or more demonstration plants. The construction of such plants will be based on preliminary feasibility studies based on the results from Phases 1 and 2.

Work Plan

Phase 1 should require a maximum of one year for assessment and planning. Phase 2 will last for approximately three years: 2.5 years for experimentation and 0.5 years for reporting. The duration of Phase 3 will depend heavily on the complexity of the process modifications to be implemented. A minimum of two years would be expected.

Funding

Phase 1 and 2 could be carried out on a task- or cost- shared basis. The extent of the work will depend upon the number of participants, their interests and the resources they are able to provide. A minimum of three countries or companies should participate to guarantee a total effort of at least 10 person-years per year. The funding of Phase 3 will likely be best accomplished on a cost-shared basis.

Intellectual Property

The IEA Implementing Agreement on Hydrogen Production and Utilization has provisions for the protection of information and intellectual property of the Participants. They secure that “Arising information regarding inventions shall be owned in all countries by the inventing Participant”. It can be assumed that this will be applicable also in the proposed new Tasks, thus providing adequate protection of the intellectual property of the Participants.

Appendix III Companies participating in the questionnaire

No.	Company	Country	General	Interest in Task 16	Task 17
1	Husky Oil Operations Ltd.	CAN	Yes	4	1, 2, 3
2	Norsk Hydro ASA	NOR	Yes	1, 2, 3, 4	2, 3
3	Eka Chemicals Rjukan AS	NOR	Yes	3	4
4	Syncrude Canada Ltd.	CAN	Yes		1
5	Statoil	NOR	(Yes)		
6	Falconbridge Nikkelverk A/S	NOR	No		
7	Husky Oil Ltd.	CAN	N.A.		
8	Eka Chemicals AB, Albyfabriken	SWE	Yes	1	4
9	PPG Canada Inc.	CAN	N.A.		
10	Norsk Hydro Electrolysers AS	NOR	Yes	2	
11	Nynas AB	SWE	No		
12	REPSOL	ESP	Yes		3
13	Cellulose Attisholz AG	SUI	No		
14	Surefabrik Schweizerhall	SUI	N.A.		
15	Novartis CP Monthey SA	SUI	N.A.		
16	Carbagas	SUI	No		
17	Giovanola Frres S.A.	SUI	Yes	3	
18	Clariant AG	SUI	N.A.		
19	Novartis International AG	SUI	No		
20	Iwatani Industrial Gases Corp.	JAP	N.A.		
21	Nisseki Mitsubishi Corp.	JAP	N.A.		
22	Sumitomo Seika Corp.	JAP	N.A.		
23	KK. Suzuki Shokan	JAP	N.A.		
24	Japan Energy Corp.	JAP	N.A.		
25	Shinko Pantec Corp.	JAP	N.A.		
26	Nihon Sanso Corp.	JAP	N.A.		
27	Targor Iberica S.A. (BASF Espanola)	ESP	No		
28	CEPSA (La Rabida)	ESP	N.A.		
29	FMC Foret	ESP	No		
30	ELNOSA	ESP	N.A.		
31	Quimica del Cinca S.A.	ESP	No		
32	Shell Hydrogen	USA	Yes		
33	Rock Hydrocarbon	USA	N.A.		
34	Chevron Products Co.	USA	No		
35	The BFGoodrich Company	USA	No		
36	Solvay Interox Inc.	USA	No		
37	PROTON Energy Systems	USA	Yes	3, 4	2, 3, 5
38	Huron Tech Corp.	USA	No		
39	Kerr-McGee Chemical Corp.	USA	Yes	3	5, 6
40	Weyerhaeuser Company	USA	N.A.		
41	San Joaquin Refining Company	USA	Yes		1
42	Marathon-Ashland Petroleum Inc.	USA	N.A.		
43	Mallinckrodt Inc.	USA	N.A.		
44	Teledyne Brown Eng. Energ. Syst.	USA	Yes	3, 4	
45	Western Electrochemical Company	USA	N.A.		
46	Cross Oil Refining	USA	Yes	3, 4	1
47	Carburos Metalicos S.A.	ESP	Yes	Yes	Yes

No.	Company	Country	General	Interest in Task 16	Task 17
48	Texaco Inc.	USA	Yes	Yes	Yes
49	International Fuel Cells	USA	Yes	2, 4	2, 3, 4, 6
50	Elektro-Chemie Ibbenbüren GmbH	GER	No		
51	Siemens/KWU	GER	No		
52	HGC Hamburg Gas Consult GmbH	GER	Yes	2	2
53	Wintershall AG	GER	Yes	1	1, 3, 6

Appendix IV Outline of the proposed Task

Task Objective

The central objective of this Task is to increase the created economic value per unit of hydrogen used in today's large scale industrial applications. The Task seeks to promote the afforded changes in the bulk use of hydrogen and enhance all measurements that will improve the underlying conditions and limitations. Naturally, this program will have to focus on a few, select processes. These will be defined by the participants' needs.

Scope

The scope of this Task includes all large scale processes that do not use hydrogen solely as an energy carrier. The Task focuses especially on those industrial processes with a high hydrogen demand and incomplete consumption of hydrogen during the process. New materials, systems and strategies will be tested and their performance will be evaluated in laboratories, computer simulations and demonstration plants. This will include economic and ecological aspects, as well as the influence on the quality of respective products. Furthermore, the connections to other areas of hydrogen technology cannot be neglected. Production, transport, storage and safety account for basic limitations in the use of hydrogen. The choices of manufacturing methods and the raw material sources are key to the sustainability of the entire system.

Means

The integral character of hydrogen as both an energy carrier and a commodity must be considered in all fields of research and development. It is recommended that an evaluation of known processes, research activities and demonstration of technologies be included in this Task.

As appropriate, the work will be carried out in cooperation with other IEA Implementing Agreements. To accomplish the above mentioned objectives, the participants of academic institutions and industry will undertake research, development and demonstration activities within the framework of the following highly coordinated Subtasks:

Subtask A: Hydrogen consumption in large scale processes

This subtask covers today's main industrial processes' consumption of hydrogen. In particular, it will include the use of hydrogen for hydro-treating and ammonia and methanol production.

Current bulk processes using hydrogen need an upgrade in efficiency of hydrogen use and energetic parameters. Any unnecessary degrading of hydrogen must be avoided. A more careful use of the hydrogen provided will increase the created economic value per unit of hydrogen. The aims of the collaborative work are to:

- lower the energy and cost of processes:
- find new processes or modify existing ones to improve the carbon dioxide balance: and
- improve the overall efficiency of hydrogen driven large scale processes.

Research and construction of demonstration plants have to be done in cooperation with the respective industries. The needed efforts could be split into three activity areas.

Goals:
- Lower temperature and, thus, energy costs of processes
- Advances carbon dioxide sequestration technologies
- Develop new catalytic systems for denitrogenation and desulfurization
- Demonstration improved efficiency

Milestones:	01/2000	Begin R&D
	09/2001	Preliminary reports/Decision about further program
	01/2002	Design of demonstration plant(s)
	07/2002	Construction of demonstration plant(s)
	01/2003	Begin demonstration phase
	12/2003	Final reports

Activity A1: Efficiency of hydro-treating processes

Hydrotreating to saturate aromatic and olefinic compounds in petroleum, fats and oils industries uses large amounts of hydrogen. The desulfurization and denitrogenization of fossil commodities also demands for intense hydrotreatment. However, raw materials availability, as well as legal and technical requirements, change. Existing processes need to be modified. This includes such activities as the catalytic removal of sulfur and nitrogen.

Activity A2: Re-engineering of nitrogen-based processes

As ammonia demand and production is declining in some highly industrialized regions the parameters for construction of respective plants have to be changed to meet the new economic requirements. The production plants for ammonia and its related products have to be re-engineered to allow for the industrial synthesis of new nitrogen-based chemicals.

Activity A3: Improvement of synthetic fuels' production

Today, the production of synthetic fuels, in particular methanol, is one of the most important consumers of hydrogen. The demand for these products is expected to grow steadily during the next decades. This growth may be even more rapid if methanol does, in fact, become a major substitute for petrol. Technical and industrial processes need to be developed where carbon species are upgraded into economically attractive products. This includes effective use of the limited hydrogen supplies.

Subtask B: Hydrogen supply for large scale processes

It is not sufficient to increase the efficiency of consuming processes alone. Supply must also be considered. This Subtask aims to:

- intensify the use of hydrogen by development and enhancement of upgrading or purification technologies and on-stream analysis methods, as well as lowering the costs for these units;
- improve the economic and ecological efficiency of hydrogen supply sources through more sensible use of by-product hydrogen; and
- strengthen the merchandising capacity for hydrogen by lowering the costs and encouraging multi-user solutions.

Research, development and realization of the necessary changes to the supply system afford the participation of the respective industries.

Goals:
- Use a greater share of by-product hydrogen
- Increase market share of merchandised hydrogen
- Improve transport logistics for hydrogen
- Lower cost of long distance mass transport of hydrogen
- Improve purification, upgrading and analysis systems for hydrogen

Milestones:	01/2000	Begin report phase
	06/2000	Reports on: 1. Deficits in hydrogen supply and merchandising 2. Technical requirements for more effective transport

	3. Cost effectiveness of hydrogen supply sources
07/2000	Begin R&D
09/2001	Preliminary reports/Decision about further program
01/2002	Design of demonstration hydrogen supply network/Guidelines
01/2003	Begin demonstration hydrogen supply network
12/2003	Final reports

Activity B1: Efficiency of hydrogen sources

Every process using hydrogen demands special qualities and quantities of this commodity. The final decision for the use of a special hydrogen source is not only dependent of the respective process, but also the regional availability of hydrogen supplies. A review for each individual process is necessary to identify opportunities for an overall increase in economic efficiency and a reduction of ecological damage. In particular the increased utilization of by-product hydrogen will be necessary to realize this goal. The key to improve the existing supply mechanisms, aside from better logistics, lies in better standardization of purification and analysis systems.

Activity B2: Strengthening of hydrogen merchandising

As hydrogen supply changes from a mere captive to a merchandise business substantial developments must be made. Supply logistics have to account for a rapidly growing demand. This can be done through utilization of multi-user and perhaps even multi-gas pipeline networks, with purification and analyses systems operating at pipeline outlets. Regionally, shared transport logistics under independent control are needed. Some of the new requirements for hydrogen transport can be met by adaptation of conventional systems. However, some new materials and systems will have to be developed, tested and implemented. Apart from needed research, the set-up of demonstration plants and strengthening of market potential may be necessary.

Subtask C: Assessment of hydrogen driven large scale processes

The building of the future hydrogen economy requires a better base of data. This must include organized data collection and data processing with adequate tools. Only by taking these measures can the hydrogen savings potential in bulk processes and the growth potential of new or niche processes be calculated. The objectives of this Subtask are to:

- define the framework for a better reporting system on large scale hydrogen use;
- provide means for selection and prioritization of alternative large scale processes; and
- facilitate mechanisms for incorporating feedback from implementation of these processes.

The acquisition of data and the comparison of computer models to reality may only be carried out with the participation of the above mentioned industries.

Goals:
- Improved data acquisition for on-site use of (esp. by-product) hydrogen
- LCA methodology development
- Data processing for activities from the other Subtasks
- Prioritized listing for alternative hydrogen using processes

Milestones:	01/2000	Begin report phase
	06/2000	Reports identifying LCA tools and needed inputs
	07/2000	Begin process evaluation
	12/2001	Plant and Transportation Network Design Guidelines
	12/2002	Report on estimated impact of new processes
	12/2003	Final reports

Activity C1: Systems analyses of large scale processes

The modification and implementation of hydrogen technology affords a careful analysis of the expected environmental and socioeconomic impacts. Therefore studies have to be undertaken that include life cycle analyses at least for key processes. The results of this modeling work should allow for an assessment of alternative processes. Special attention should be given to possible processes with carbon-neutral flows of materials and fuels and to the analysis of carbon dioxide reduction and mitigation potential.

Activity C2: Improved data and report system on hydrogen transport and use

To gain an overall understanding of hydrogen consumption and supply, all contributions to this system need to be known. Currently a significant lack of data exists for the on-site use of by-product hydrogen and in total hydrogen use in non-western countries. Thus, a better organized reporting system on hydrogen use is urgently needed. This has to be defined and implemented in close co-operation with the respective industries and with other organizations, including governments.

Preliminary Time Schedule

This Task should enter into force on January 1, 2000. It should remain in force for three years. Extension for both the research and demonstration phases may be considered.

Milestones:	09/1999	Workshop for Task definition
	10/1999	Outline R&D plans
	01/2000	Begin R&D
	09/2001	Preliminary reports/Decision about further program
	01/2002	Design of demonstration plant(s)
	07/2002	Construction of demonstration plant(s)
	01/2003	Begin demonstration phase
	12/2003	Final reports

Level of Effort

Operating agent and subtask leaders will each require 0.5 person year (py) per year. Subtask A will require 1.5 py per process for the first year and 2.5 py per year per process for the second and third year. During the demonstration phase an additional 1 py will be required for coordination. Subtask B will require 3 py in the first year and approximately 6 py in the second and third year. In the fourth year, 2 py will be needed for coordination and reporting. Subtask C will require 1 py per year for each process.

Costs

Funding for the Task activities will be a combination of task- and cost-shared contributions. The majority of the basic and applied research effort can be done on a task-shared basis. However, the demonstration phase will be more practically carried out through cost-shared support. Throughout the duration of the Task, funding should also be available for a Scientist Exchange Program.