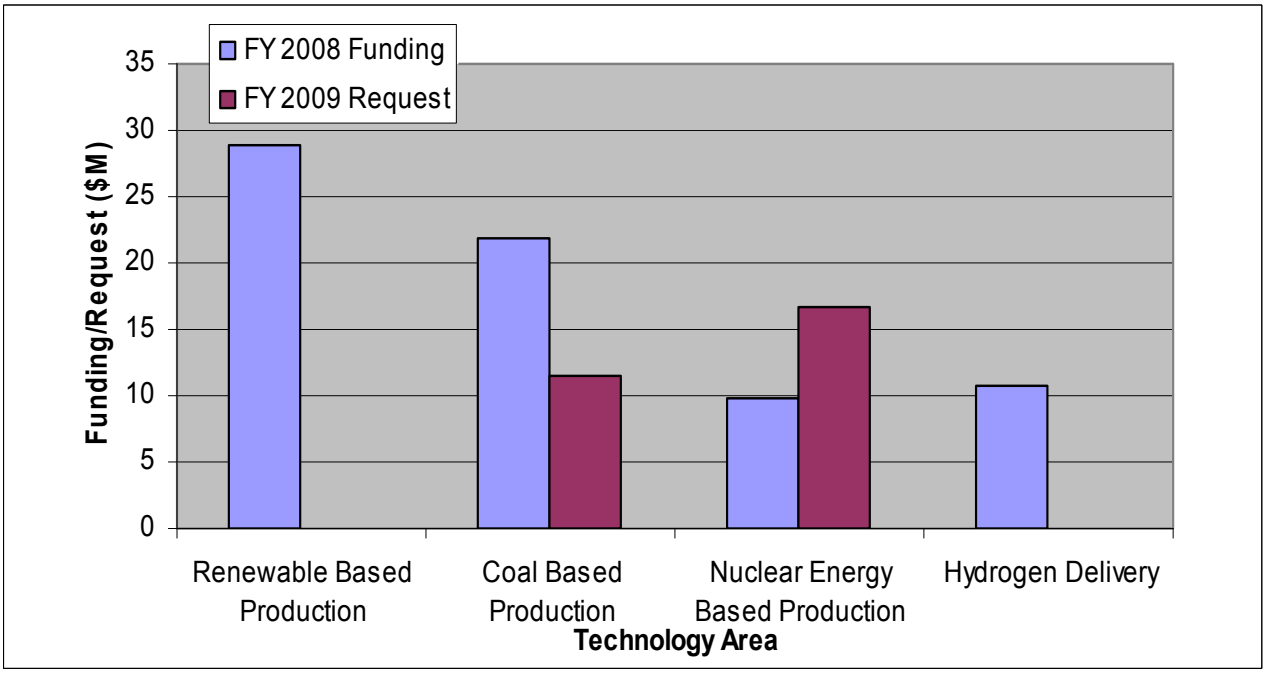
2008
Hydrogen Production and Delivery
Summary of Annual Merit Review Hydrogen Production and Delivery Subprogram

Summary of Reviewer Comments on Hydrogen Production and Delivery Subprogram:

This review session evaluated hydrogen production and delivery research from all DOE activities working on the President's Hydrogen Fuel and Advanced Energy Initiatives, including: the Offices of Fossil Energy, Nuclear Energy, and Energy Efficiency and Renewable Energy. The production and delivery projects are generally considered to be well-aligned with the goals and objectives of the Hydrogen Program.

The production projects include diverse energy sources and technologies for hydrogen production including natural gas reforming, water electrolysis, bio-derived renewable liquids reforming, biomass gasification, solar-driven thermochemical cycles, nuclear-driven thermochemical cycles, photoelectrochemical direct water splitting, biological hydrogen production, and hydrogen production from coal. The delivery projects reviewed included the next stage of development of the H2A Delivery analysis models, and several of the key hydrogen delivery research efforts such as pipeline embrittlement, new fiber reinforced polymer pipeline and linings, and compressor research. Overall, the projects were judged to have made considerable progress in reducing both projected capital and operating costs and in improving material properties. Reviewer concerns and recommendations varied considerably by project and are summarized below.

Hydrogen Production and Delivery Funding by Technology:



Majority of Reviewer Comments and Recommendations:

In general, the reviewer scores for the production and delivery projects were high to average, with scores of 3.9, 3.1 and 1.9 for the highest, average and lowest scores, respectively. The scores are indicative of the technical progress that has been made over the past year for DOE competitively selected and Congressionally directed projects. Recommendations and major concerns for each project category are summarized below.

Bio-Derived Liquids Reforming: New technology being developed for distributed reforming from bio-derived liquids (e.g. ethanol, sugars) will build on distributed reforming from natural gas technology while helping to solve outstanding issues with on-site hydrogen production to reach the bio-derived liquids cost goal of $3.00/gge by 2017. Two primary recommendations emerged from the reviews. First, the catalyst development tasks must move forward and be successful if the reforming of bio-derived liquids is to meet the DOE production cost targets. Second, all projects need to utilize H2A production modeling to provide consistent cost estimates.

Electrolysis: In general projects in this area were scored favorably. Two projects ended in FY08, one continued, and 2 were new starts. Most of the projects were regarded as well-aligned with current program goals and objectives. The projects focused on increasing stack efficiency and decreasing capital cost. Innovative new membranes presented were able to increase the efficiency to above that of the 2012 DOE targets and advanced manufacturing techniques along with new designs were presented that are projected to significantly reduce capital costs. The reviewers noted: 1) long term durability of the membranes must be tested, 2) the advanced membranes being developed need to be integrated into stacks and tested and 3) balance-of-plant development is needed to increase system reliability while reducing system cost. The newly started projects will be addressing these important issues.

Biomass Gasification: Three projects in this area were reviewed; two projects evaluated the potential for central high temperature biomass gasification; the other researching the potential of central plant, low temperature, single step, aqueous phase reforming of hydrolyzed biomass. The project scores ranged from 2.5 to 3.7. Projects scoring higher were noted to have significant technical advancements since last year and to have a focused project plan, which was followed closely.

Solar-Driven High Temperature Thermochemical: Two presentations and two posters were reviewed in this topic area. The projects were favorably rated for their collaborative efforts and technical skills and abilities of the researchers. Recommendations for improvement included to ensure that the calculation of overall system efficiency is consistent for each cycle, to complete all material balances, and to identify and resolve waste disposal issues. Finally, the reviewers responded favorably to the centralized H2A analysis that TIAX is coordinating.

Photoelectrochemical Hydrogen Production: The reviewers noted that the teaming approach that was used in some of the projects in this area was effective and necessary to achieve the DOE targets. Several of the projects received high ratings from the reviewers. Nearly all the projects were viewed to be aligned with the program's long-term goals. The projects have achieved good scientific progress in materials research and have established effective collaborations. The addition of theoretical activities to this area was seen by the reviewers as necessary.

Biological Hydrogen Production: The projects in this area were highly rated and the general conclusion from the reviewers was that the researchers are moving toward the DOE goals in this long-term renewable hydrogen production area. The scientific methods used in the majority of the projects are seen as cutting edge and the collaborations are effective and productive.

Separations: Reviewers commented, similar to prior year reviews, that there is a great need for investigators to test their hydrogen separation and purification membranes using realistic, mixed gas streams and to complete cost analyses. The potential for membrane technology to reduce the on-site hydrogen production footprint (by eliminating the PSA unit) and to reduce capital costs were frequent comments. Overlap with DOE Office of Fossil Energy membrane separations work was noted.

Hydrogen from Coal: The projects reviewed in this area received mostly favorable ratings from the reviewers. Reviewers observed that the projects were in alignment with the DOE Hydrogen Fuel Initiative and Hydrogen from Coal Program goals and objectives. The reviewers suggested that the projects need to advance the technology to the point where experiments using actual or close to actual gas streams are being performed. Specifically, the reviewers noted that the membranes need to be tested in the presence of impurities. The membranes also need to go through temperature cycling to assess mechanical stability. Finally, the reviewers noted that free standing membranes may be difficult to implement in a real world system.

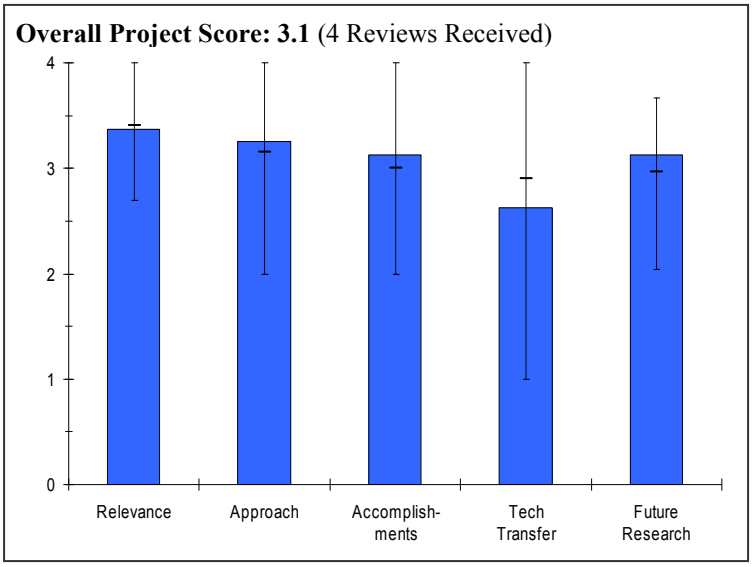
Hydrogen Production Using Nuclear Energy: In general, the projects reviewed in this area were scored favorably. Reviewers approved of the breadth of collaboration for some projects and the well-focused approach of other projects. The projects were judged to be well-aligned with the program's goals. As in 2007, reviewers recommended that research be driven by materials and cost. Specific recommendations were made to understand durability and degradation of the high temperature electrolytic cells.

Hydrogen Delivery: The reviews recognized significant and very relevant progress in the pipeline research. The reviews also complimented the broad spectrum of collaboration across industry, national labs and universities as well as a good mix of theory, modeling and experimental work. The reviewers suggested benchmarking results achieved in this program with Technology Validation results or with field installations, e.g. hydrogen embrittlement of existing pipelines. Reviewers also suggested measuring the effect of hydrogen impurities on pipeline and storage system performance and on the cost for purification.

Project # PD-01: Low-Cost Hydrogen Distributed Production System Development
Frank Lomax; H2Gen Inno. Inc.

Brief Summary of Project

The objectives for this project are to 1) design, build and test a 565 kg/day hydrogen plant for 99.999% pure hydrogen to meet the Department of Energy hydrogen $3/kg cost target for steam methane reforming and pressure swing adsorption; and 2) develop a catalyst suite based on our current technology suitable for use with fuel grade ethanol to facilitate renewable hydrogen production.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.4** for its relevance to DOE objectives.

- This project is highly relevant toward meeting Department of Energy's short term objectives.
- Project supports achievement of Department of Energy cost targets for distributed natural gas reforming hydrogen production.
- It is not clear that the project is working toward the Department of Energy efficiency goals.
- The development of low cost sources of larger quantities of hydrogen is highly relevant.
- Development of small, distributed reforming technologies will be necessary for Department of Energy to meet Hydrogen Fuel Initiative Goals.

Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

- The approach was sound and ended up proving to be successful.
- The PI is knowledgeable about the market requirements for the hydrogen generation plant (for current hydrogen markets such as metal processing and chemical manufacturing) and appears to be focused on meeting these requirements.
- It is not clear that H2Gen is focused on meeting the requirements of the vehicle refueling market.
- H2Gen has identified the bottlenecks in the original product and has implemented improvements in the second generation product to overcome the bottlenecks of the first.
- The presentation did not include discussion of all the barriers identified; thus, it is not possible to evaluate the contribution of this project in terms of overcoming fuel processing manufacturing barriers, O&M barriers, feedstock issues, or control and safety.
- It was difficult to evaluate the approach taken, since little information was provided in the presentation on the details of the hydrogen production system.
- The approach seems very good.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.1** based on accomplishments.

- H2Gen made substantial progress toward meeting Department of Energy goals with its first design plant.
- The improvements that were identified and implemented should close the gap but additional data is needed to validate this conclusion.

- Production is at 565 kg/day rather than 1,500 kg/day; thus, some work is required to translate the efficiency and costs to those appropriate for a 1,500 kg/day plant that would be directly comparable to the Department of Energy targets. This translation was not shown in the presentation. During Q&A, the PI indicated that the H2A cost of hydrogen is about $2.90/kg hydrogen, which is close to the Department of Energy goal.
- The hydrogen output and efficiency of the prototype plant are good, albeit the hydrogen output capacity is a little short of the target.
- The cost of the plant is not given (proprietary). Hopefully, it is less than the cost of present hydrogen reforming facilities.
- The cost per kilogram of hydrogen is not given.
- Good progress. Very quick identification of heat transfer problem and redesign of plant to correct. Comparison between the performance of the General Motors 5001 and General Motors 5002 will be valuable.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.6** for technology transfer and collaboration.

- The collaboration with catalyst provider and host site were both effective, resulting in a successful project.
- Working with Sud Chemie is appropriate.
- Partnership with a national lab or one of Department of Energy's analysis contractors could be considered. Such a partner could use H2A to help H2Gen translate this project's results to the correct scale and units to compare with Department of Energy's targets.
- It appears that there is essentially no technology transfer or collaborations on this project.
- Sud Chemie's role is not clear.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.1** for proposed future work.

- The future plans are to enter full commercialization, while taking orders now.
- Under timeline, it is indicated that the project is complete.
- Future work does not, but should, include additional efficiency improvements to the process to meet the Department of Energy targets.
- It is appropriate for the commercialization of the product to take place without Department of Energy funding.
- Future work related to ethanol is appropriate.
- The PI expressed difficulty with measuring hydrogen purity at the levels that are currently assumed to be required. While probably not an appropriate direction for this project, work on hydrogen quality/impurity measurement instruments should be considered by Department of Energy.
- Future work is stated, but the project is indicated to be complete.
- Focus on additional fuels is a good direction for future research.

Strengths and weaknesses

Strengths
- The project demonstrated successful implementation of advanced, more expensive catalysts in such a way that supports lowering overall costs of the production while at the same time improving reliability and longevity of the system relative to other commercially available reformers.
- Project has seemingly strong commercialization potential.
- PI is focused on requirements for current hydrogen markets.
- Team has identified bottlenecks in the project and corrected for them in a second generation product.
- Development and demonstration of a low-cost hydrogen production facility.
- Project focus on identifying and correcting engineering issues.

Weaknesses
- It is not apparent that the Department of Energy cost and efficiency targets have been met.

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- It is not clear that the project intends to continue to improve cost and efficiency of the process.
- It is not clear that the team is focused on meeting the requirements of the vehicle refueling market.
- Little technology transfer from the Department of Energy support. Only benefit to the company.
- Very little cost information was presented. It is not clear whether the Department of Energy cost target was met.
- Very little information was presented on operating costs.

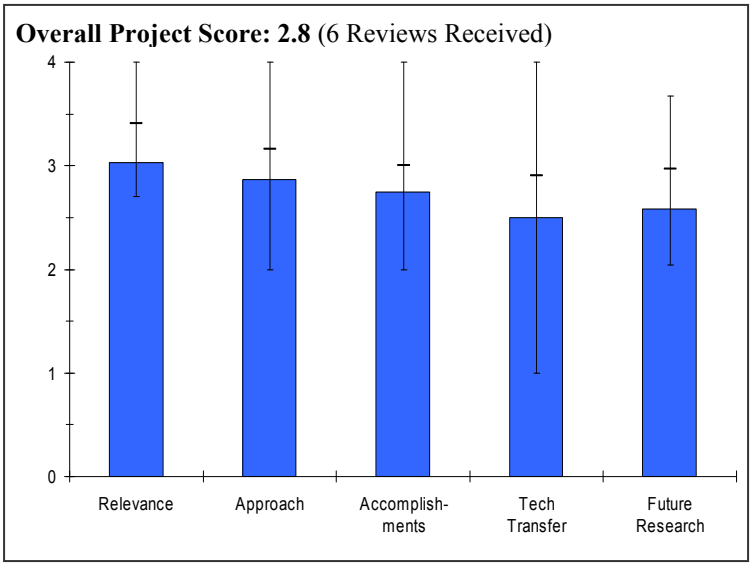
Specific recommendations and additions or deletions to the work scope

- Consider partnering with a National Laboratory or Department of Energy contractor to do H2A cost and scaling analysis.

Project # PD-02: Bio-derived Liquids Reforming
Yong Wang; Pacific Northwest National Laboratory

Brief Summary of Project

The overall objective of this project is to evaluate and develop bio-derived liquid reforming technologies for hydrogen production that can meet the Department of Energy 2017 cost target of <$3.00/gge. The specific objectives for this project are to 1) identify at least one catalyst having the necessary activity, selectivity, and life at moderate temperatures to justify scale-up; 2) provide input for H2A analysis to determine potential economic viability and provide guidance to the research and development; 3) identify and control the reaction pathways to enhance hydrogen selectivity and productivity as well as catalyst; and 4) provide preliminary data for H2A analysis.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.0** for its relevance to DOE objectives.

- How does this technology differ from other advancing ethanol reforming technologies with Virent, National Renewable Energy Laboratory, and Ohio State University?
- Project is within Department of Energy bio-derived liquids to hydrogen mission.
- With cost of ethanol production rising, does this approach still have relevance?
- There is no sense of connection to overall outcomes.
- Excellent, clear and steady presentation style.
- Solid review of reaction pathways and kinetic controls.
- Very clear explanations of the chemistries.
- Relevance is clear; but I'm not up to speed on why the comparisons to (and exploration of) the aqueous phase processes are necessary!
- The availability of inexpensive bio-derived liquid feedstocks is rather questionable (barring advances in conversion of ligno-cellulosic matter); however, given the existence of such a feedstock, the proposed work is reasonable.
- The project studies hydrogen production from bio-derived liquids, especially ethanol. Hydrogen today is made from natural gas, a fuel in short supply and whose price is rapidly increasing. Developing other sources seems "relevant".
- Biofuels are an important part of mix of fuels from which hydrogen can be produced for use in fuel cells. Pacific Northwest National Laboratory provided test results from Rh/CeO_2-ZrO_2catalyst to H2A analysis.
- Work reveals hydrogen can be produced from ethanol for $3/kg consistent with Department of Energy targets.
- In helping to elucidate the reaction mechanism for sugar and alcohol reforming with select catalysts the project supports the goal of reduction in fossil fuel dependency.

Question 2: Approach to performing the research and development

This project was rated **2.9** on its approach.

- H2A cost analysis with $1.07 cost may not be relevant at this time.

- It would be appropriate at this stage in development, now that many variables have been identified, to see a full cost analysis presented with several market contingencies.
- The idea of fuel produced in situ is appropriate, however can enough feedstocks be made available to provide the ethanol?
- Very methodical (almost pedestrian) approach regarding temperature assessments of catalytic activity.
- Need to explore other supports (beyond ZnO).
- Need to explore other metals (beyond Co species).
- What about porosity effects of support structures?
- What next? Need more details on catalyst down-select and other process.
- Approach is ok, but why not study two inexpensive readily available catalyst materials rather than rhodium? (Co-based is fine.)
- Assumptions in H2A analysis are rather questionable.
- The project focuses on two reforming catalysts, one rhodium-based and the other cobalt-based, very conventional formulations.
- Researcher is leader in reforming.
- Researcher has theoretical and analytical and experimental tools to conduct reformer research.
- Pacific Northwest National Laboratory understands role of variables such as space velocity, catalyst and steam/carbon ratio in reforming and their role in achieving project goals.
- I think the project could benefit significantly from collaboration with Ohio State University. Also I am unclear how much of this work is being leveraged by Virent. This likely came out during the Virent presentation which I missed.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.8** based on accomplishments.

- Perhaps the goal can be more clearly stated to find a low cost catalyst with optimal performance.
- Definitely a solid paper with clear process understanding and progress.
- Need to explore more broadly, e.g., effects of different steam/C ratios; does the short-lived methane plan provide insights?
- Need to better understand why the aqueous processes matter in this paper/project.
- The PIs should comment on how reproducible the data are (conversion, stability, etc.).
- Good progress on stability front, but longer durations must be targeted.
- Rather conventional experiments were described, with nothing surprising. Catalysts were synthesized, and reduced in Pacific Northwest National Laboratory laboratories.
- Improved ethanol catalyst by factor of 4. Improved catalyst life through modification of catalyst support.
- Gained further insights into role of side-reactions leading to concepts to further improve hydrogen selectivity.
- Identified dehydration pathway—methane and ethylene production—as the undesirable dead-end of ethanol reforming.
- Reaction either dies or cokes up. Substantial progress made on increasing lifetime of rhodium-CeO_2-MO_2 catalyst.
- Generated good understanding of strengths and weaknesses of Co/ZnO catalyst system and proposed approaches for catalyst improvement..
- The project seems to be on track for meeting the cost targets. The 4x improvement in rhodium life for vapor phase ethanol reforming and the improvements in conversion and selectivity for the APR rhodium with base system are significant steps forward towards achieving the research objectives. However a lot of work still needs to be done to improve catalyst activity and to define optimum reaction conditions to obtain the right balance of selectivity, conversion and reactivation.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.5** for technology transfer and collaboration.

- Collaboration is noted in the presentation, however the identification of individual technology development is also highlighted and it is unclear how the collaboration is working. Virent has their own technology with stated results for aqueous phase reforming.
- Mentioned collaboration (or data-exchange) with DTI and Virent; but what about other learnings (from Ohio State University work? From other parties?).
- How have feedback from DTI, Virent, etc. affected this project?
- Could be better outlined, but on the whole, ok. Good, strong team.
- There were no useful collaborations with catalyst suppliers.
- Collaborating effectively enough with Virent. Ohio State University is working on Co-Rhodium with other supports than ZrO. May need to collaborate more with Ohio State University.
- As stated earlier I think more can be done with Ohio State University and I missed the Virent presentation to better understand how they will use the mechanistic information.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.6** for proposed future work.

- Future plans must consider the effect on the economy of using food based feedstocks for fuel consumption.
- Success in cost reduction highly dependant on ethanol price volatility and catalyst costs.
- Unclear from presentation how the benefits will unfold or when.
- In comparison to other groups' developments and progress, unclear on the benefit of this approach.
- Go/No go decision should be made at this time.
- Not very clear re: major thematic conclusions?
- Would new pressure experiments affect overall process costs?
- Where would the PM versus NPM comparisons lead to?
- What about effects of impurities?
- More detail would have been welcome.
- Perhaps better to focus on less expensive materials.
- Revisit (if possible) H2A analysis assumptions.
- Needs to continue to update and include cost of precious metals in planned work.
- Plans to downselect ethanol catalyst which should be done.
- How does space velocity effect ethanol catalyst life?
- More rigor could be adopted in characterizing changes in surface active sites under varying synthesis and reaction conditions. For instance it would have been helpful to see Raman, x-ray diffraction and TEM studies for pre- and post-reactions.

Strengths and weaknesses

Strengths
- Developing an understanding of catalyst research under certain moderate to low temperature conditions.
- Excellent presentation of process chemistries and understanding of temperature/pressure effects that have been studied.
- Strong team.
- Appear to be hitting targets (perhaps should set more challenging targets).
- Future focus on fundamentals is a step in the correct direction.
- The collaboration with Virent and completion of preliminary H2A analysis demonstrates pre-commercial viability.

Weaknesses
- Lack of clarity of met targets, hard to understand benefit.
- Progress seems slow, but it's possible all efforts were not conveyed in presentation.
- Not clear about why certain alternative catalysts were chosen, e.g., why not Ni-based systems? Why not other catalyst alloys?
- Questionable assumptions in financial analysis (revisit if possible).

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- Need to show reproducible data - why no error bars?
- Need to expand efforts in characterizing the reaction mechanisms.

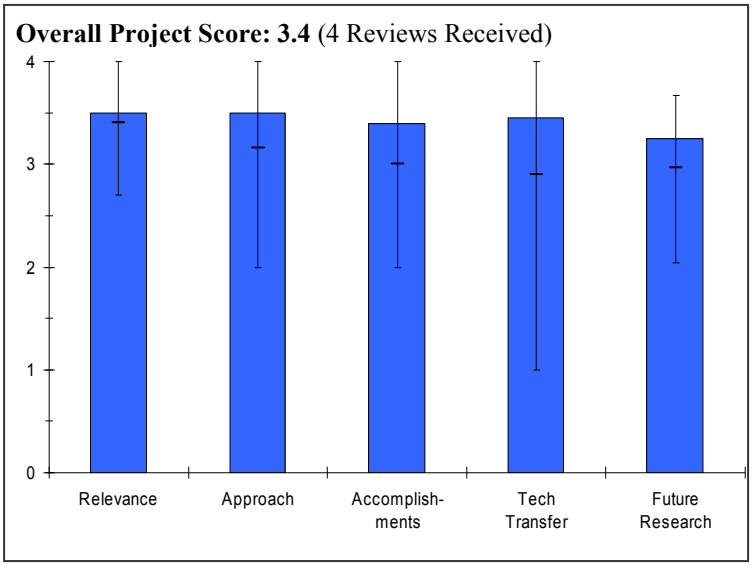
Specific recommendations and additions or deletions to the work scope

- More clarity and milestones with detailed explanation of how this differs from other advancements in this area.
- Tie together performance milestones with progress in the lab. Explain relevance more clearly.
- May want to consider removing the rhodium component if cobalt-based catalysts are more effective.
- Catalyst fabrication is a complicated but well understood technology. There is a vast literature on Fischer Tropsch (FT) Co-based catalysts and a good set of suppliers for these materials. It is critical that well-characterized catalysts are used for a study of this sort, and that data are taken that show reproducibility and catalyst performance degradation. Reduction is essential for activation; however passivation is also essential. The so-called egg shell catalysts would be highly appropriate and work well. Pressured processing will result in chain growth on Co, and those FT-like products should be looked for. It would be good for the Department of Energy to establish codes and standards for all projects pertaining to catalyst preparation, reduction, storage and measurement. If "home brew" catalysts are used, results need to be compared to results obtained using well characterized, commercial materials. Results should also be shown for several preparations of the same catalyst to demonstrate reproducibility. Although reforming ethanol is understood, bioethanol may contain impurities and learning about fuel processing of contaminated ethanol could reward. The reforming reactions are highly energetic, and modeling should include reacting CFD that includes descriptions of 3D temperature profiles. Even small samples can "hot spot".

Project # PD-03: Analysis of Ethanol Reforming System Configurations
Brian James; DTI

Brief Summary of Project

The objectives for this project are to 1) assess cost of hydrogen from bio-derived liquids (emphasis on ethanol); and 2) reflect recent research. This includes interacting with Department of Energy laboratories and contractors. The researchers will supply catalysts composition, performance and potential configurations. The output of this work is 1) system/configuration definition; 2) performance specifications and optimization; 3) capital cost estimation; and 4) projected hydrogen $/kg.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- Assess cost of hydrogen production from bio-derived liquids.
- Ethanol reforming work done at H2Gen, Pacific Northwest National Laboratory, Ohio State University, and other Department of Energy-contractor institutions are considered in this work.
- This project supports hydrogen production R&D by evaluating the cost of distributed production of hydrogen using steam methane reforming of ethanol and recommending R&D pathways that are most likely to meet the Department of Energy goals.
- Distributed reforming of bio-derived liquids is seen as a potentially very important pathway for the transition to the use of hydrogen for fuel cell vehicles and other energy applications. It avoids the need for a large hydrogen delivery infrastructure while providing hydrogen produced from domestic resources with near-zero net greenhouse gas emissions.
- The analysis effort provided by this project is very important to help guide the direction of the distributed reforming research within the Department of Energy Production Program. It provides clear insight as to the cost leverages of the various options being investigated.

Question 2: Approach to performing the research and development

This project was rated **3.5** on its approach.

- Reformer capital costs and reformer manufacturing costs are addressed in this project.
- Department of Energy cost targets are analyzed using experimental data obtained in a number of Department of Energy-funded projects.
- Multiple configurations are examined.
- The approach is effective.
- The assumptions appear to be appropriate.
- The analysis approach being taken is excellent. The project has defined and characterized the distributed ethanol reforming technologies that are being investigated for hydrogen production. DTI is working with all the distributed ethanol reforming projects funded by Department of Energy to gather the information needed for the proper configuration and performance of these technologies. It is using sound analysis and cost estimating tools including HYSYS, DFMA, and H2A.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.4** based on accomplishments.

- Six different configurations were analyzed.
- A critical system level evaluation was carried out.
- The impact of integrated membrane on overall catalyst bed size was evaluated.
- Pros & cons of tubular and annular heat exchange reactor were examined.
- Key assumptions and observations were very well explained.
- Various process configurations have been identified, described, and compared.
- It appears that the project is on schedule and is producing the intended results.
- Excellent progress has been made on this project. The various distributed ethanol reforming technologies and process configurations have been defined and fully analyzed for cost and energy efficiencies, identifying all the key cost leverages. This information will enable the Production Program to properly guide research efforts in this area of hydrogen production.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.5** for technology transfer and collaboration.

- Collaborated and transferred data from Pacific Northwest National Laboratory, Ohio State University, and multiple Department of Energy-contractors (H2Gen, Pall, and Virent).
- DTI appears to be collaborating with most or all of the ethanol reforming projects sponsored by the Department of Energy Hydrogen Program, giving them access to current data on the technology and research.
- DTI is clearly collaborating with all the Department of Energy funded distributed ethanol reforming projects.
- DTI is reporting out on this project through the Department of Energy Distributed Bio-Derived Liquids Reforming Working Group.
- The information being generated by this project is very important to those researching distributed hydrogen production technologies and other hydrogen stakeholders. It is important for the results to reach the full hydrogen community through future meetings and/or through publication.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.3** for proposed future work.

- Since this project is going to end in September 2008, not much was presented for future work, except completing the system comparisons and examining aqueous reforming system.
- This work should be continued in FY 2009 and other options listed on slide #5 should be looked into.
- The system comparisons will allow Department of Energy to prioritize ethanol reforming R&D pathways with the most potential to achieve the targets.
- The proposed future directions appear to be appropriate.
- Future work should include some examination of non-ethanol bio-derived liquids for comparison.
- Emphasis was on wrapping up this project, and little was described beyond tasks to do that.

Strengths and weaknesses

Strengths
- Good background in H2A analysis program.
- Good knowledge of ethanol reforming hierarchy.
- Good collaboration with multiple Department of Energy contractors.
- Collaborations with Department of Energy ethanol reforming projects provide access to the best available data on ethanol reforming processes including membrane reactors, which is very positive since the value of the analysis depends on the accuracy and appropriateness of the parameters and assumptions.

- The process comparisons presented allow objective assessment of potential ethanol reforming pathways and are a valuable tool for decision-makers to identify research priorities.
- Distributed reforming of bio-derived liquids is seen as a potentially very important pathway for the transition to the use of hydrogen for fuel cell vehicles and other energy applications. It avoids the need of large hydrogen delivery infrastructure while providing hydrogen produced from domestic resources with near-zero net greenhouse gas emissions. The analysis effort provided by this project is very important to help guide the direction of the distributed reforming research within the Department of Energy Production Program. It provides clear insight as to the cost leverages of the various options being investigated.
- The analysis approach being taken is excellent. The project has defined and characterized the distributed ethanol reforming technologies that are being investigated for hydrogen production. DTI is working with all the distributed ethanol reforming projects funded by Department of Energy to gather the information needed for the proper configuration and performance of these technologies. It is using sound analysis and cost estimating tools including HYSYS, DFMA, and H2A.
- The PI knows H2A very well and also knows how to use that code very well. Moreover, his presentation and slides were exceptional.

Weaknesses

- Partial oxidation and oxygen transport membrane were not presented; there may be other pathways that should be studied and compared.
- Much of the analysis turns out numbers in the units of dollars. Unfortunately the value of the dollar is rapidly changing, and thus the value of studies that utilize dollars is fuzzy. It might be better to invent some "basket of currencies" that would compensate for this. This is especially important for any project that uses global commodities, steel, copper, etc., and consumes fuels that are traded globally. One could also just invent a "current dollar" unit, and provide a formula to change modify result to "today's" dollars. Better yet, the calculations could be done in Joules or other engineering units, leaving the currency markets for MBA types.

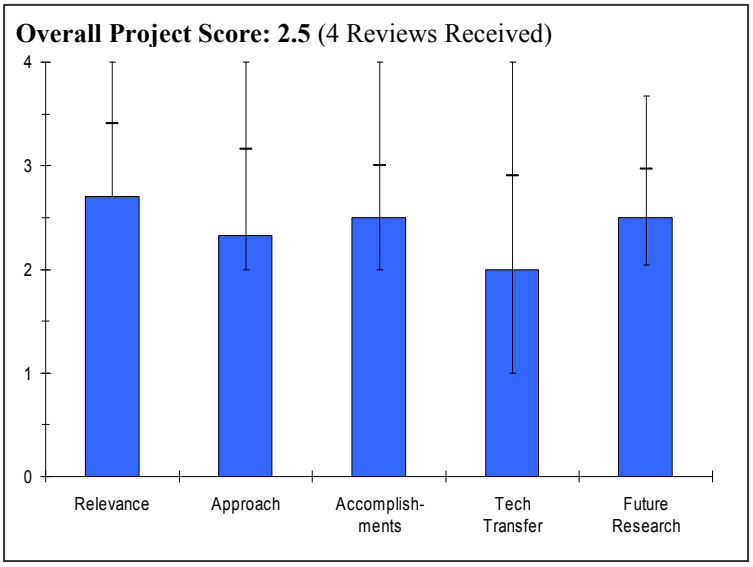
Specific recommendations and additions or deletions to the work scope

- Perform H2A analysis for other options listed on slide #5.
- It is surprising to see the cost numbers very close to each other for most of the options analyzed in this study. Please check for accuracy.
- Include some analysis of other bio-derived liquids besides ethanol for comparison.
- This project should be extended to cover all distributed reforming technologies for all possible bio-derived liquids. This would include; partial oxidation/fast catalysis of bio-oils, mixed alcohols and FT liquids from biomass gasification, and other bio-derived liquids; oxygen transport membrane/water splitting assisted reforming; and any other technologies or bio-derived feedstocks of interest.

Project # PD-04: Pressurized Steam Reforming of Bio-Derived Liquids for Distributed Hydrogen Production
Shabbir Ahmed; Argonne National Laboratory

Brief Summary of Project

The objective for this project is to develop a distributed hydrogen production process 1) from hydrated ethanol and other bio-derived liquids; 2) using a pressurized steam reforming reactor; 3) to develop an efficient hydrogen production/purification process by reducing the hydrogen compression penalty. The rationale for this project is that steam reforming of liquid fuels at high pressure can reduce hydrogen compression costs. In addition, high pressure reforming is advantageous for subsequent separations and hydrogen purification.



Question 1: Relevance to overall DOE objectives

This project earned a score of **2.7** for its relevance to DOE objectives.

- Distributed production scale of hydrogen from ethanol and other bio-liquids (feedstock flexibility).
- Lower capital - liquid compression to obtain high pressure reforming without costs of gas compression.
- Lower capital - production and separation/purification combined in one vessel.
- Higher Yield - removal of hydrogen from reaction vessel provides more hydrogen favorable reaction kinetics.
- The work is attempting to produce hydrogen from ethanol, which is a goal of the Hydrogen Production Program. However, the results do not show much promise for this approach.
- Supports Hydrogen Initiative and Department of Energy RD&D. Rational for the project is that successful results will reduce hydrogen compression costs therefore the cost of hydrogen production. Project did not provide specific target for the cost reduction.
- Reforming ethanol makes little sense. Ethanol is too valuable in fuels to be destroyed to make hydrogen. It would make more sense for the Program to focus more on other bio-derived liquids that cannot be used in motor fuels.

Question 2: Approach to performing the research and development

This project was rated **2.3** on its approach.

- Very early in the development phase of a combined unit operation approach to reforming and separation/purification. The PI has correctly identified the major technical barriers in the pursuit of an advanced reactor/separator single unit operation.
- The project is attempting to conduct ethanol reforming at high pressure – which tends to increase methane production and decreases the hydrogen production. In addition, this increases cost, steam requirements and increases the potential for coke production. Overall, the approach does not appear to have much benefit, and the work does not appear to show any advantages over a lower pressure process.
- The use of high pressure to produce a high pressure product stream does not appear to be reasonable. If membrane separation is used – a low pressure hydrogen stream will be produced. Even if PSA is used – the hydrogen will be produced at a lower pressure than in the reformer and still require additional compression.
- Project approach is focused on the reduction of hydrogen compression cost.
- Technical and economical feasibility of high pressure reforming of bio-derived liquids are main focus areas to achieve the above.

- Project plans to incorporate membrane technology for the removal of oxygen, carbon dioxide and hydrogen toward achieving technical feasibility. This approach may lead to new critical research targets and new collaborations.
- Project at present is not technically feasible unless new membrane technology to remove carbon dioxide is available and will facilitate reaching the technical and economical targets of this project.
- Chose simplest of feeds. Ethanol reforming easier than for other heavier bio feedstocks. Pros/Cons of reforming at high pressure well known. High pressure only has value if easier membrane separator or less costly compression. No work balancing these factors. Should have started with simple studies to choose best pressure.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.5** based on accomplishments.

- Lab run shows >4 mol H_2 /mol EtOH which approaches the 70% energy efficiency goal (according to PI).
- Up to approx 5.6 mol H_2 /mol EtOH predicted with thinner membrane.
- Up to approx 4.5 mol H_2 /mol EtOH predicted with lower GHSV (gas hour space volume).
- Initial indicators are positive in terms of overall energy balance.
- Work appears to have been ongoing for two years (with a one year break).There appear to be relatively few results from the work. Some high pressure work has been conducted, and all the results indicate that the proposed approach has little benefit over a lower pressure process.
- In general it appears that most of the conversion is occurring from the pre-thermal reactions. There is some additional conversion over the catalyst - but this appears to be very limited. Some improvement may result from the added membrane separation - but again, only very limited improvement.
- The project does not appear to be achieving any of the Department of Energy targets.
- The work does not appear to address the cost of constructing a larger scale unit. However, with all the potential problems, it is likely that cost will be well above the Department of Energy cost targets.
- Project is at technical feasibility research phase, and it also seems to be at a Go/No-Go decision point. Experimental data from high pressure steam reforming of bio-derived liquids provided key results for the combined effect of temperature, pressure and space velocity on the hydrogen yield.
- Research results provided key discoveries toward objectives. Results suggest new membrane is needed to remove carbon dioxide to improve methane conversion and to yield high purity hydrogen.
- Proving methane yield up at higher pressure, hydrogen yield lower. Good technical work but not surprising. Program is generating good data but the results are not surprising. Using rhodium, palladium in process. No appreciation that these materials are outlandishly expensive and makes the approach expensive. No analysis of costs. Using expensive feed (ethanol) with expensive materials little step out potential.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.0** for technology transfer and collaboration.

- The project does not have strong collaboration outside the lab.
- Technology transfer appears very limited. No peer reviewed publications are identified. There are some limited presentations. Membranes were obtained from REB – but these appear to be low performance membranes with limited hydrogen flux (less than 10 $cm^3/cm^2/min$).
- Based on project progress status and results, there is a close coordination between PI, other Argonne divisions and REB research & Consulting.
- No evidence of collaboration.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.5** for proposed future work.

- Better performance data with the existing system (repeatability and experience) should be developed before evaluating the impacts of oxygen or carbon dioxide membranes. The PI indicates up to 5.6 mol H_2 /mol EtOH with palladium membrane

- The future work is still focusing on the initial objectives from the start of the project. Little progress has been made.
- The presenter is suggesting alternate approaches such as carbon dioxide separation and oxygen membranes. It is not clear that there would be any benefit of employing these new approaches.
- The PI has planned good future work, based on the critical technical results obtained. Technically and economically feasible transport membranes are critical for this project to reach successful conclusion.
- Need to do more work on analysis. These are well known chemistry and membrane separators. Little to no work looking at costs/effectiveness.

Strengths and weaknesses

Strengths
- Conceptually this is a very economic and efficient approach to bio-based reforming.
- This is a needed engineering project as it is not developing new catalyst or membranes but is building knowledge and experience in the development, design, and operation requirements of systems to produce hydrogen.
- PI demonstrates a very good understanding of the fundamentals.
- Technical feasibility research plan, execution of the technical plan.
- Critical analysis of variables affecting hydrogen yields.
- Identification of critical hurdles, i.e. carbon dioxide and oxygen transport membranes' inclusion in the future research.
- Good experimental data.

Weaknesses
- Scale is very small (0.07 gm/min).
- Need more (repeatability) and longer duration (degradation) runs.
- All of the results presented indicate that the use of high pressure has no benefit and in fact has a deleterious effect.
- High steam concentrations will likely be necessary, which will further increase the cost of this approach.
- Economic targets for the key processes, i.e. high temperature and pressure, transport membranes, catalyst types and quantity.
- Key Go/No-Go decision points.
- Economic feasibility target for the project is missing.
- No appreciation that costs are high due to metals. No analysis of Pressure optimization. Little step out here. Old chemistry, expensive catalysts and separators.

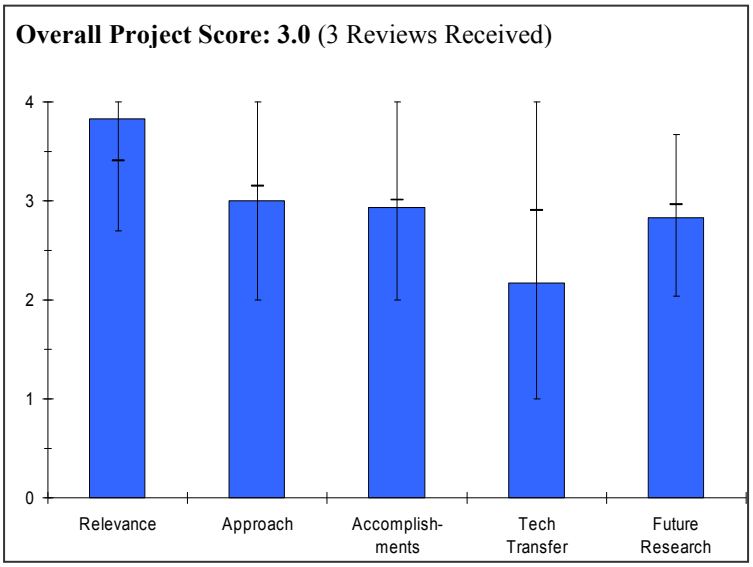
Specific recommendations and additions or deletions to the work scope

- This work needs to be published as it provides barrier indicators to others contemplating or pursuing the combined membrane reactor concept. It also provides design conditions/performance metrics for the membrane system that would be incorporated in such a system.
- Project should include studies with elevated permeate pressure in order to minimize pure hydrogen compression energy requirements.
- Investigate and measure possible ethanol decomposition in the vaporizer section. Develop controls if this is occurring.
- The work does not appear to be making any significant advancement. Department of Energy should consider terminating funding for this effort.
- Cost related key Go/No-Go milestones need to be added.
- Cost dependent technical targets need to be identified and built in to Go/No-Go decision points.
- Go/No-Go analysis for the technical feasibility.
- To be novel and add value it must step out away from ethanol and away from platinum group metals.

Project # PD-05: Investigation of Reaction Networks and Active Sites in Bio-Ethanol Steam Reforming Over Cobalt-Based Catalysts
Umit Ozkan; Ohio State University

Brief Summary of Project

The objective for this project is to acquire a fundamental understanding of the reaction networks and active sites in bio-ethanol steam reforming over Co-based catalysts that would lead to 1) development of a precious metal-free catalytic system which would enable low temperature operation (350-550°C), high ethanol conversion, high selectivity and yield of hydrogen, high catalyst stability and minimal byproducts such as acetaldehyde, methane, ethylene and acetone; and 2) enabling hydrogen production from renewable sources at low cost. Ohio State has identified the active sites and reaction mechanism and characterized the deactivation mechanism.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.8** for its relevance to DOE objectives.

- Non-precious metal catalyst development is necessary for long-term matching of Department of Energy cost targets.
- Renewable ethanol reforming is definitely part of the Department of Energy hydrogen goals.
- Developing a renewable pathway to cost effectively produce hydrogen is critical to the Hydrogen Initiative.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- Iterative approach allows feedback. What is the strategy for long-term selection of material? Inclusion of Doctor Hadad is commendable.
- Use of cobalt catalyst is good.
- Mechanistic degradation studies are very useful.
- Use of molecular simulation may provide interesting information and direction for future development.
- Need to concentrate on operating reforming conditions under more realistic case (lower H_2/EtOH ratio and no dilutent addition).
- Need to investigate effects of impurities on realistic H_2/EtOH ratio. Would the effects be magnified with lower H_2/EtOH ratio?
- Using a PSA recovery of 85% is not realistic due to limitation/requirement on impurity levels in product hydrogen stream.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.9** based on accomplishments.

- Catalyst characteristics work is impressive. Acidity has been correlated to coking (this confirms expectation).
- Reporting conversion of ethanol is not useful. Suggest mol/mal EtOH.
- Investigating lactic acid impurity effects distracts from catalyst development. Stick to one fuel (neat or impure).

- Have made good progress in understanding failure mechanisms.
- Longer life studies need to be done- 100 hours is short, 1,000 hours would be more useful.
- They need to increase the weight hourly space velocity.
- They need to run experiments without dilutents.
- Good progress in catalyst formulation and testing work and the application of H2A model to obtain preliminary cost data. Need to consider testing the catalyst for more extended period of time (more than 100 hours).

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.2** for technology transfer and collaboration.

- Still early in the development process, okay to wait for tech transfer.
- Collaboration with other academics is a positive.
- They have made many presentations and published many papers.
- Collaborations with partners outside of the university are not apparent.
- This project is in its early research stage which does not allow for tech transfer at this point. However, more collaborations with other universities/national labs might be needed to share lessons learned.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.8** for proposed future work.

- Strength: Doctor Hadad simulation.
- Weakness: Engineering test on catalysts that is far from acceptance.
- Catalyst testing under more realistic conditions is needed and planned.
- Proposed research addresses important issues of catalyst life.
- Further testing of impurity effects under realistic H_2O/EtOH ratio is warranted.
- The future work proposed is in line to address the key barriers.

Strengths and weaknesses

Strengths
- Material characterizations.
- They are using a step-wise approach.
- Trying to understand the failure mechanisms is very important.

Weaknesses
- Reporting of reaction results.
- Scope is getting too broad — systems, cost, realistic conditions, time on stream…
- Research has focused on unrealistic conditions.
- They need to increase the weight hourly space velocity.
- They need to operate without any gas diluents and at higher ethanol concentration.
- Increased lifetime studies are needed, or increasing the weight hourly space velocity to do an "accelerated" test.
- Lacks realistic operating conditions so far.

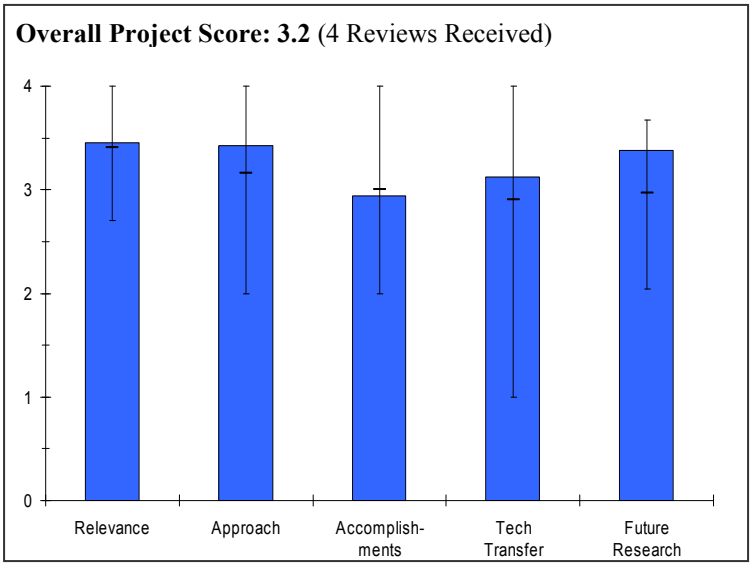
Specific recommendations and additions or deletions to the work scope

- They should de-emphasize system analysis for a catalyst development project.
- Maintain focus on catalyst formulations.

Project # PD-07: Integrated Hydrogen Production, Purification & Compression System
Satish Tamhankar; Linde

Brief Summary of Project

The overall objective of this project is to develop an integrated system that directly produces high pressure, high-purity hydrogen from a single integrated unit. The specific project objectives are to 1) verify feasibility of the concept, perform a detailed techno-economic analysis and develop a test plan; 2) build and experimentally test a proof of concept (POC) integrated membrane reformer/metal hydride compressor system; 3) build an advanced prototype system with modification based on the POC learning and demonstrate at a commercial site; and 4) complete final product design capable of achieving the Department of Energy 2010 hydrogen cost and performance targets.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- Project aligns with needs of Department of Energy Production Program.
- Hydrogen from natural gas or liquefied petroleum gas using a membrane reactor and thermal compression.
- Lower capital – combined unit operations.
- Lower energy – thermal compression with reformer heat.
- Higher Yield – removal of hydrogen from reaction vessel provides more hydrogen favorable reaction kinetics.
- The feedstock flexibility, reduction in parts counts, high hydrogen purity and elimination of compression steps all help to move the Program Multi Year Plan forward for achieving the cost and efficiency targets for hydrogen production and moves us closer to reducing dependence on foreign oil.
- Very relevant in the area of low cost hydrogen production, process intensification and flexible feedstock capable reformer.

Question 2: Approach to performing the research and development

This project was rated **3.4** on its approach.

- Approach is very good.
- The approach combines good engineering and pilot scale testing to the complex integration of two systems membrane reactor and thermal compressor.
- The project has done well to incorporate Design For Manufacturing and Assembly (DFMA) concepts even in the current POC stage.
- The approach to minimize system components and process intensification is well in line to address the key cost barriers.
- It appears the operational issues the PI has faced so far might be contributed by an integrated approach which might not have allowed for much flexibility and controllability.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.9** based on accomplishments.

- Consider third party economic modeling of systems costs and comparing with other technologies.
- The heat exchanger shown is very novel and should be looked at for synergies in other parts of the Hydrogen Program. Also recent work with neutron analysis (analyzing fluid flow during operation) can be used to optimize design.
- Consider long-term verification testing to demonstrate robustness of system.
- Achieved conversions that were 55-60% lower than target, however system modifications (optimizing membrane to change reaction equilibrium) theoretically brings this up.
- Manufactured multi-stage, dual-line hydride heat exchanger fabricated for continuous operation.
- The fabricated equipment and pilot scale of this project provide valuable data and operational experience.
- The reduction in part counts, the ease in which the fluidized bed membrane can be modified or repaired, the leveraging of heat and mass balance all will hopefully contribute to the fully integrated system meeting the efficiency and cost goals. Further, the use of multiple feedstocks with varying levels of impurities needs validation.
- Comparing the updates of last year to this year, the PI has faced with various operational issues to get the integrated system up and running. The PI so far does not have a great deal of operational data to report.
- The issues with membrane stability, startups/shutdowns, and the ability to recover hydrogen from permeate and retentate steams to allow for 100 bar pure hydrogen remain.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.1** for technology transfer and collaboration.

- Linde is a commercial developer. I do not know if Linde plans to create a business unit to supply the technology (a plus) to the market or use it internally for their own hydrogen business development (a minus - since this would slow the market adoption).
- Linde is working closely with the membrane developer.
- Linde is working closely with the thermal compressor developer.
- Collaboration includes MRT and Ergenics Corp.; would have been helpful to partner with a university as well.
- Good collaborations with membrane and hydride compressor partners.
- Might need to have independent third party look at the hydrogen cost.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.4** for proposed future work.

- Future plans and Go/No Go decision points clearly delineated.
- Testing of the hydride compressor in-situ will provide valuable, practical data and experience.
- A previous goal was to reduce the membrane thickness but tests have shown that pinholing was a problem so settled on 25 microns. Also the modularization of the fluidized bed membrane demonstrates systematic progression.
- Go/no go decision on next phase should also consider a run hour target that the system must achieve (without performance loss) and a full analysis of the impurities in the product hydrogen stream to confirm that it meets fuel cell grade (current 50 ppm on some impurities might be too high).

Strengths and weaknesses

Strengths
- The system is built from off the shelf components.
- Novel heat exchanger.
- The scale of this project provides a very good basis for testing and collecting performance design data and building economic models (particularly compared to the many lab / table top projects).
- Good run times (>100 hrs), good experience gained.
- This is really two projects in one: membrane reactor combinations and the integrated hydride compressor.

- The collaboration appears to be a mutually beneficial partnership.
- A good pathway/approach to reducing capital cost.

Weaknesses
- Limited testing for 100 hours.
- System sensitivity to impurities not addressed.
- The project depends on good membrane performance, tolerance to coking and life. Longer runs are needed.
- Still have not validated integrated system.
- The unintended consequences of the integrated approach might be increased control complexity; durability/lifetime issues (increased operating costs).

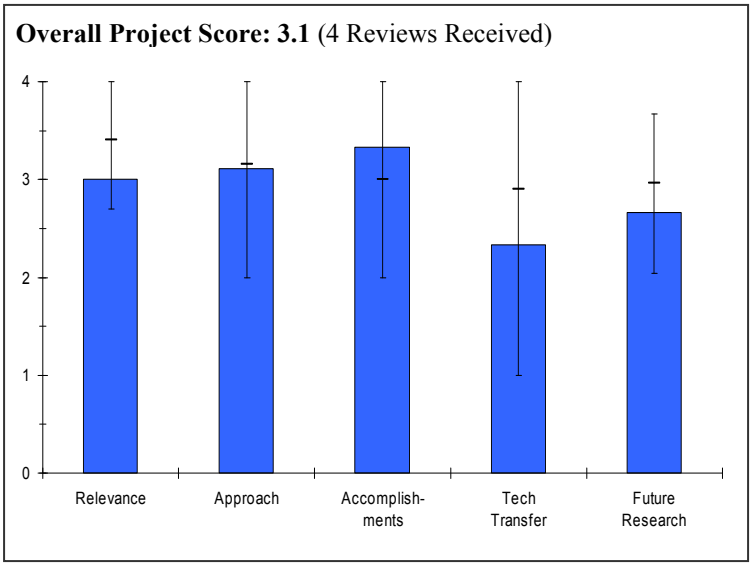
Specific recommendations and additions or deletions to the work scope

- Consider adding economic analysis and energy balance for process under development.
- Complete integrated installation (i.e., installation of the hydride compressor) and obtain run times >100 hours.
- Need to set a run hour target that the system must achieve (without performance loss) before moving to next step.
- Conduct a full analysis of the impurities in the product hydrogen stream to confirm that it does meet fuel cell grade (current 50 ppm on some impurities might be too high).

Project # PD-08: Zeolite Membrane Reactor for Water-Gas-Shift Reaction for Hydrogen Production
Jerry Y.S. Lin; Arizona State University

Brief Summary of Project

The overall objective of this project is a fundamental study for the development of a chemically and thermally stable zeolite membrane reactor for water-gas shift reaction for hydrogen production. The specific project objectives are the 1) synthesis and characterization of chemically and thermally stable silicalite membranes; 2) experimental and theoretical study of gas permeation and separation properties of the silicalite membranes; 3) hydrothermal synthesis of tubular silicalite membranes and gas separation study; and 4) experimental and modeling study of membrane reactor for water-gas shift reaction.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.0** for its relevance to DOE objectives.

- The objective was to increase yield & lower capital costs. This could be done by removal of hydrogen via membrane from reaction vessel provides more hydrogen favorable reaction kinetics.
- The work was on developing a membrane for separations.
- The work is focusing on the development of a hydrogen separation membrane for use with the water-gas-shift reaction. This is a need for hydrogen production and addresses both hydrogen separation and process intensification. The work supports the Department of Energy Hydrogen Program objectives.
- Unfortunately, the approach will not produce a high purity hydrogen stream (or a high purity carbon dioxide stream). The best H_2 separation factor appears to be around 65 (with reasonable permeance - although below the target level). It is highly likely that a subsequent polishing step will be required and this may have a large impact on the overall cost.
- If other impurities are present in the stream (for example - sulfur), this will also diffuse through the membrane to some extent and additional clean up steps may be necessary for both the hydrogen and carbon dioxide streams.
- Project supports critical cost reduction goal of distributed hydrogen production from natural gas and renewable liquids.
- Project qualitatively anticipates that successful results will achieve Department of Energy hydrogen production cost targets.
- Specific project targets need to be provided toward achieving hydrogen production cost targets i.e., $1.60/gge at the plant gate by 2012.
- Material development in the photoelectrochemical arena is clearly relevant, especially if such materials could improve over photovoltaics/electrolyzer systems (not sure why funding by Department of Energy is inconsistent).
- Use of iron oxide alloys is a good start, but not particularly innovative and mixed oxides may not have been considered early enough.

Question 2: Approach to performing the research and development

This project was rated **3.1** on its approach.

- Approach is to modify zeolites. Researchers keep working with zeolite which is 25 + years old. What are needed are new materials and structures.
- The microwave synthesis and CVD for membranes may be applicable to hydrogen production from other materials.
- This is a fundamental university/academic effort that will provide a moderate purity hydrogen product. This is a reasonable project for a university and the work appears to be obtaining some good data and results.
- The hydrogen purity will be somewhat low. Department of Energy was probably aware of this when the project was selected.
- It is highly unlikely that the work will provide significant data to evaluate scale-up.
- Good technical project plan.
- Technology seems to be technically feasible. Cost analyses needs to follow to validate that the successful technical results yield significant reduction in hydrogen production toward achieving Department of Energy cost target.
- Solid, systematic approach and selection criteria.
- It is not clear how the materials selection process leads to practicable large-scale reactions.
- It is not clear how the different morphologies lead to different properties, except for area and path length effects.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.3** based on accomplishments.

- The experimental zeolite selectivities (hydrogen separation factor - H_2/CO_2) are 50, compared to 20,000 for palladium. This low separation factor will require multi-stages or other equipment (both adding costs) for down stream hydrogen purification.
- The work has led to some advancement in membrane preparation (CVD and microwave techniques). The performers have prepared tubular membranes and have conducted a number of tests with the prepared membranes. Thin active layers - 3 micron - have been prepared on supports.
- Testing has been conducted with gas mixtures and has shown the ability to achieve separation. Including water in the feed was also an important factor.
- The work has been flexible enough to change the membrane composition when the original materials performed lower than expected.
- Tests have indicated that the membranes are resistant to sulfur compounds and this is an important factor for membrane lifetime.
- The work has identified some new water-gas-shift catalysts with about the same performance as commercial materials.
- The work has demonstrated separation above Knudsen separation levels, which demonstrates that some form of selective adsorption is in effect.
- Project accomplished majority of its Phase 1 milestones.
- Project reported good results and accomplishments towards technical milestones.
- Progress report on Department of Energy barrier for the hydrogen cost reduction as a result of the technical accomplishments needs to be clearly discussed.
- Targeted hydrogen selectivity of 50 will potentially provide significant reduction in hydrogen production cost. Project objectives should include resulting economic accomplishments.
- High throughput screening achieved.
- Somewhat Edisonian approaches to processing and synthesis methods which led to different hematite phases but similar to XRD's - why?
- Not clear why the different surface treatments lead to different IPCE's (and whether such structural variations are metastable).

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.3** for technology transfer and collaboration.

- The researchers need some industrial partners, currently it is composed of only university partnerships.
- The performers have been very active in publishing the results of their work and indicate 36 publications - many in peer reviewed journals.
- The project lacks any input from industry. All of the participants are academic. It would be a major benefit to collaborate with an industry partner to get a commercial perspective. It is unlikely that any commercial product will result without this type of collaboration.
- Project progress report suggests that there is some coordination between collaborators.
- Although a member of the photoelectrochemical working group, the paper does not show clear collaborations with theoreticians for Density Functional Theory (DFT) modeling, nor with the other teams.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.7** for proposed future work.

- The project needs to directly address the overall production of hydrogen using the membrane/reactor system.
- The project needs to show membrane performance targets that directly relate to economic hydrogen production and purification.
- The work is following the original work plan and appears to be on schedule. The future work will evaluate the membrane separation under water gas shift conditions - which was the objective of the project.
- The near-term work should consider testing at higher pressures. Pressure could have a significant impact on the separation factor.
- Plans are exclusively for the technical improvements of the proposed technology.
- Economic feasibility and addressing Department of Energy hydrogen production-related cost reduction targets need to be included in project's future milestones.
- Recognition that hematite modifications may not be fruitful?
- Move to other mixed oxides appropriate.
- Need for continued post-processing modifications; but there must be attempts to correlate performance to structural changes due to such surface modifications.

Strengths and weaknesses

Strengths
- It appears to be a very good academic team, strong fundamentals in zeolite structure and chemistry.
- They have expanded the current vast body of knowledge on zeolite use in membranes and have designed a reactor test unit to hold a tubular membrane.
- This is a good academic scale project that is providing some solid fundamental information.
- Synthesis and modification of silicate membranes for separating hydrogen and carbon dioxide produced by water-gas-shift reaction.
- Research and analysis of technical feasibility of silicalite and DDR Zeolite membranes.
- Production of silicalite membranes with high H_2/CO_2 perm-selectivity, potentially over 50.
- New water-gas-shift catalyst with improved chemical stability for sulfur dioxide and hydrogen sulfide.
- Solid, systematic piece of work.
- Clear progress on showing changes to surface area, path lengths, and effects of electrocatalyst additions.
- While only conceptual, the project discussed reaction design process.

Weaknesses
- Membrane hydrogen selectivity is low at 50.
- They need to envision and model the entire system. What equipment and costs will be required to obtain commercial hydrogen purity if this membrane is used?
- Ultimate system scale (area per unit of hydrogen) is likely to be high and costs need to be determined.
- 10 atm operating pressure will limit tube diameter/design and likely increase costs.
- The work needs to address the final potential costs. This should be done with an industry partner.
- There will be a problem with the hydrogen purity if it is to be used with a fuel cell.
- Comparison with other existing and on-going similar technologies in terms of technical and economic advances.

- Economic analysis of the accomplished technical advancements.
- Milestones related to the hydrogen production cost are not included.
- No clear guidance from theoretical calculations (DFT).
- Somewhat singular focus on the hematite systems.
- The project needs new hosts.

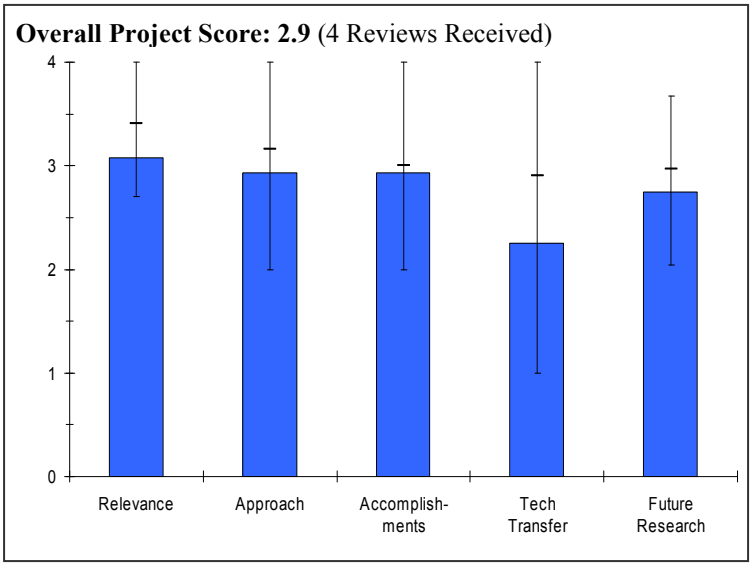
Specific recommendations and additions or deletions to the work scope

- A back of the envelope calculation of total equipment needed and costs to meet hydrogen purity requirements should be performed. A calculation of the "practical" selectivity and permeability values should be made and the project should address the barriers that must be overcome to reach those practical values.
- Project needs to focus on the membrane reactor system and product purity requirements. Currently the focus seems to be mostly on membrane fabrication.
- Multi-lumen tubes are a geometry that can boost area while lowering costs. This may be an option to bring zeolite membranes into practical/economic operating ranges.
- Include examining the effect of increased pressure as soon as possible.
- Cost reduction-related milestones need to be added.
- Discussion and analysis of project results and targets in reference to other similar technologies in terms of technical and economical advancements.
- The project should include Go/No-Go decision points to address key technical and economical milestones.
- The project should move to mixed oxides (ternary systems).
- The project needs to secure consistent funding support.

Project # PD-10: Low Cost, High Pressure Hydrogen Generator
Monjid Hamdan; Giner Electrochemical Systems LLC

Brief Summary of Project

The overall objective of this project is to develop and demonstrate a low-cost, moderate pressure proton exchange membrane water electrolyzer system that 1) reduces stack capital costs to meet Department of Energy targets; 2) increases electrolyzer stack efficiency; and 3) demonstrates 1,200 psig electrolyzer system. The objective for the past year was to field test the electrolyzer system at the National renewable Energy Laboratory. Further development of a high-strength, high efficiency membrane is recommended. Development of a low-cost, long-life separator is required.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.1** for its relevance to DOE objectives.

- Design & Development of PEM electrolyzers is an important area, not just for water electrolysis, but also for application in thermochemical cycles.
- Clearly a relevant project, but there are already proton exchange membrane-based electrolyzers that are commercial (e.g., the DESC systems-the "old" Proton Energy systems).
- The project needs to clarify why the Giner approach is different from those of Proton and Stuart, and others.
- While the objectives are relevant, the project seems to be limited to bringing Giner Electrochemical Systems, LLC up to cost parity with others in the proton exchange membrane electrolysis community and towards parity with alkaline technology.
- To be significantly relevant, the technology must be economically scalable to hydrogen production rates several orders of magnitude higher than is being addressed.
- Electrolysis is one of the key current hydrogen production methods for decentralized hydrogen (no major hydrogen infrastructure required).
- Decreasing capital cost and improved efficiency (two major barriers) are addressed by this project.
- Cost of electricity is a major issue to economic deployment. The Giner Electrochemical Systems, LLC proton exchange membrane stack electric cost is projected to be 30% less costly.
- Validation of the improved stack performance has been completed at National Renewable Energy Laboratory.
- The 2007 testing has generally achieved the Department of Energy targets for distributed water electrolysis.
- The capability to meet the 2012 and 2017 Department of Energy targets was orally discussed.

Question 2: Approach to performing the research and development

This project was rated **2.9** on its approach.

- Nice job. Especially in enhancing efficiency and complexity of components while simultaneously improving components' performance.
- The technical approach provides a good pathway to show the improved performance of the advanced membrane and overall electrolysis cell.
- This is the end of the current program – additional experimentation and required scale-up will be performed under a new contract.

- Reducing complexity of the system through parts-count reduction. Simplified anode/cathode side membrane support structure fabrication by reducing assembly from nine parts to one single piece. Incorporated thermoplastic cell frame - molding process reduces cell cost by 40%. Total cell stack reduction of 40+ parts to sixteen parts.
- Developed lower-cost materials and fabrication methods for cell components, increased operating current density and systems innovations to replace high cost, high maintenance components. National Renewable Energy Laboratory validation testing of cell has not included DSM in last test campaign.
- The approach does not address life, durability or scale-up questions of the membrane/cell.
- The choice of 1200 psig operating pressure seems arbitrary, without a rationale.
- Good breakdown of where the improvement could be made component-wise, but where are the major innovations?
- Titanium separation example is good; but need to explain its limitations.
- Support structure for 2-mil "Nafion" is meaningful only if the system is subject to cyclic testing - steady state tests will not reveal weaknesses such as de-lamination, etc.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.9** based on accomplishments.

- They reported very good progress, one question is why large difference between the Giner Electrochemical Systems, LLC tested cell performance & the stack performance?
- They demonstrated advanced membrane in 160 cm^2 cell and demonstrated 28 cell unit that produced 0.25 kg/hr at 1200 psig at National Renewable Energy Laboratory.
- National Renewable Energy Laboratory validation testing of cell have not included DSM in last test campaign.
- Short term results are better than comparison cell – potential improved performance at lower pressure and lower cost – limited information provided on National Renewable Energy Laboratory tests.
- Additional data is needed, including longer term durability operation.
- Further scale-up is required (possible two cell area scale-ups).
- Use of thermoplastic and molded components has been practiced by other companies already.
- Use of thinner membranes has been done before.
- DSM approach has not been thoroughly checked out, relative to long-term durability.
- The Program seems to have advanced Giner Electrochemical Systems, LLC proton exchange membrane capability, but has not advanced the state of the art.
- Advancements of membrane life and system costs are based on analysis/claims/projections and not demonstrated performance.
- The operating pressure is not significant.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.3** for technology transfer and collaboration.

- It's not clear that the accomplishments indicate a successful team.
- General Motors and Center for Technology Commercialization are partners. General Motors has provided membrane information and expertise on other components. Nothing mentioned about scale-up or mass manufacturing.
- The role of other partners is not clear (General Motors was a cost-share partner and helped with bipolar plates and membranes; but General Motors' interests are in fuel cells, not electrolyzers.) Center for Technology Commercialization role is unclear.
- Not sure if further tech transfer programs are being conducted.
- There is no evidence of outside collaboration other than cost sharing.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.8** for proposed future work.

- Development of new membranes under the new grant is a step in the right direction.
- This is the end of the current program - additional experimentation and required scale-up will be performed under a new contract.
- The performer identifies that work will be continued to develop the lower cost, high efficiency membrane with emphases on continued reduction of stack capital cost and stack scale-up to a 290 cm^2 active area.
- Giner Electrochemical Systems, LLC acknowledges and identifies areas that need progress, but a significant portion only brings Giner Electrochemical Systems, LLC proton exchange membrane to cost parity with others.
- Longer duration runs will be performed.
- The program details are not discussed.
- Program is complete.
- Need greater clarity as to: Giner productivity more for the market places? Beyond National Renewable Energy Laboratory testing, what next?

Strengths and weaknesses

Strengths
- Development of improved components. Meeting major milestones.
- Approach to reducing capital cost of the electrolysis cell membrane system by reducing separate parts is an excellent approach.
- Experimental cell valuations appear to be making good progress.
- Costs are expected to be lower – particularly electricity cost, which is a major concern with distributed electrolysis.
- Based on the progress reported, Giner Electrochemical Systems, LLC appears to have the technical competency required to eventually complete the work.
- Well explained.
- Good component-by-component improvement.

Weaknesses
- Stack performances were much lower than cell performances and the differences were not explained?
- Electrolysis requires inexpensive electricity to meet the Department of Energy target goals.
- Need more details on National Renewable Energy Laboratory evaluation and future work.
- Still needs additional experimentation and scale-up to validate 2010 Department of Energy target.
- The project starts out behind the state-of-the-art and behind other technologies and has not yet caught up or advanced.
- The PI needs to develop "system-integrated" improvement plans.
- The PI needs to clarify the roles of partners and how active were the collaborators in this program.

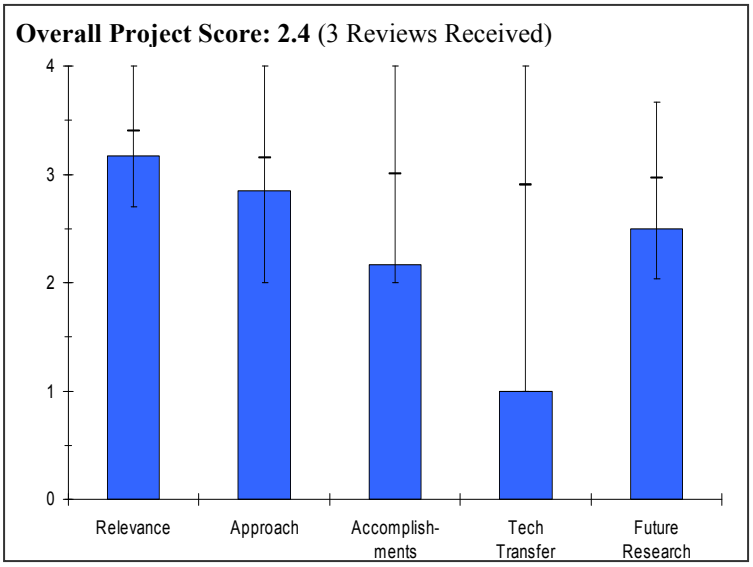
Specific recommendations and additions or deletions to the work scope

- If the project is to be continued, high emphasis needs to be placed on membrane durability and life.
- Operating pressures should either be lowered to 100-400 psi or raised to greater than 5,000 psi.
- Water electrolysis programs (to make sense) must be tied to possible direct DC renewable sources. Otherwise, water-electrolyzers are indeed items in commerce already.

Project # PD-11: Hydrogen Generation from Electrolysis: 100 kg H_2/day Trade Study
Stephen Porter; Distributed Energy Systems

Brief Summary of Project

The objectives of this project were to 1) establish a pathway to larger proton exchange membrane systems (100 kgH_2/day with growth to 500 kgH_2/day); 2) optimize for capital cost and energy efficiency (emphasis on cell stack and power supply); and 3) refine focus area for future research. Proton Energy Systems performed trade studies and made a conceptual design of a 100 kgH_2/day electrolyzer.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.2** for its relevance to DOE objectives.

- The work supports the Hydrogen Initiative to a limited extent.
- Economic scale-up, not technology, is a major hurdle for water electrolysis to produce hydrogen. Proton Energy Systems builds and sells commercially 12kg/day hydrogen production units into niche markets. Project addressed scale-up (value-engineering) of their systems for the distributed hydrogen fuel market.
- Proton exchange membrane electrolytes – good topic for R&D; useful for water electrolysis and for thermochemical cycles.

Question 2: Approach to performing the research and development

This project was rated **2.9** on its approach.

- Have identified barriers, but the barriers are not new. High capital cost, low system efficiency, difficult integration schemes with renewable electricity generation system are some known barriers.
- Not much suggestion on how to overcome the barriers.
- No suggestion that is new and different from known efforts to overcome the barriers.
- Very linear engineering process approach to scale-up. Would have been nice to pursue some 'what ifs', which really go outside the envelope.
- The approach adopted is good.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.2** based on accomplishments.

- The work scope was rather limited.
- The presentation materials are confusing. It appears the electrolyzer capital cost in 2011 is 1,676 $/kW and the Department of Energy target for a scaled-up unit in 2012 is 400 $/kW. No discussion or explanation given how the Department of Energy target can be accomplished in one year.
- Identified the integration of optimal power supply and cell stack designs (stack size and operation in series) as the key trade-offs.
- Final results do not meet Department of Energy 2012 targets in terms of energy efficiency, hydrogen cost or capital costs.
- Good accomplishments though efficiency appears to be low.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **1.0** for technology transfer and collaboration.

- This information is not available in the presentation. It is assumed that most work is done at the sponsoring organization.
- Optimization of their own technology, in-house.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.5** for proposed future work.

- This project is complete; future focus areas are relevant.

Strengths and weaknesses

Strengths
- Project is COMPLETE.

Weaknesses
- Project is COMPLETE.

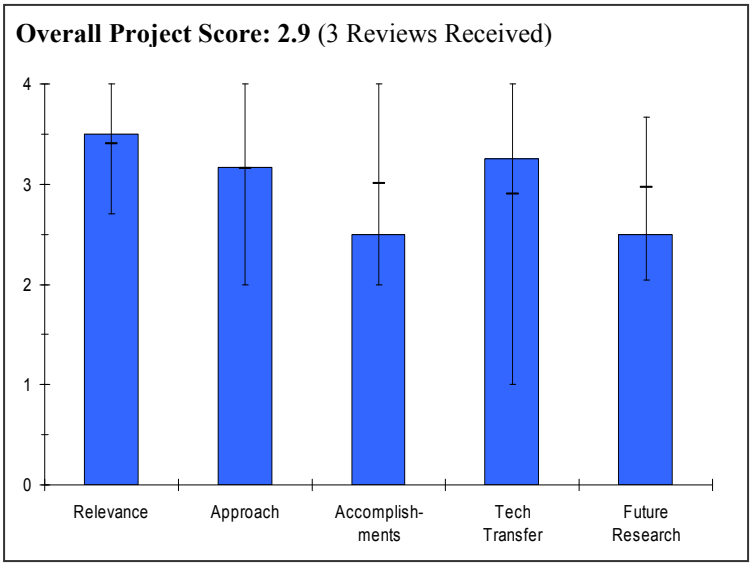
Specific recommendations and additions or deletions to the work scope

- Project is COMPLETE.
- Future work should also include membrane/catalyst work to enhance efficiency (if possible).

Project # PD-12: Development of Water Splitting Catalysts Using a Novel Molecular Evolution Approach
Neal Woodbury; ASU

Brief Summary of Project

The objectives of this project are to 1) design and synthesize a peptide based electrocatalyst for water splitting using principles learned from photosystem II; 2) optimize the function and stability of this electrocatalyst through iterative creation and analysis of libraries; and 3) develop efficient water splitting catalysts required for effective electrolysis. Arizona State has designed metal binding peptide to use as starting sequences and has demonstrated the utility of light directed synthesis methods for creating libraries of peptides. Additionally, electrochemically directed synthesis of peptides with a limited number of side chains has been developed.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- The use of biological and biologically inspired materials holds a lot of promise for new materials for water splitting.
- This work uses a novel approach to develop manganese-based water splitting catalyst systems and is in line with Department of Energy objectives.
- The project appears relevant, but the presentation lacked information on why this method is better than existing methods.
- The project aligns well with the President's Hydrogen Fuel Initiative in its effort to develop an efficient catalyst for splitting water into hydrogen and oxygen.
- It is expected that the catalyst coating on an electrode will help drop the required voltage of 2.2 volts of electricity required to produce hydrogen to 1.3 or 1.2 volts, which would be an energy savings of 40 percent.
- This aligns well with the overall Department of Energy goal to produce hydrogen at lower cost.

Question 2: Approach to performing the research and development

This project was rated **3.2** on its approach.

- The milestones and technical barriers are clearly laid out for the project.
- They have integrated high throughput methods to address a focused issue of creating and understanding a metal cluster binding environment and associated activity.
- They have abandoned light directed synthesis in favor of chip based combinatorial synthesis which has allowed the project to move forward.
- Approach seems logical. The CombiMatrix approach allows direct synthesis on addressable electrodes.
- The technical approach is logically laid out through six milestones to develop improved catalysts.
- By observing nature where photosynthesis catalysts aid the conversion of carbon dioxide in the air into sugars, the project team is evaluating potential manganese-based catalysts.
- Peptides will be used to develop an array of material combinations as potential catalysts. The best catalysts should be selected and tweaked for further testing and development.

PRODUCTION AND DELIVERY

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.5** based on accomplishments.

- They have made some progress towards addressing their project goals.
- They have not yet shown water splitting and it is not clear just how close they are to achieving this goal.
- They have borrowed and successfully integrated chip-based chemistry with computer aided design to create libraries, which can be used to probe interactions well beyond their initial manganese cluster concept.
- To date, there are not a lot of results.
- Net result: no difference between control and test peptides with no explanation if this is a good or bad result.
- Progress is satisfactory on the establishment of a baseline for evaluation.
- Encountered challenges with chemical deposition methods of catalysts on electrode surfaces.
- Developed an alternate method for deposition based on electrochemical synthesis.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.3** for technology transfer and collaboration.

- They have demonstrated collaboration with chip manufacturers and addressable electrode system manufacturers.
- There is one non-governmental partner (CombiMatrix Corporation) and one academic partner. Technology transfer into a commercial venture might occur through CombiMatrix, but it is unclear if this company is large enough to secure private sector financing and implement product development, manufacturing, and sales/marketing.
- Significant R&D may be needed before this concept becomes commercially feasible and attractive for investors.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.5** for proposed future work.

- They have identified an approach for the synthesis, and the future work will focus on resolving some of the teething issues with the new technology (side chain effects, surface preparation, synthesis approaches).
- It's not clear how this will lead to advancements.
- The proposed future research appears sufficient to reach the milestones.
- Given that this work is fundamental, the final end product should be more clearly defined to determine if further research in this area is warranted.

Strengths and weaknesses

Strengths
- They have developed a rich platform technology that can be applied to focused combinatorial screening of structure function relationships.
- Good approach to testing large numbers of samples.
- The project PI is aware of current issues facing his research efforts, e.g. the instability of the electrode surfaces to chemical synthesis procedures, and he is developing alternate synthesis methods.
- Teamed up with CombiMatrix and Dr. Bill Armstrong for help and guidance on the use of electrochemically directed synthesis (as opposed to light-directed synthesis in their original plan).

Weaknesses
- It is not clear that this approach and the results achieved so far will allow this team to achieve a viable water splitting device.
- In particular, the new approach shows no difference between control and test peptides +/- manganese.
- There was not enough in the presentation discussing the potential impacts of this work.

- The effort to understand, replicate, and translate a natural process catalyst that facilitates the conversion of carbon dioxide into sugars into a usable coating on an electrode to aid water spitting is somewhat ambitious to be accomplished within the remaining one year timeframe.

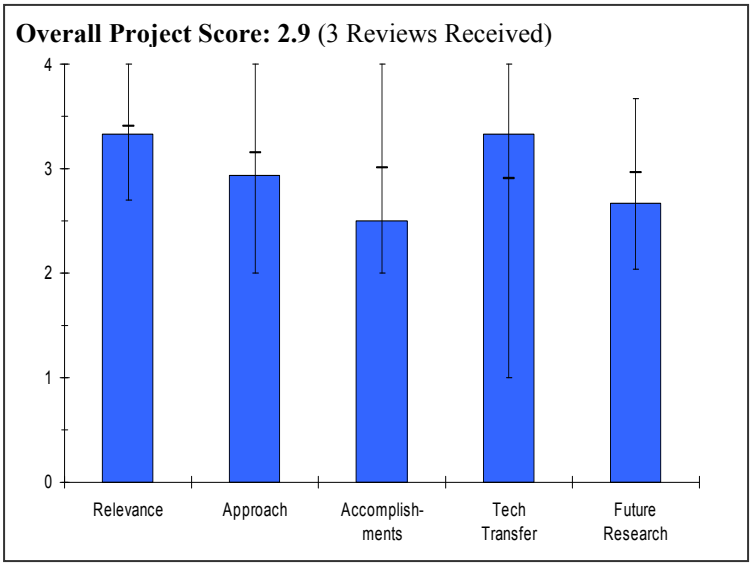
Specific recommendations and additions or deletions to the work scope

- Some Go/No-go criteria should be established to determine if this concept warrants further investigation. The concept itself appears reasonable, but other competing technologies within the entire spectrum of hydrogen production might render this approach (and hence this research effort) unwanted.

Project # PD-13: Development of Solar Powered Thermochemical Production of Hydrogen from Water
Nate Siegel; STCH Collaboration

Brief Summary of Project

The overall objective of this project is to select one or two cost competitive solar powered hydrogen production cycles for large scale demonstration. The specific objectives of this project are to 1) develop solar receiver concepts; 2) perform experimental validations of the key components of prospective cycles; and 3) produce economic models of all prospective cycle using a common methodology and assumptions. The feasibility studies are progressing and the solid particle receiver has been demonstrated. Other receiver concepts are nearing demonstration and the H2A analysis is underway.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- Thermal chemical water splitting for hydrogen production is within the Department of Energy Hydrogen Program project portfolio.
- The project addresses the application of solar thermal energy to the production of hydrogen.
- It does not appear to be on a critical pathway, even within the production/delivery portfolio.
- Making hydrogen from high temperature heat must be of interest.

Question 2: Approach to performing the research and development

This project was rated **2.9** on its approach.

- They developed the different chemical cycles to the point where a techno-economic analysis could be made which was used in the down-selection process.
- The development focused on cycles, materials and reactors, which are the correct areas.
- Consideration should be given to decreasing operation and maintenance requirements.
- More work should be done on long-term stability.
- The project appears to address the barriers, especially U and X.
- The project appears to be doing a good job at integrating work that is being done at several facilities.
- It appears that the selection of possible cycles was made at an earlier date. It would have been helpful to review the criteria used and to discuss how each of these materials meet the criteria. For example, was mechanical strength an issue, or particle density? How about particle size? Thermo?
- What will be the criteria used in the Go/No Go decision on continuing work with any given thermochemical cycle?
- STCH has assembled an excellent collection of collaborators, continuing work on an old, and well-studied problem. The current emphasis is a design-to-cost effort, with some laboratory scale exploration of key unit operations. As before, projected unit operations remain technically challenging.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.5** based on accomplishments.

- Technical progress has been made on developing the different cycles, but after five years, more progress would be expected.
- H2A analysis has been done on several of the cycles; it needs to be done on all of the cycles.
- The H2A analysis should include operation and maintenance and spent material disposal costs.
- Standardized method for calculating efficiency needs to be made.
- Materials development for the reactors and receivers needs to be addressed.
- Material degradation and long-term stability need to be investigated.
- It appears that smaller particles give better performance; what is the limit envisioned in terms of handling fine powders?
- Because so many cycles were being developed, it was difficult to assess progress in any one area or with any specific material. It would have been more helpful to focus on one material as an example and treat in depth, in order to provide the reviewer with a better understanding of the depth of the investigation, criteria used for Go/No Go, etc.
- At this stage of development, it is difficult to assess how seriously to take any H2A analysis unless critical assumptions are also listed.
- Planning and economic projections have gone well. However the technical challenges remain. The plan is to down-select to one (or perhaps two) of the reaction schemes and then pour all efforts into that concept. This could work. However if all the remaining concepts have problems, then that down-selected concept has problems. The team should have concluded they will select zero or one.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.3** for technology transfer and collaboration.

- There seems to be strong interaction between the participants with defined roles.
- The degree of collaboration appears to be quite good, involving several partners. It is less clear how technology transfer will be done and what companies are possible collaborators. Perhaps it is too early to assess this latter aspect.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.7** for proposed future work.

- Life time studies on the materials in the extremely aggressive environment need to be done in order to understand the operation and maintenance costs.
- Down-selection is very important to focus the limited resources on the most promising chemistries.
- Thermal management and storage for improved efficiency and 24/7 operation is needed.
- The proposed future research is sufficiently vague and generic to make any meaningful assessment or offer helpful suggestions. Seems basically OK.
- There didn't seem to be a route that accepted the reality of an "unsolved technical barrier".

Strengths and weaknesses

Strengths
- Strong team that has begun working together.
- Down-selection to the most promising technologies is in the plan.
- Strength is involvement of many groups, potentially bringing in new ideas and approaches.
- This group has considerable technical horse (people) power.

Weaknesses
- Materials durability is not directly addressed, at least not in this presentation.
- It is unclear if the H2A analysis includes all of the costs for operation and maintenance, thermal storage capital equipment, heliostat maintenance, and materials disposal.

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- Weakness is also involvement of so many groups. It is not clear how decisions will be made and how strong the leadership is to move this project forward and to make tough decisions.

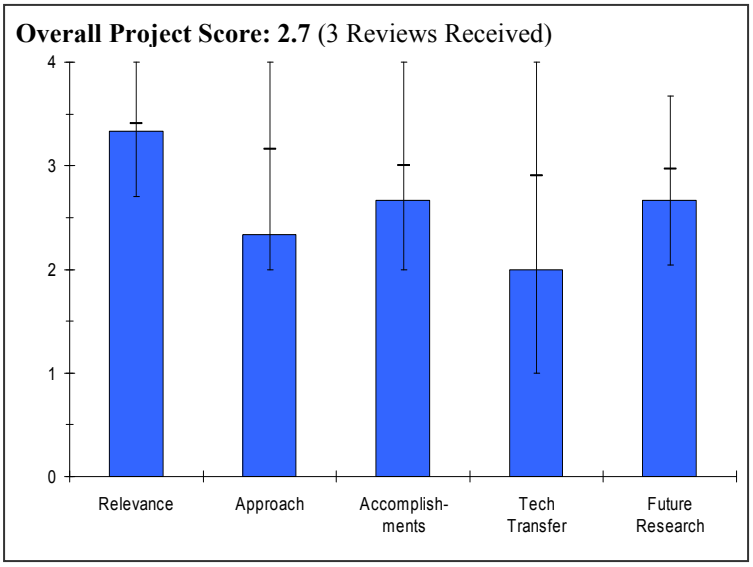
Specific recommendations and additions or deletions to the work scope

- None

Project # PD-14: Solar-Driven Photocatalytically-Assisted Water Splitting
Ali T-Raissi; UCF/FSEC

Brief Summary of Project

The objectives of this project are to 1) evaluate photo/thermo-chemical water splitting cycles that employ the visible portion of the solar spectrum for production of hydrogen; 2) select a cycle that has the best potential for cost-effective production of hydrogen from water (Department of Energy target of $3.00/kg H_2); 3) demonstrate technical feasibility of the selected cycle using solar input in a bench-scale reactor; 4) demonstrate pre-commercial feasibility via a fully-integrated pilot-scale solar hydrogen production system; and 5) perform economic analysis of the selected cycle.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- Solar driven thermochemical water splitting for hydrogen production is within the Department of Energy Hydrogen Program's plans.
- As a process for non fossil fuel hydrogen generation: An interesting combined use of photocatalytic and thermal processes for water splitting.
- This project explores a hydrogen generation technology, an area that is not currently emphasized by the Department of Energy as "relevant", even though conventional fuel supplies are limited.

Question 2: Approach to performing the research and development

This project was rated **2.3** on its approach.

- Approach seems reasonable, focusing on the key gaps in a methodical manner.
- Economic analysis is very important.
- While the investigators' approach to water splitting is reasonable, their claim to a 51% efficiency for the process is highly suspect: If visible light in 20% of the spectrum is used to generate hydrogen, the reported kinetically limited step in water splitting, then the efficiency cannot be greater than 20%.
- This project explores a well-explored thermochemical cycle for "water splitting". This cycle uses ammonia and sulfur and a variety of unit operations, including one critical step driven by solar energy. This cycle has been described for several decades and has proven difficult to optimize. The project strives to beat a hydrogen production target of $3/gge, and thus involves some effort on system design and capital cost estimates.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.7** based on accomplishments.

- The projected started Sept. 2007, but they have made solid progress.
- Initial cost analysis is promising.
- The researchers need to increase work on reactor and receiver designs.
- The researchers need to do economic analysis of the current system using current efficiencies.

- The project has only recently started and they have done a good job. Their planned methodology for partitioning the sunlight could have been better explained.
- The work was completed on a laboratory scale photochemical experiment but no indication apparent of measuring rate of reaction. Engineering analysis work done using a standard program that indicated that the $3 target might be addressed. However, the project efficiency numbers for the photochemical step were incorrect; if so the economic analyses are flawed, because the solar collection hardware is too small to provide necessary solar energy to prompt the hydrogen synthesis. The experimental tasks seemed to be in only early phases.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.0** for technology transfer and collaboration.

- They have published many papers.
- SAIC's participation is unclear.
- In cooperation with Solar Concentration System Development – about which little was said.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.7** for proposed future work.

- They need to close the cycle.
- They need to consider scale-up needs.
- Current efficiencies need to be reported as well as the efficiency of model systems.
- Must address and connect their claimed energy efficiency estimates.
- The proposed work will explore two unit operations, generating data to support the system engineering design.

Strengths and weaknesses

Strengths
- The cycle is using solar energy directly unlike other cycles which use the solar power as heat.

Weaknesses
- Their efficiency analysis should use the entire solar spectrum.
- Discussion on scale-up is needed, especially in using solids and light splitting.

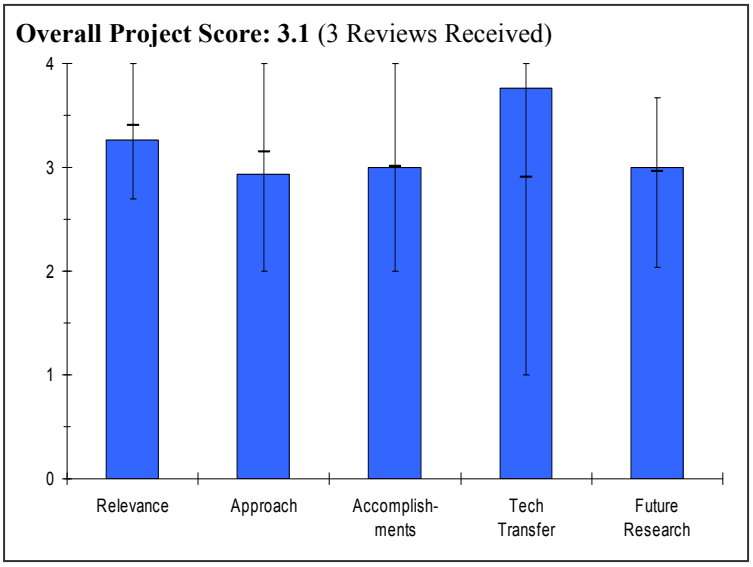
Specific recommendations and additions or deletions to the work scope

- FSEC should solicit help in the economic modeling effort, and get guidance on sizing the photo reactor and the solar collection hardware.

Project # PD-16: Hydrogen Delivery Infrastructure Analysis
Marrianne Mintz; Argonne National Laboratory

Brief Summary of Project

The objectives of this project are to 1) refine technical and cost data in H2A Delivery Models (H2A Hydrogen Delivery Components Model and H2A Hydrogen Delivery Scenario Analysis Model, HDSAM) by incorporating industry inputs and evolving technologies (revised data and analysis, enhanced model capabilities and user options, improved consideration of storage and component sizing, carrier analyses); 2) explore options to reduce hydrogen delivery cost, including storage optimization and novel carriers; and 3) develop enhanced models to assist in program planning and development.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- This will yield an excellent tool for evaluation of various distribution options.
- Department of Energy faces a number of issues and questions regarding hydrogen delivery. However, it is not clear that spending considerable resources on developing a model rather than more thorough, documented, and published studies of delivery costs is the best approach.
- Delivery represents a significant portion of the consumers cost of hydrogen; therefore, it is necessary that we understand the costs associated with the various options.

Question 2: Approach to performing the research and development

This project was rated **2.9** on its approach.

- Approach is appropriate but should address integration with the hydrogen production source assumptions such as distributed or centralized, nuclear, natural gas or electrolysis sources or even multiple "central" sites. This is important for accommodating peak demands and outages.
- The layout of HDSAM limits the user to a constrained suite of options, and the components model is extremely difficult to use. This approach severely limits the flexibility of the models.
- The delivery model seems to be continually "overtaken by events". The user cannot easily evaluate costs for new technologies. New technologies must be added by the model developers, so they are always behind the latest advances.
- Began with excellent models and refined from there.
- Refinements are extremely credible due to the high level of industry interaction.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- Excellent progress is indicated but obviously cannot yet evaluate future advances.
- Too much emphasis on liquid hydrogen.
- The users' guide should have been published with the model.

- In light of the level of funding, the process of vetting the draft version should have gone more quickly.
- Assuming Nexant's funding was linearly distributed over their performance period, the accomplishments for the past year are very good.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.8** for technology transfer and collaboration.

- The report indicates excellent coordination with others.
- The project makes good use of collaborations and appears to obtain needed input from industry and researchers.
- Great industry/consulting/national lab team.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- The inclusion of production and usage considerations should provide more focus for future cases.
- It is not clear that continued refinement of this model is necessary.
- Project is being wrapped up, but as new delivery technologies and scenarios are developed, they need to be added to the model.

Strengths and weaknesses

Strengths
- Excellent modeling capabilities and excellent coordination capabilities.
- The project makes good use of collaborations and the team is well coordinated.
- Broad range of delivery options being covered.

Weaknesses
- Seems to be limited to existing scenarios without projecting future capabilities/technologies.
- It only considers one, totally isolated centralized system and does not consider a widespread grid-type system, which could reduce storage requirements for outages.
- The model is not flexible and is very difficult to use.
- Could use more interaction with companies that deliver gases.

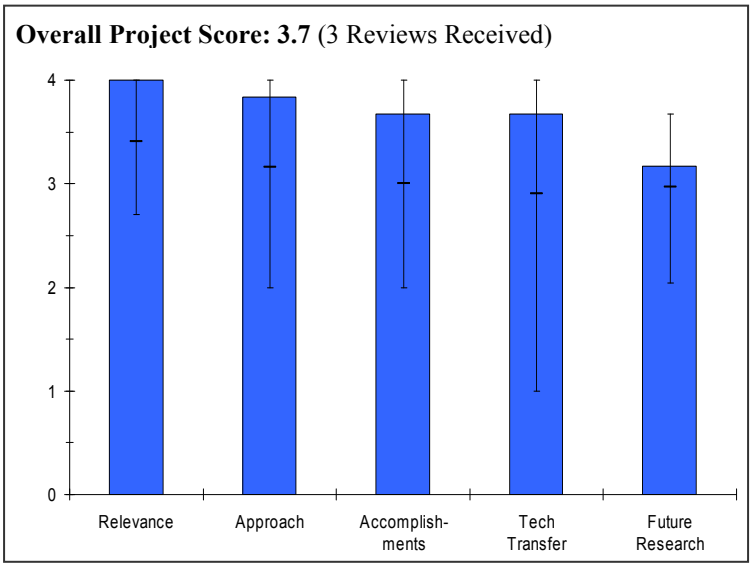
Specific recommendations and additions or deletions to the work scope

- More emphasis on compressed gas trucking, especially with new higher pressure capabilities.
- Consider adding on-site generation capabilities to model for comparison purposes, i.e. electrolysis or small steam reformers.
- The costs versus benefits of further enhancements to this model should be evaluated.
- As delivery scenarios are developed, they need to be added to the model.

Project # PD-17: A Combined Materials Science/Mechanics Approach to the Study of Hydrogen Embrittlement of Pipeline Steels
Sofronis Petros; U of Illinois

Brief Summary of Project

The objectives of this project are to 1) come up with a mechanistic understanding of hydrogen embrittlement in pipeline steels in order to devise fracture criteria for safe and reliable pipeline operation under hydrogen pressures of at least 15 MPa and loading conditions both static and cyclic (due to in-line compressors); 2) study existing natural gas network of pipeline steels or hydrogen pipelines; and 3) propose new steel microstructures. It is emphasized that such fracture criteria are lacking and there are no codes and standards for reliable and safe operation in the presence of hydrogen.



Question 1: Relevance to overall DOE objectives

This project earned a score of **4.0** for its relevance to DOE objectives.

- Project is critical to hydrogen initiatives and supports hydrogen delivery technology RD&D.
- Embrittlement is a serious failure mode of steel pipelines for hydrogen infrastructure; this study aims at a science-based approach to obtain mechanistic insights into why failures occur and the R&D products are useful to design/fabricate pipelines less prone to such failure modes. The study may lead to technical know-how development for mitigating hydrogen embrittlement issues with steel pipelines.
- This contribution is based on experimental tests and theoretical analyses, significantly contributing to addressing the issues and achieving the Department of Energy hydrogen energy technology deployment goals.
- Understanding hydrogen embrittlement is essential to mass distribution and storage of hydrogen.

Question 2: Approach to performing the research and development

This project was rated **3.8** on its approach.

- Sharply focused on the analyses of failure modes of steel pipelines for hydrogen transport infrastructure.
- Experimental and theoretical approaches are combined to clarify influence of hydrogen to materials for hydrogen pipeline.
- Approach seems to be right on target.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.7** based on accomplishments.

- The results thus far are impressive.
- The study has generated considerable insights on the mechanism of steel pipeline failures due to hydrogen transport; the researcher used pipeline samples supplied by manufacturers (air Products, Air Liquide, OSM steels).
- Identification of the fracture criteria could lead to improved pipeline designs, specifications, coating materials and processes.
- Ultimately, this could impact the cost of pipelines and M&O costs.

- Good progress has been made in the basic understanding of embrittlement but more is needed before methods of overcoming the barriers can be suggested.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.7** for technology transfer and collaboration.

- Air Products and Air Liquide, two largest hydrogen manufacturers and suppliers, are only providing pipeline specimens.
- Considering the outstanding results thus far, these manufacturers should be made interested in cost sharing and data interpretation and analysis
- Sandia National Laboratories and Oak Ridge National Laboratory are research and experiment participants.
- Experimental and theoretical approaches are combined to clarify influence of hydrogen to materials for hydrogen pipeline.
- The participants of this project have good contact with standard development organizations.
- The list of collaborators is impressive and indications are that they are being actively consulted.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.2** for proposed future work.

- Plans to build on evolving knowledge and technical know-how base.
- Appears to be a good continuation of the project.

Strengths and weaknesses

Strengths
- Solid unfolding of knowledge based on experiments and analyses of theoretical foundations.
- Project shows strong potential to progress towards a meaningful outcome.
- This project is conducted under collaboration with both experimental and theoretical groups.
- Good coordination with others.
- Solid technical capabilities.

Weaknesses
- The chemical reactions, which perhaps initiate the failure modes to then propagating to actual failures have not been studied at levels required for a complete understanding of the reliability issues.
- Comparison with other, novel materials pipelines for hydrogen transport has not been included. At least a literature study is needed.
- There is some recognition that steel pipeline is a no-go for hydrogen transport because of intrinsic chemical reactions of hydrogen with steel components, carbon, iron, etc.; a comparison with other materials of construction may shed some insights on this issue.
- Very theoretical.

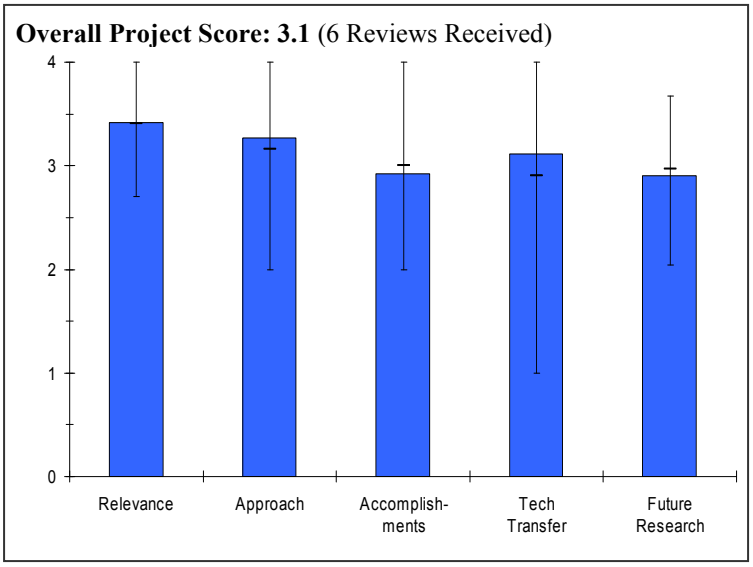
Specific recommendations and additions or deletions to the work scope

- Study the chemical reactions and kinetics of hydrogen with iron, carbon, etc., and how the reactions cause initial defects to further propagate the failures.
- In depth study of chemical mechanisms, electro-mechanical mechanisms and relating to the physical (e.g., hydrogen diffusion) failure modes ultimately causing mechanical fractures.
- Coordinate this with the similar task by Sandia National Laboratories for practical applications.

Project # PD-18: Materials Solutions for Hydrogen Delivery in Steel Pipeline
Doug Stalheim; Secat/ORNL

Brief Summary of Project

The objective of this project is to develop materials technologies to minimize embrittlement of steels used for high-pressure transport of hydrogen. The deliverables are to 1) identify steel compositions/microstructures suitable for construction of new pipeline infrastructure; 2) develop barrier coating for minimizing hydrogen permeation in pipeline and associated processes (on hold per the Department of Energy); and 3) understand the economics of implementing new technologies.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.4** for its relevance to DOE objectives.

- Very relevant to establishing next steps regarding current infrastructure or new infrastructure.
- Pipelines are important but can steel pipelines contribute to meeting Department of Energy targets. I thought the problem was welding and this program does not appear to address this. Not clear that their team understands the big picture. Comment was made that maybe existing pipeline could be use connected to hydrogen—massive picture that natural gas pipelines will be needed for natural gas.
- This project is relevant to Department of Energy's goals.
- As this project explores the potential to use existing, commercially available steel materials, and includes a task to study the economics, it contributes to addressing the barrier of high capital cost.
- Additionally, the study of the effects of hydrogen relative to the material composition and microstructure addresses the barrier of materials issues with hydrogen embrittlement.
- Pipelines are the most cost effective shipment method; however, barriers to hydrogen shipment must be addressed before long distance pipelines can be used.

Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

- Methodical, clear and forward looking.
- Clear explanation of where they are and where they are going.
- Approach to this problem appears to be good. Have had to defer some work due to funding issue.
- The project is too narrowly focused on microstructures. Other aspects of steel composition could be important.
- Too few analyses have been conducted to assess the effects of variability in microstructures.
- Project contributes to the determination in the feasibility of using certain grades of commercially available steel and alloys for hydrogen pipeline delivery.
- Logical approach and testing being conducted within a limited, focused group of materials (limited manufacturers and materials grades).
- Extensive team partnering is a strength.
- Communication with other projects needs to be established to maximize the benefits of the experiment and calculation/theoretical activities (of other delivery projects).
- Low risk for technical feasibility in testing the commercial steel and alloy materials.

- It is not clear how applicable the test results of the subject materials will be towards other materials fabricated by other manufacturers, nor whether manufacturers can accommodate the microstructure improvements needed. Understanding the mechanisms appears to be critical to extrapolate the focused studies to be helpful in the broader sense.
- The four tasks outlined are appropriate for advancement of the technology.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.9** based on accomplishments.

- Progress is proportional to funding.
- The project is only 25% complete, while being 75% of the way through the time. Very little progress has been made.
- Multiple commercial pipeline materials have been tested from one manufacturer, including microstructure imaging, the effect of hydrogen on the mechanical properties of steel (ex-situ testing), and studies of hydrogen-induced cracking.
- Studies in pure hydrogen provide a baseline.
- Testing apparatus is complete for in-situ high pressure hydrogen testing.
- Extensive amount of work in selecting and characterizing candidate materials.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.1** for technology transfer and collaboration.

- Impressive list of collaborators, definitely necessary for this type of analysis.
- Cannot tell the time each partner participated.
- In-situ test in hydrogen atmosphere is important in cooperation in SECAT consortium.
- Fairly good collaboration with laboratories.
- The project includes many team members including private companies, national laboratories and universities.
- It is not clear that the extensive collaboration is being fully utilized except for the testing capabilities provided by Oak Ridge National Laboratory.
- Three Project team is an excellent vertical alignment from R&D entities to a pipeline owner, but could be improved with the inclusion of a hydrogen pipeline owner.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.9** for proposed future work.

- Very focused program, Object is achievable.
- Evaluation of in-situ fatigue testing is highly expected.
- Task 3 activities and the codes and standards integration in Task 4 do not appear in the presented future plans.
- The presentation did not include milestones or stage gates/decision points (i.e. define a clear decision point at which the material compositions and microstructures are either feasible or not, and alternatives need to be explored).
- Future activity includes an economic evaluation.
- The project needs to more clearly define test criteria.
- In-situ high pressure hydrogen testing will be conducted.
- Future work does not seem to go all the way to revising codes and standards.

Strengths and weaknesses

Strengths
- Businesslike approach, results focused.
- Focused program testing steels in hydrogen environment.

- Project addresses the barriers of cost and material challenges.
- Technically feasible and focused approach.
- Strongest point is the vertically integrated team.

Weaknesses

- This is a focused "development/communization" program and not propane, which will have any ability to dramatically lower the cost of steel pipelines. Department of Energy programs should lead to step-outs, not the materials.
- Major conclusions are based on a very small number of samples.
- In determining whether existing pipelines and commercially available baseline and alloy materials are feasible for a hydrogen economy, then accelerating testing/aging of steel, hydrogen with impurities, an understanding of the mechanisms for degradation, and safety thresholds would appear to be a high priority. Criteria for continuing with existing steel chemistry/microstructure should be defined (versus at what point alternatives should be pursued).

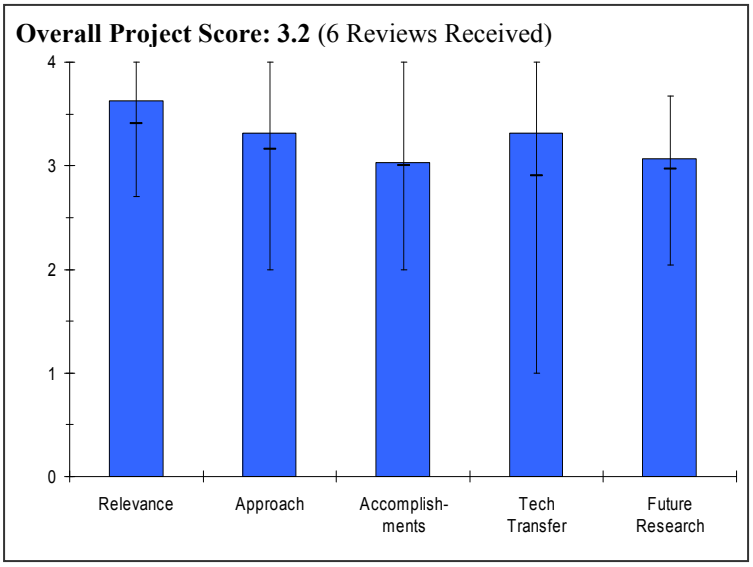
Specific recommendations and additions or deletions to the work scope

- Asses how "impure" hydrogen affects these results.
- Add oxygen to hydrogen, see how this travels, purify at end of pipe.
- Add impurities to allow pipelines to "work" with hydrogen, purify at end of pipe.
- Hydrogen pipelines currently exist. The project should include evaluation of the aging of existing pipeline if feasible.
- Agree with Department of Energy's decision to put coating work on hold, at least until a favorable cost/benefit analysis has been prepared and adequately reviewed.

Project # PD-19: Composite Technology for Hydrogen Pipelines
Barton Smith; ORNL

Brief Summary of Project

Oak Ridge National Laboratory will investigate the applicability of composite pipelines in use in oil and gas gathering operations and develop a path forward for hydrogen delivery. The cost scenario shows composite pipeline will meet the Department of Energy 2012 goals and are close to the 2017 goals. The hydrogen compatibility of pipeline materials is acceptable. The pipeline leakage rates are better than predicted.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.6** for its relevance to DOE objectives.

- It is not clear what specs the Program is trying to achieve. Department of Transportation rules for pipeline? American Society of Mechanical Engineers?
- If so, is there any interaction?
- Composite pipelines may offer a low cost, no hydrogen embrittlement option to metal.
- The objectives are critical but success of composite pipe materials obviously depends upon competing technologies.
- Project is focused on reducing the cost of hydrogen pipelines by using fiber-reinforced polymers to manufacture the pipelines.
- Project appears to have significant potential to reduce the cost of hydrogen pipelines to meet the Department of Energy targets.
- Clearly relevant to the goals of the RD&D plan, regardless of whether or not the end-use will specifically address hydrogen-fuel-cell-powered vehicle infrastructure.

Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

- The Program should be given access to the current technology validation program for hydrogen stations to retrieve materials for testing. Already many of the existing stations have 2-5 years of high pressure hydrogen exposure in cyclical stressed conditions. Of course the PIs have limited access to the other program (and also influence) and this should be coordinated through Department of Energy program managers.
- Immersion test may not be the best way of testing without a pressure differential across the tube wall.
- What are the technical specifications that need to be met (beyond cost)?
- Composites experience in natural gas industry provides a good basis for this work. Barriers are mostly known. Project approach is logical and straight forward.
- Investigation of commercially available materials is an approach to low cost pipeline.
- The approach is satisfactory although it should include other alternative composite pipes, not just Fiberspar.
- Testing of HDPE, PA, and PPS pipelines for hydrogen permeability, tensile strength, and materials compatibility is appropriate and necessary.
- Pressure and temperature effects are appropriately considered.
- Surface treatments and associated testing will yield valuable data on the ability to improve the permeability of polymer pipelines.

- Overall approach is effective.
- Project is addressing pipeline capital costs and hydrogen embrittlement.
- Approach does not yet include thermal fatigue effects on composite pipe assembly. Will such effects be implemented along with future mechanical fatigue experiments?

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- Accelerated aging tests would have been more meaningful had a pressure differential been maintained across the pipe. This could have provided both permeation and strength data on a hydraulically loaded pipe. The aging test performed (immersing the entire pipe in a static 1000 psi hydrogen environment at 60 degrees Celsius) is only an indicator of the effect of hydrogen on the materials, not pipe performance.
- I would suspect that hydrogen permeation may decrease over time as the liner surface is fouled with other constituents.
- Acceptable pipeline materials compatible with hydrogen are proposed. This result supports activity to evaluate the practicality of pipeline transportation of hydrogen.
- Accomplishments appear good but it has taken two and a half years to reach an understanding of one material.
- Good progress is being made in testing HDPE, PA, and PPS pipelines for hydrogen permeability, tensile strength, and materials compatibility. Permeation coefficients, tensile properties, and hydrogen leakage results from the tests were presented.
- Surface treatments and associated testing appear to be underway.
- Project appears to be progressing toward achieving technical millstones within the anticipated timeframe.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.3** for technology transfer and collaboration.

- The two major composite pipe manufacturers and major liner materials companies are on the team.
- Collaborations appear satisfactory but should be expanded to include other material suppliers.
- Collaborations are appropriate.
- Partners appear to be working closely with the PI.
- Manufacturers of additional polymer types should be considered for inclusion in the project to include additional polymers.
- Potential customers (pipeline purchasers/installers/maintenance) should be consulted to enable transfer of the technology to industry at the appropriate time.
- Strong collaboration with pipe, liner, and coupling manufacturers is evident.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.1** for proposed future work.

- Beginning code work early is essential.
- Plan is limited in terms of pipe lengths (i.e. sample size) and number of joints.
- Needs to focus more on overcoming barriers.
- Proposed research is appropriate and should be funded.
- The cost and pipeline performance impacts of variations in pipeline manufacturing process conditions should be studied to understand potential issues of onsite pipeline manufacturing.
- Brittle fracture in fiber-reinforced polymer materials is always a concern even for buried pipe structures due to environmental acids. In particular, crevice corrosion around couplings may be a concern. Future plans should include experiments aimed at assessing whether crevice corrosion around couplings will lead to brittle failure of fiber-reinforced polymer.

Strengths and weaknesses

Strengths
- Builds on natural gas experience and includes commercial fiber-reinforced polymer fabricators.
- Good depth of technical understanding.
- Good coordination with material supplier.
- Good test and analytical technical abilities.
- Composite pipeline testing is elucidating the performance and properties of polymer pipelines.
- Project is contributing to development of necessary codes and standards for composite pipelines.
- Approach has potential to meet Department of Energy pipeline cost targets.
- The project is globally relevant to hydrogen infrastructure.
- Project is likely to generate useful reference data and standard protocols for hydrogen pipeline testing.

Weaknesses
- The immersion test may not accurately reflect the embrittlement effects or diffusion issues.
- Project presentation did not address installed costs, only states that scenarios meet 2012 Department of Energy goals.
- Project is concentrating on 4' nominal pipe. This may have limited application. Large diameter (>6") fiber-reinforced polymer composite pipe may have inherent cost and installation disadvantages.
- Does not give data to support cost effectiveness of pipe material.
- Is not able to generalize to other alternative materials.
- Given the 20% deviation in the results of testing 3 samples, a larger sample size is needed.
- A limited number of coupling, pipe, and liner structures have been selected.

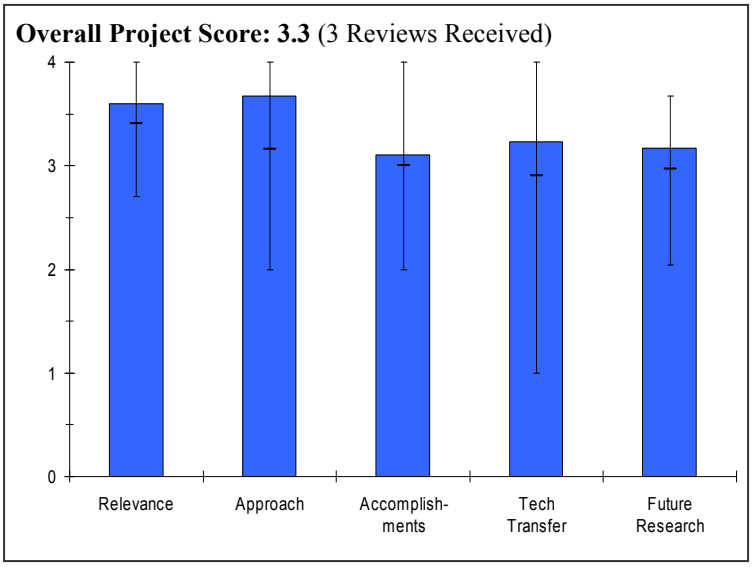
Specific recommendations and additions or deletions to the work scope

- This is for Department of Energy Program management: coordinate the access to materials aged in Technology Validation Program (hydrogen stations), be it storage cylinders or reformers or other materials exposed to high pressure and/or high temperature hydrogen.
- Calculate if the costs of fluorination offset the amount of hydrogen saved.
- Calculate pressure drop - standard fiber-reinforced polymer pipe plus 0.5 cm liner may have much smaller ID than nominal steel pipes that will result in higher pressure losses per linear foot of pipe. This pressure loss may be offset somewhat (but not completely) by surface smoothness.
- Theorize the differences between hydrogen service and natural gas (is there a hydrogen induced cracking mechanism in fiber-reinforced polymer?). This exercise may strongly support fiber-reinforced polymer use in hydrogen.
- Determine any special requirements for pipe line inspection "pigs".
- Determine corrosion protection requirements for buried joint fittings.
- Include some type of bench-mark for alternative materials such as exiting pipe material.
- Include other composite materials and pipes for evaluation.
- Consider the cost and pipeline performance impacts of variations in pipeline manufacturing process conditions.
- Increase the sample size used in the testing effort to account for the large deviation (20%) in the results.

Project # PD-20: Hydrogen Permeability and Pipeline Integrity/Fiber Reinforced Composite Pipeline
Thad Adams; SRNL

Brief Summary of Project

The objectives of this project are to 1) investigate the influence of weld fabrication microstructure (especially weld heat affected zones [HAZ]) on hydrogen compatibility; 2) measure hydrogen transport (diffusivity) in HAZ materials; 3) determine HAZ material susceptibility to hydrogen embrittlement; 4) focus evaluation of fiber reinforced composite (FRP) piping for hydrogen service applications; and 5) assess the structural integrity of the FRP piping and leakage of existing commercial available FRP joint designs and joint components.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.6** for its relevance to DOE objectives.

- Two projects were presented in this talk. One was on hydrogen pipeline integrity and the other is on fiber-reinforced composite pipeline (fiber-reinforced polymer). Both projects are important to address issues involved in transmission/distribution of hydrogen.
- Both projects in this presentation are relevant to the Department of Energy Hydrogen Program.
- The hydrogen permeability and pipeline integrity project ended in March 2008. The fiber-reinforced polymer project should be combined with PD-19. I don't see any justification to having PD-19 & PD-20. PD-20 involves collaboration with Oak Ridge National Laboratory and PD-19 is an Oak Ridge National Laboratory-led project. Good synergy to combine these two projects.
- Fiber-reinforced polymer is the only Pipeline program that can possibly meet Department of Energy targets. Welding in steel P/L's is also a key element of the cost of P/L's.

Question 2: Approach to performing the research and development

This project was rated **3.7** on its approach.

- The hydrogen permeation and integrity part of this project is finished. Test samples from actual weldment was prepared and tested for hydrogen solubility, diffusivity, & permeability at sub-atmospheric pressure and moderate temperatures.
- The approach for the fiber-reinforced polymer part of the project is to investigate fiber-reinforced polymer joint types & determine hydrogen leakage rates. This seems to be a good approach for this task.
- Well focused programs. Clearly focused on milestones and deliverables. Refocusing correctly on fiber-reinforced polymer work with Oak Ridge National Laboratory.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.1** based on accomplishments.

- Determined that effect of microstructure on diffusivity of hydrogen in pipeline steels is critical to aiding understanding of hydrogen embrittlement. It is well-known in materials science that microstructures influence the materials property. It is not clear what this work has accomplished other than stating that structure-property-

processing is important. One could open any book on materials science and find the statement that structure-property-processing are interlinked. It is good to see that this part of work is terminated in March 2008.
- Higher hydrogen leakage rates were measured in fiber-reinforced polymer and the reason for this is not known at this time. Oak Ridge National Laboratory and Savannah River National Laboratory are going to get together to analyze the results. It is not possible to measure the progress towards objectives.
- Good progress. Helping Oak Ridge National Laboratory. Little money, getting data. Focus has been too much on weld materials permeability. Should work more on fiber-reinforced polymer.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.2** for technology transfer and collaboration.

- Good collaboration between Savannah River National Laboratory and Oak Ridge National Laboratory.
- Praxair provided the welded samples for analysis.
- Role of Edison Welding Institute is not clear.
- Collaborations with Oak Ridge National Laboratory. No others apparent.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.2** for proposed future work.

- Plans to determine the cause for higher leakage rates is not included in the future plan. It is important to determine the reason for the higher leakage before proceeding with the other planned activities.
- The rest of the future plans are reasonable.
- It is good that the weld work stopped and work redirected to fiber-reinforced polymer. Do more.
- Test planning of fiber-reinforced polymer materials, joints, and fiber-reinforced polymer pipeline system are expected to be extensively carried out based on their experience on pipeline testing.

Strengths and weaknesses

Strengths
- Collaboration between Oak Ridge National Laboratory and Savannah River National Laboratory.
- Good strategy to measure the diffusivity, solubility, and permeability.
- Courage to end the hydrogen permeability and integrity portion of the project back in March 2008.
- Experience of material testing for hydrogen pipeline

Weaknesses
- Not following up on analyzing the reasons for higher leakage rates.
- Needs to be more work with manufacturers focusing on mp processes, consistency, on site mp etc and how that affects leak rate.
- Lack of experience of plastic materials and fiber-reinforced polymer.

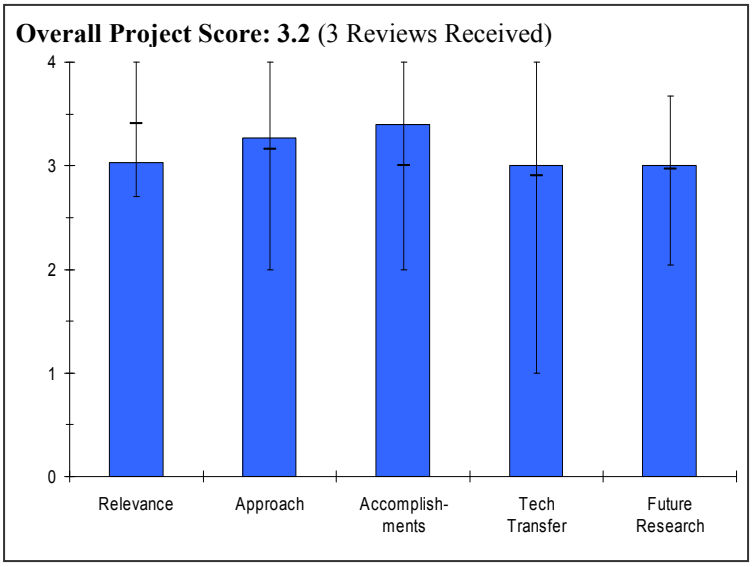
Specific recommendations and additions or deletions to the work scope

- Combine the fiber-reinforced polymer task with PD-19.No need to keep two different projects.
- Determine the cause for higher leakage rate and fix this problem before proceeding with rest of the future plans.
- Need to decrease steel effort and P/L working group and increase efforts and collaborations in fiber-reinforced polymer work.

Project # PD-21: Innovative Hydrogen Liquefaction Cycle
Martin Shimko; Gas Equipment Engineering Corporation

Brief Summary of Project

The objectives of this project are to 1) design a practical hydrogen liquefaction cycle that significantly increase efficiencies over existing technologies; 2) produce a small-scale (100-500 kg/day) hardware demonstration of a hydrogen liquefaction plant; 3) use low/no risk development components that scale to 50,000 kg/day plant size; and 4) document a significant reduction in the total cost of hydrogen liquefaction at the 50,000 kg/day production level.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.0** for its relevance to DOE objectives.

- Goal of reducing energy losses associated with hydrogen liquefaction is important and should make use of liquid hydrogen delivery system significantly more attractive.
- Increasing cycle efficiency from Linde volume of 30/35% to 45% is a worthy goal, but there remains the question of whether one can more clearly approach Quack "practical limit" of 60%. Author claimed this cycle would be too costly, but did not prove it.
- If efficiencies of liquefaction could be significantly increased, this project would be more relevant but this does not seem to be realistic.

Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

- Approach good, particularly in use of low/no risk development components. Intermediate step of producing a small-scale hardware demonstration is good. Massachusetts Institute of Technology experience is a plus.
- The approach is good regarding the technology but it concludes that liquefaction efficiencies cannot be increased enough to be critical to overcoming barriers to the extensive use of liquid hydrogen.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.4** based on accomplishments.

- Use of para/ortho equations of state good, as is development of "simple" cycle simulation program leading to examination of several cycle options and optimizations
- Good progress is made toward improving the technology but it doesn't appear to be enough to overcome barriers.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- Not clear how much technology transfer is applied.
- Good collaborations appear to have occurred with indicated partners but expansion to others in the industry should be taken.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- The investigators appear to have adequately defined possible limiting problems and have done a reasonable job of estimating cost. Future efforts are well-defined. Doing catalyst heat exchange development incoming year is appropriate.
- Development of the catalytic heat exchanger may be of interest.
- Demonstration of a pilot plant does not seem warranted regarding the achievement of Department of Energy Hydrogen Plan goals.

Strengths and weaknesses

Strengths
- Excellent approach to significantly reducing process efficiency losses and thus reducing cost associated with conversion of hydrogen to liquid state (which appears to be an attractive delivery and storage option).
- The project does advance hydrogen liquefaction technology.

Weaknesses
- Necessity of liquid nitrogen.
- The improvements identified do not appear to overcome barriers.

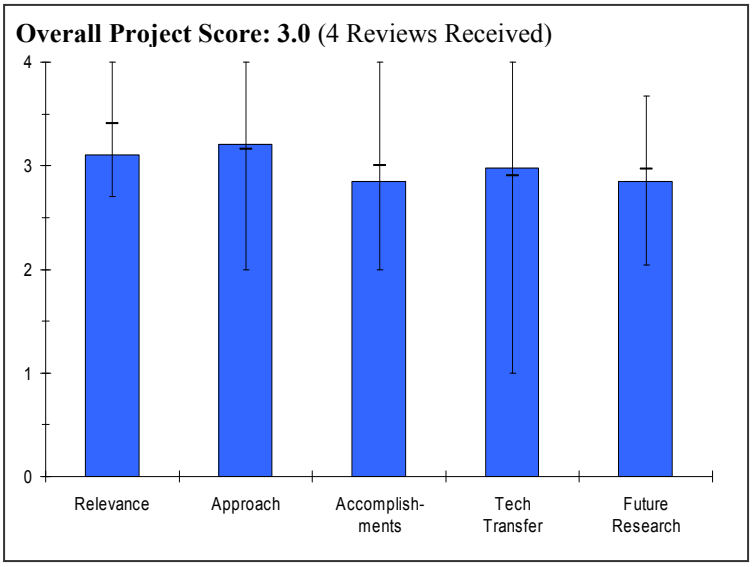
Specific recommendations and additions or deletions to the work scope

- Combine the objective to lower the hydrogen temperature rather than the just liquefactions.
- Use this technology for hydrogen storage such as cryo-absorption.
- Continue the work on catalytic heat exchangers.
- Refine the cost/efficiency study work.
- Do not build a pilot plant.

Project # PD-22: High Pressure, Low Temperature Hydrogen Tube Trailers
Salvador Aceves; LLNL

Brief Summary of Project

The objective of this project is to demonstrate inexpensive hydrogen delivery through synergy between low temperature (200 K) hydrogen densification and glass fiber strengthening. Colder temperatures (200 K) increase density ~35% with small increases in theoretical storage energy requirements. Low temperature are synergistic with glass fiber composites. Glass composites (~$1.50/kg) minimize material cost. Increased pressure (7,000 psi) minimize delivery costs. Dispensing of cold hydrogen reduced vehicle vessel cost ~25%.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.1** for its relevance to DOE objectives.

- High pressure tanks are certainly one alternative to storing hydrogen in the future.
- Unless there is a huge breakthrough in hydrogen storage, future hydrogen fuel cell vehicles will probably use at least a combination of hydrogen storage materials and high pressure tanks.
- A lot of work has already been done on high pressure tanks and the current technology is already being readily used, so this work is a little more long-term, focused on lowering the cost of the composite tanks.
- If the hydrogen storage subprogram achieves their targets, the value added of this project to the Hydrogen Program is significantly lower.
- There are significant issues related to cold hydrogen storage such as slow hydrogen release over time if a vehicle is parked for extended periods.
- This method provides superior strength at lower temperatures, but this assumes that the tank temperature remains low over long periods of time. If the tank weakens over time as it heats up, this could be a significant issue.
- Obviously low temperature will increase gas density which will lead to reduced tank volume per unit mass of hydrogen.
- Indications are that glass fiber strength increases at low temperature (good), but not clear that overall tank strength increase with low temperature.
- Cost of cold glass fiber and the cost of carbon fiber truck systems approach each other at high volumes. Glass meets the target at lower delivery volume, but question whether Department of Transportation would accept design.

Question 2: Approach to performing the research and development

This project was rated **3.2** on its approach.

- The project is investigating glass fiber composites, which is an interesting potential substitute for carbon fiber that would provide added strength and potentially lower the delivery cost to less than $1/gge.
- The project seems a little disjointed with work on composite tanks, cold hydrogen storage, and large tube trailers.

- The tensile testing of the glass fibers is not working. There are too many variables surrounding the glass fibers (humidity, temperature, time at temperature) that must be addressed to make any sense of the data. In addition, the fibers are breaking very randomly and close to the holder.
- The tensile data is confusing and hard to discern. Since several individual fibers are being tested at once, the stress strain curves are stepped and this makes it hard to determine anything from them.
- The issue of water weakening the fibers is a concern since it will be nearly impossible to keep water out as there may always be a little water in the hydrogen. It would be vital to know if the tank had been exposed to water, and this would not be something easily measured over time at very low levels.
- Clearly laid out goals and deliverables.
- Concurrent engineering a plus.
- Testing samples consisting of multiple fibers imbedded in resin matrix is the right way to go (critical).
- Novel approach to reducing the cost of storage tanks.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.9** based on accomplishments.

- The progress was slower than expected and most of the work presented was based on concept rather than actual data.
- It was hard to determine the results of the project over the last year versus the results of the project overall. Presenting the status of the project at the time of the Annual Program Review last year and then specifically stating the accomplishments over the last year would have helped.
- Given the amount of time spent they have made great progress in this development.
- Myth busting of glass fiber reliability refreshing.
- Progress appears to be somewhat slow – need to get to testing of full samples (fibers in matrix) as soon as possible.
- Accomplishments are limited, but funding was very limited.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- Three separate collaborators who all have significant experience in the area of composite tanks.
- Little evidence was given about how the collaborations are specifically benefiting or contributing to this project.
- Team assembled makes sense; they seem to be working well together.
- Having Quantum on board is very important since they have been a real leader in fiber-wound tanks for high pressure operation.
- Industrial partners are significant.
- Adding Department of Transportation as a partner/advisor would be beneficial.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.9** for proposed future work.

- Very little offered as far as their proposed future work beyond the cryogenic tensile testing and the work with Department of Transportation to make their tube trailer viable.
- Potential weaknesses already identified, plans for remediation already discussed - great!
- What needs to be done is fairly obvious and it looks like they are headed that way, except that there is no mention of pressurization/depressurization cycling tests or temperature cycling tests.
- Proposed research appears to be hampered by funding limitations.

Strengths and weaknesses

Strengths
- The proposed concept does have the potential to lower the vessel cost by 25%.
- Very applicable knowledge regardless of hydrogen production pathway.
- Good team.
- Out of the box thinking to reduce cost.

Weaknesses
- The concept has several potential issues that could prevent it from being a viable option.
- The tensile testing at cryogenic temperatures has resulted in very little usable data.
- Nothing spelled out for cumulative damage analysis.
- Considering the controls that must be implemented to maintain dry, cold fibers in practice, appears to be adding considerable risk to the application.

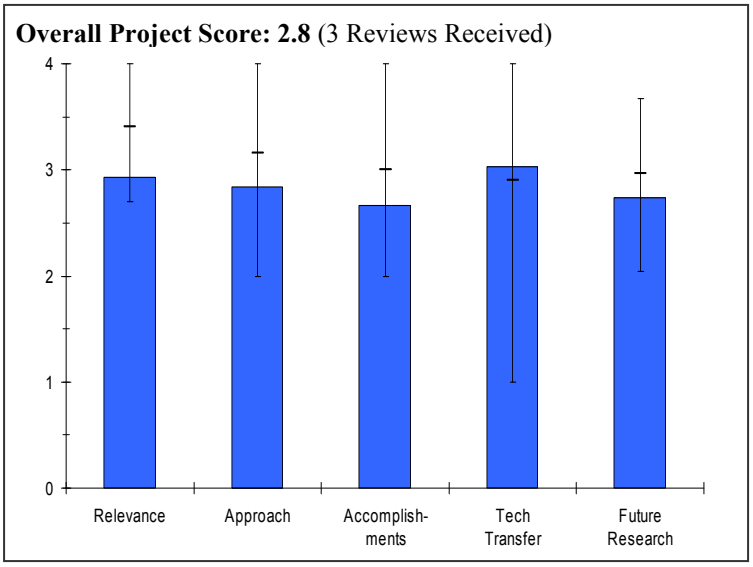
Specific recommendations and additions or deletions to the work scope

- The group should try to develop alternative ways to measure the strength of the glass fibers rather than the current tensile tests. Similar to tensile testing ceramics, the data will probably never show consistent results.
- The cryogenic tensile testing should be deemphasized.
- Complete cost analysis of construction for scale.
- Revise costing analysis with current parameters in H2A.
- Explore real world scenario for how this would be used in real world conditions, I think this idea is promising, let's see what real world conditions would be necessary to pursue to full fruition.
- Continue and add funding to explore real world.
- Find another group, vendor or lab to build one of these trucks – even a scaled down model to invite private sector development.
- Ultimate failure tests for tanks at purposed operating temperatures. Cumulative damage analysis for multiple cycles of pressure, temperature.
- Recommend an independent risk/benefit analysis of the technology and the application.

Project # PD-23: Reversible Liquid Carriers for an Integrated Production, Storage and Delivery of Hydrogen
Bernard Toseland; APCI

Brief Summary of Project

The objective of this project is to enable a liquid carrier concept. This includes a economic study to determine the concept's viability. This project supports the liquid carrier by developing a dehydrogenation reactor system for hydrogen delivery. The packed bed reactor works well, but design limitations limit the reactor efficiency. Thin-film catalysts (useful for monoliths and microchannel reactor) can be made with high catalyst efficiency. Monolith reactors are useable, but flow instabilities will cause design limitations. Micochannel reactors still look like the most viable alternative.



Question 1: Relevance to overall DOE objectives

This project earned a score of **2.9** for its relevance to Department of Energy objectives.

- Carriers could reduce distribution cost but need to consider total well to wheel cost
- While a hydrogenated fluid could be relevant in theory, no data is supplied to explain this. Thus the relevance of this project is questionable.
- The indicated distribution costs appear to be far from other alternatives.
- Project addresses hydrogen carriers for both onboard and offboard hydrogen regeneration.
- Potential to meet hydrogen production, delivery, and storage targets is not clear.

Question 2: Approach to performing the research and development

This project was rated **2.8** on its approach.

- Prototype reactor tested in lab.
- Large gas flow and variable flow challenges identified.
- N-ethylcarbazole carrier system is six weight percent hydrogen.
- The approach seems reasonable within hydrogenated fluid technology but it is not indicated that it will significantly overcome barriers.
- It is unknown if the fluid, N-Ethycarazde is appropriate other than for academic purposes.
- Consideration of multiple reactor configurations was appropriate.
- The results presented provide sufficient data to downselect to the microchannel reactor design for the prototype.
- A system-level analysis is needed to determine whether onboard dehydrogenation in general is likely to be an effective and consumer-acceptable approach.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.7** based on accomplishments.

- Packed bed reactor mass transfer limits identified.
- Effectiveness factor in packed bed.
- Microchannel reactor allows modular design and turndown for variable hydrogen production.
- Evaluation of dehydrogenation reactors appears competent and thorough.

- How this progress will overcome barriers is not indicated.
- Data obtained thus far supports a Go/No Go decision on the reactor designs.
- Progress against the Department of Energy delivery targets for carrier hydrogen content and carrier system energy efficiency was not presented.
- The cost estimates for this project are significantly (~2x) higher than the Department of Energy targets, and it is not clear that all of the relevant costs are included in the PI's cost estimate.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- Mix of industry and national laboratories.
- Coordination with partners to date has not been indicated.
- Future coordination regarding the source of hydrogen and end use is indicated.
- No collaboration with component suppliers such as for thin film or micro-channel components is indicated.
- Pacific Northwest National Laboratory is an effective partner for microchannel reactor work.
- A fuel cell partner and an original equipment manufacturer partner (unknown at this time) are included in the project. More collaboration with these partners in the early stages of the project is needed to assess potential system issues and show-stoppers related to both technology transfer capability and consumer acceptance.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.7** for proposed future work.

- Reactor selection and test facilities.
- It is not clear how the proposed future tasks will overcome barriers.
- Future plans are appropriate.
- Conduct a system-level analysis of the viability and consumer acceptance potential of an onboard dehydrogenation system. Include an onboard Go/No Go decision in future plans.

Strengths and weaknesses

Strengths
- Economic analysis completed using Aspen and H2A models.
- Good understanding of the overall liquid fluid dehydrogenation technology.
- Project has considered multiple reactor configurations.
- Project addresses hydrogen carriers for hydrogen production, storage, and delivery and is relevant to the Department of Energy goals.

Weaknesses
- Original equipment manufacturer partner not yet identified.
- Microchannel reactor cost not yet identified.
- Required solutions/advancements are not identified and quantified.
- Analysis costs are very high.
- Assessment of this project's reactors' performance against the Department of Energy goals was not shown.

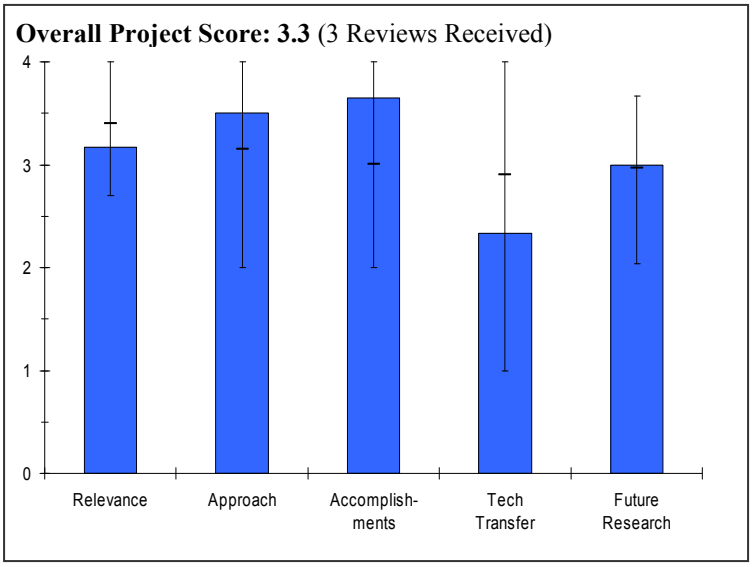
Specific recommendations and additions or deletions to the work scope

- Review toxicity data for carrier liquid.
- Define specifically what cost/technological improvements are required for liquid fluid hydrogen carriers to overcome Department of Energy distribution barriers and relate the barriers to hydrogenated fluid parameters.
- In terms of these improvements, define the technological improvement required.
- Assess the potential of the systems considered in this project against Department of Energy's goals for carrier content and carrier system energy efficiency.
- Conduct a system-level evaluation of the ability of onboard carrier system to meet market demands.

Project # PD-24: Coatings for Centrifugal Compression
George Fenske; ANL

Brief Summary of Project

The objective of this project is to identify and develop as required, advanced materials and coating that can achieve the friction, wear and reliability requirements for dynamically loaded components (seal and bearing) in high-temperature, high-pressure hydrogen environments prototypical of pipeline and forecourt compressor systems. The reliability and efficiency of hydrogen compressors will depend on the tribological performance of critical bearings and seals. Knowledge of the tribological performance of materials and coatings in hydrogen environments is currently insufficient to design reliable, efficient hydrogen compressors. The rule of thumb/target is friction <0.1.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.2** for its relevance to DOE objectives.

- Good relevance to improving pipeline and forecourt compressors.
- Appears to be very important if high pressure gaseous hydrogen is selected as delivery method of choice.
- There certainly could be benefits coming from this activity, but it is not clear that this is high priority.

Question 2: Approach to performing the research and development

This project was rated **3.5** on its approach.

- Good approach. Very logically indentified, evaluated, characterized, developed and engineered.
- Could consider some kind feedback upon final testing.
- Program assumes being right the first time.
- Excellent systematic approach.
- Good approach; although, hydrogen impurities could have a significant impact on materials selected.
- Focused on critically loaded components.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.7** based on accomplishments.

- Slow progress due to funding constraints. Not their fault.
- Screening of types of coating excellent: homing in on Argonne National Laboratory DLC6 appears appropriate.
- Establishment of test facilities and initial research accomplishments are appropriate.
- Results for DLCs very impressive.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.3** for technology transfer and collaboration.

- Working with MITT (compressor company). Could they work with more relevant compressor manufacturers?
- Doesn't appear to be a lot of coordination with others (notable VTT Tech Research Centre of Finland).
- Project benefits from the inclusion of a bearing manufacturer performing parallel research.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- Long list of materials to be tested.
- Good approach regarding microscopic studies for wear mechanism definition and studying embrittlement and crack behavior.
- Needs to address thermal loads for various scenarios-how much and how fast will heat build up.
- Good plan for continuation of this project and identification of a suitable coating material.

Strengths and weaknesses

Strengths
- Well thought out technical approach.
- Appears to have identified a promising coating approach.
- The PI understands the issues and approaches to a solution.

Weaknesses
- Choose more commercial partners not just someone who is funded by Department of Energy.
- Lack of integrated analysis of thermal loads.
- Lack of a broad team and a compelling reason for the work to be done.

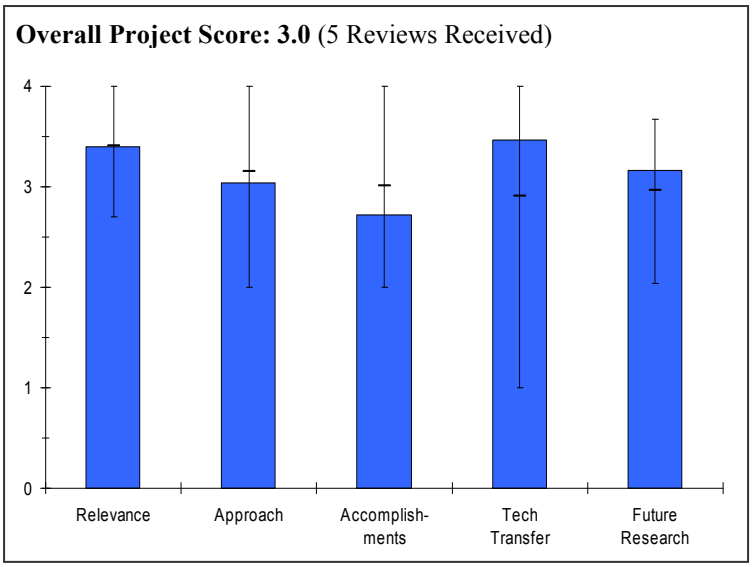
Specific recommendations and additions or deletions to the work scope

- Continue at current level as long as project priority keeps it above the funding limit line.

Project # PD-25: Sulfur-Iodine Thermochemical Cycle
Paul Pickard; SNL/GA/CEA

Brief Summary of Project

The objective of this project is to evaluate the potential of the sulfur-iodine cycle for hydrogen production using nuclear energy. Sulfur cycles have the potential for high efficiency. The approach of the project is to construct and operate an Integrated Lab Scale experiment to investigate the key technical issues. This will provide a basis for nuclear hydrogen technology decisions.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.4** for its relevance to DOE objectives.

- Perhaps the front-runner cycle for turning heat into hydrogen is some question about whether you want to connect this process to a nuclear reactor.
- The fact that the work will be providing a baseline for Nuclear Hydrogen Program decisions is valuable.
- The production of hydrogen driven by nuclear energy through the sulfur iodide thermochemical cycle has the potential to produce immense amounts of hydrogen without any emissions using only domestic resources.
- Removing hydrogen from the water-gas-shift reactor favors the conversion of carbon monoxide to hydrogen.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- Project divided nicely between three groups, some key interface areas seem to be left out. One worry I had was discovering that only ceramic materials worked for the high temperature contactor between the nuclear-heated fluids and the decomposing sulfuric acid. I was also concerned that the hydrogen may not be free enough of iodine for use.
- Integrated lab scale approach with the three modules and interface skid should facilitate testing and performance improvements.
- It is not clear how much hydrogen would be produced for various future system sizes.
- It is reasonable to use the extractive distillation process at this point; however, there should be more work on moving towards a reactive distillation technology.
- Catalyst and materials durability is a significant issue.
- There seems to be a lot of steps in this cycle, which will result in higher costs for capital, operations and maintenance, and controls.
- This is a large, well funded collaborative effort utilizing state of the art science and being performed by excellent scientists and engineers.
- The overall approach that has been taken of initial lab work, and scaling up to the fully Integrated Laboratory System is excellent. The Integrated Laboratory System can provide the information needed for scale-up to a pilot plant operation.
- Three separate excellent research groups (GA, Sandia National Laboratories, and CEA) are each responsible for one of the three steps but also collaborate with each other well. This is a very sound way to approach this complex project.
- An effective stable catalyst for the sulfuric acid decomposition is critical to success. It is good that there is separate focused effort on this issue.
- The research needed on materials of construction for the Bunsen reaction and HI decomposition areas will be done in FY09. It might be appropriate to increase the funding in this important area to ensure it is successfully completed on time vs. the Nuclear Hydrogen Initiative schedule.

- The Nuclear Hydrogen Initiative Program call for pilot plant operations at a 1 MW scale (~240 kg of H_2/day) and an engineering scale operation linked to a natural gas NP reactor in 2019 at a 50 MW scale (~12,000 kg of H_2/day). This engineering scale operation will be very expensive. Smaller scale pilot plant and engineering scale operations (perhaps .5 MW and 5 MW) should be adequate prior to commercial scale.
- Initial work on membrane reactor development followed by fabrication and testing seems reasonable.
- Low cost ceramic membranes are preferable over palladium membranes.
- Weakness: Mole sieve membrane sensitivity to water and hydrogen sulfide is not addressed.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.7** based on accomplishments.

- Built pilot scale reactor-separators. Some materials and separation issues left for later – to some extent this is legitimate, to some extent, not. Expect more for this "mature" technology. I do not believe the hydrogen cost numbers presented.
- The price tag for this work is high but good progress has been made and partners are providing some funding.
- It is not apparent how much in kind cost share is being provided.
- The graph of hydrogen price versus electricity costs is good information, however more information on the assumptions for the economic analysis should have been provided, such as projected system size and catalyst costs.
- For the resources made available for the project, progress seems modest.
- Materials is a significant focus of the project, but materials development was minimally discussed.
- It seems a major cost for this technology would be operation and maintenance. It is not clear how this was addressed in the H2A.
- Excellent progress has been made. The three Integrated Laboratory System units have been constructed and put in place to be run in an integrated manner at GA. Each unit has been started up and operated separately.
- It appears the project in general is right on the original schedule that was set except the Bunsen unit is a little behind.
- More progress (and therefore effort?) is needed on the sulfuric acid decomposition catalyst. It is critical to the success of this process.
- It is early in terms of data from the Integrated Laboratory System but there was no attempt at comparing Integrated Laboratory System or lab data performance with the assumptions used in the process cost estimate. This would be very helpful to understand how close the proven process performance is to the projected performance and cost estimate.
- Process simulation has been completed to show 84% efficiency. The researchers have not addressed if coke formation is thermodynamically predicted at these conditions, especially considering such a large amount of hydrogen is being removed from the raffinate stream.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.5** for technology transfer and collaboration.

- Excellent group. Excellent collaboration.
- Involvement by their industry and international partners is significant and provides value to the research.
- There seems to be strong collaboration and well defined roles between participants.
- There is excellent collaboration across the research groups working on this project at GA, Sandia National Laboratories, CEA, and INL.
- The project has published papers and presented at most of the key conferences so that people interested in this project and technology can follow its progress.
- Having one or more private sector nuclear energy companies as a member of the project could add additional value and insight.
- Collaborating with USC, Chevron, and Johnson Matthey. Not clear on the distribution of effort.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.2** for proposed future work.

- Key issues are recognized. Not so clear how they will be addressed.
- The proposed future work on catalyst durability, materials issues at high temperature, and optimizing the hydrogen output will be important to the success of the technology and should be completed.
- Planned work should include more catalyst development.
- They need to operate the complete integrated system.
- Increased life time tests need to be done.
- The future work plan is very good and fits well with the overall Nuclear Hydrogen Initiative program.
- It would be helpful if the Future Work Plan extended out to 2011 which is when the Department of Energy Nuclear Hydrogen Initiative Program will make its decision on what process will be used for the Nuclear Hydrogen Initiative Pilot Unit.
- Proceeding towards scale-up.
- No indication of decision points.

Strengths and weaknesses

Strengths
- Separation and materials issues; catalyst degradation issues are unresolved and appear hard to resolve. I don't believe the hydrogen cost numbers based on the materials cost + complexity of the process.
- There is a strong team that is well funded.
- The cycle they are developing is strong candidate for use in thermochemical water splitting.
- The production of hydrogen driven by nuclear energy through the sulfur iodide thermochemical cycle has the potential to produce immense amounts of hydrogen without any emissions using only domestic resources.
- This is a large, well funded collaborative effort utilizing state of the art science and being performed by excellent scientists and engineers.
- The overall approach that has been taken of initial lab work, and scaling up to the fully Integrated Laboratory System is excellent. The Integrated Laboratory System can provide the information needed for the Pilot Plant unit.
- Membrane reactor will favor water-gas-shift conversion.

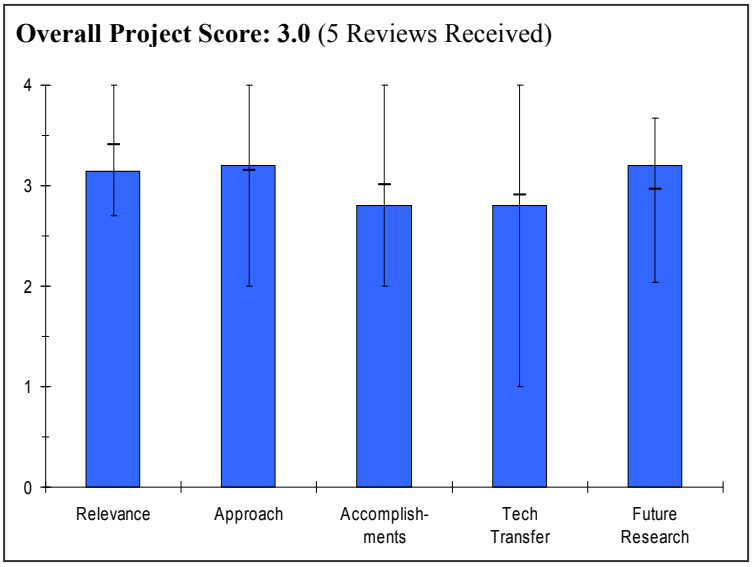
Weaknesses
- Separation & materials issues; catalyst degradation issues are unresolved and appear hard to resolve. I don't believe the hydrogen cost numbers based on the materials cost + complexity of the process. Safety worries about alumina reactor in close integration with a nuclear reactor - I would like to see a less brittle, less permeable material at this location.
- They need to increase the focus on material durability and lifetime tests.
- For the H2A analysis, they need to make sure to understand the operation and maintenance costs.
- The process has many steps and is relatively complex.
- More effort and progress is needed on the sulfuric acid catalyst.
- More effort and progress is needed on materials of construction for the Bunsen reaction and HU decomposition areas.
- It would be very helpful to compare the data from the lab and Integrated Laboratory System unit to the assumptions used in the cost estimate and to discuss how to close the gaps if there are any.
- Sensitivity of membrane to hydrogen sulfide, water is not addressed.

Specific recommendations and additions or deletions to the work scope
- More emphasis on materials and separation issues. Also address how this system might affect nuclear reactor if, for example, a leak appeared at he high temperature reactor - how do you clean up the helium loop? What are the likely capital and energy costs from cleaning up the various streams?
- Increase the effort on the sulfur dioxide decomposition catalyst.
- Increase the effort on materials of construction for the Bunsen reaction and HI decomposition areas.
- Confirm that coking is not thermodynamically predicted at water-gas-shift with 90% hydrogen removal.
- Review component / plant efficiency, cost, durability with respect to the assumed process conditions (S/C, temperature, pressure, hydrogen permeated through membrane, etc.).

Project # PD-26: Hybrid Sulfur Thermochemical Process Development
Bill Summers; SRNL

Brief Summary of Project

The overall objective of this project is to develop and demonstrate the hybrid sulfur thermochemical process as a viable option for large-scale hydrogen production using nuclear energy. The goal for fiscal year 2008 is the development and testing of an SO_2 depolarized electrolyzer (SDE) using a proton exchange membrane-type cell design. That includes to 1) optimize the HyS process design, update the flowsheet and perform cost analysis in conjunction with an industry partner; 2) continue to identify and develop improved cell components to reduce sulfur crossover and increase cell efficiency; 3) conduct single cell SDE testes at elevated temperature and pressure; and 4) install and test a multi-cell SDE with 100 lph hydrogen capacity.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.1** for its relevance to DOE objectives.

- A nice version of the heat to hydrogen cycle.
- The research is relevant to the program; however, without any cost analysis it is impossible to tell if it might meet program targets.
- Thermochemical water splitting supports the Department of Energy Hydrogen Fuel Initiative objectives.
- The production of hydrogen driven by nuclear energy through the hybrid sulfur cycle has the potential to produce immense amounts of hydrogen without any emissions using only domestic resources.
- The hybrid sulfur cycle is a far less complex cycle than the sulfur iodide cycle and thus would seem likely to be more robust in its commercial operation.
- This project involves proposed technology to manufacture hydrogen from high temperature heat.

Question 2: Approach to performing the research and development

This project was rated **3.2** on its approach.

- Concentrating on the electrolysis part - doing a fine job. Assumes the sulfuric acid decomposition & separation step is well developed; announces heat exchange and materials problems are solved. Too much effort on scale-up, not enough on development.
- Leveraging work on the acid decomposition step being performed by the Sandia National Laboratories team is a good approach and ensures the project is integrated with other research in progress.
- They are focusing on the key components.
- They need to identify and focus their development on the critical path (electrolyzer catalyst and membrane component development).
- The efficiency of the electrolyzer needs to be improved, even if they achieve their targets, the efficiency will be less than 40%.
- In the reviewer's opinion, they should focus on high temperature membranes which require less or no water, not a proton exchange membrane fuel cell.

- They may want to consider operating at a higher pressure, which may enable them to increase their operating temperature.
- Savannah River National Laboratory has teamed up with other organizations (Westinghouse, Giner, University of South Carolina, and Sandia National Laboratories) with particular expertise germane to the hybrid sulfur cycle resulting in a very good team to tackle the challenges involved with this effort.
- The project has identified the key challenges and is focused on research to overcome them. They include sulfur crossover through the membrane, a membrane with improved ion conductivity, a better and longer lasting catalyst, and good flow field/diffusion media for sulfur dioxide transport.
- Good laboratory apparatus have been and are being developed to do the needed research.
- The activity explores one unit operation in one of the more promising chemical schemes for high temperature water splitting. The activities are well focused.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.8** based on accomplishments.

- Good progress. Still over voltage is quite high – S generation in electrolyzer is problematic.
- Project funding is at a reasonable level for the work being accomplished.
- Project has accomplished important milestones; however these milestones are based on completion of tasks and not achieving quantitative results with the work.
- No information was provided on projected costs even though their plant cost analysis task is nearly complete.
- Their progress seems modest for the time and resources available for the project.
- They need to improve their electrolyzer. They may be able to increase their efficiency and possibly their durability by using a high temperature stack.
- Significant progress is being made and the effort remains on schedule.
- Significantly improved membranes that reduce sulfur crossover and enable higher temperature operations have been identified and tested.
- Catalyst work is progressing.
- A multiple cell unit has been designed, built and operated.
- An integrated plant design has been further optimized for efficient use of heat and power coupling a natural gas NP reactor to the hybrid sulfur operations to reduce hydrogen costs.
- Considerable progress, but challenges remain.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.8** for technology transfer and collaboration.

- Excellent collaboration
- Collaboration with partners to leverage proton exchange membrane R&D and process design work is apparent.
- The roles of some partners (universities, Westinghouse) are not clear.
- There seems to be a strong team, but interactions are not apparent at least in the presentation.
- There is good collaboration between the organizations working together on this project.
- They project has issued several publications and given talks at several meetings but it has not gotten the results of this effort to a broad enough audience of potential stakeholders and other scientists who might have ideas that could help the project. Presenting at conferences such as those of the American Chemical Society, National Hydrogen Association and Fuel Cell Conference could be very helpful.
- Collaborations appear internal and with vendors.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.2** for proposed future work.

- Seems prepared to address key issues.
- Multiple approaches have been identified to address the sulfur deposition problem. It will be important to solve this problem while still increasing cell efficiency.
- Focus on the electrolyzer development is appropriate for the future work.
- Improved H2A analysis needs to be done.
- The future work plan covers the key research areas and needs of this effort.
- The project has identified the key challenges and is focused on research to overcome them.
- The described activities were those to complete testing of their electrochemical reactor. However that small scale device could solve one part of the cycle they are working on, the sulfuric acid--to-sulfur dioxide problem persists. It is necessary but not sufficient.

Strengths and weaknesses

Strengths
- Good project - some progress.
- The simplicity of the process compared to other nuclear hydrogen work is a plus.
- They have a strong team.
- They are working on the critical issues.
- The production of hydrogen driven by nuclear energy through the Hybrid Sulfur cycle has the potential to produce immense amounts of hydrogen without any emissions using only domestic resources.
- The Hybrid Sulfur cycle is a far less complex cycle than the sulfur iodide cycle and thus would seem likely to be more robust in its commercial operation.
- Savannah River National Laboratory has teamed up with other organizations (Westinghouse, Giner, University of South Carolina, and Sandia National Laboratories) with particular expertise germane to the hybrid sulfur cycle resulting in a very good team to tackle the challenges involved with this effort.
- Significant progress is being made and the effort remains on schedule.
- Their electrochemical concept is sound, and could work. The team is solid.

Weaknesses
- No discussion of projected cost of hydrogen production. Even having a rough estimate of this is very important.
- The project does not seem well organized.
- Sulfur crossover will not be solved by a physical barrier as described in the presentation. Since a proton exchange membrane fuel cell uses water as the electrolyte and sulfur is miscible in water, they will always have significant sulfur crossover. They need to select a membrane that does not use water in order to decrease the crossover. The second reason that the fuel cells experience crossover is low kinetics, therefore increasing kinetics will significantly decrease their crossover.
- The key challenges of this effort may be difficult to overcome in time for the 2011 Nuclear Hydrogen Initiative planned decision on the process to scale-up to the Pilot Plant operation. Given the potential of the hybrid sulfur process, it may be appropriate to increase funding to this effort vs. the S-I process effort.

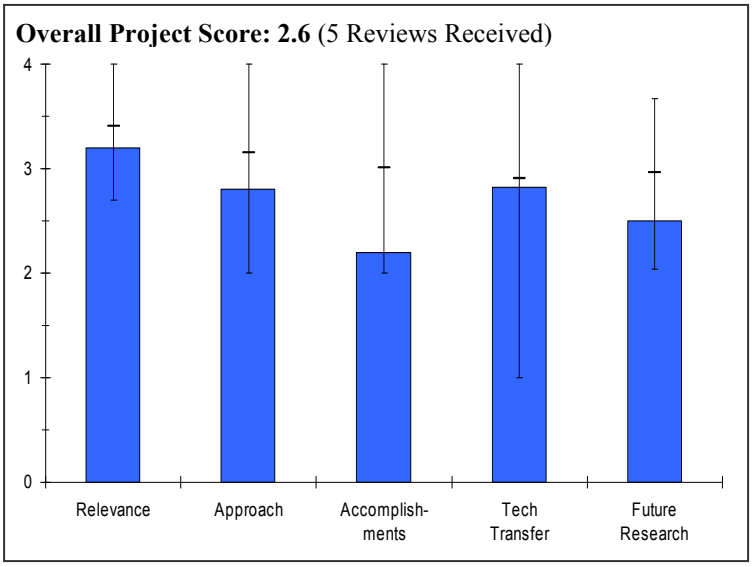
Specific recommendations and additions or deletions to the work scope

- A Go/No Go decision point based on hydrogen cost/system durability (specifically requiring a solution to the sulfur crossover issue) should be required by the Program.
- This is a very promising cycle for hydrogen production driven by nuclear or concentrated solar energy. The funding for this project should be increased. And the effort expanded to try to make more progress at a quicker pace.
- Savannah River National Laboratory is working with a proton exchange membrane fuel cell concept. The electrolysis cell design can be far simpler than the hydrogen-oxygen fuel cell. Some thought needs to be given to electrode design.

Project # PD-27: Laboratory-Scale High Temperature Electrolysis System
Steve Herring; INL/ANL/Ceramatec

Brief Summary of Project

The objectives of this project are to 1) develop efficient solid oxide electrolysis cells building on solid oxide fuel cell research; 2) decrease cost, increase durability; 3) determine reasons for long-term cell degradation; 4) optimize plant designs; 5) co-electrolyze CO_2 and steam to CO and hydrogen; 6) develop designs to apply nuclear heat and hydrogen to heavy petroleum and oil sand upgrading; and 7) integrate nuclear energy sources and fossil/biomass carbon sources for hydrocarbon synthesis.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.2** for its relevance to DOE objectives.

- Project aligns with needs of Department of Energy hydrogen production program.
- This project is developing high-temperature electrolysis for hydrogen production and therefore supports the President's Hydrogen Fuel Initiative.
- Addresses few cross-cutting barriers.
- High temperature electrolysis pertains to the Department of Energy Hydrogen Program.
- Hydrogen is produced at 1.3V at a nuclear reactor site in thermal contact with the nuclear reactor. Although this represents a modest increase in efficiency in the power used to make hydrogen, it is not clear that this increase makes up for the great increase in capital cost, and the great decrease in generator siting flexibility of putting the electrolysis unit next to a nuclear reactor.

Question 2: Approach to performing the research and development

This project was rated **2.8** on its approach.

- Approach is very good.
- Approach depends on availability of high temperature nuclear heat. It is a very long range goal.
- It appears cell degradation studies are going on since 2003 - what else can be done? No new ideas are presented to investigate the cell degradation behavior.
- This project should integrate with activities going on in SECA program.
- They have identified the critical issues and are working them in parallel.
- It would have been nice to have more discussion on the electrolyzer development.
- Carbon dioxide processing seems to be a diversion from the hydrogen production goal of this project.
- Mostly electrode potential was addressed, not durability and this was the largest show stopper. Too much emphasis on scale-up, not enough on development.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.2** based on accomplishments.

- FY08 technical objectives were clearly presented; however, there was no presentation on stack performance or degradation, and no assessment of alternative interconnect materials. In fact there has been not degradation testing initiated to date in FY08.This project is falling short of its listed objectives.
- A technical issue arising from steam corrosion in the balance of plant leading to chromia formation and contamination of the electrolyzer stack has not been addressed from last year. This problem was been solved by the fossil energy industry and a solution should be easily found by working with suppliers to the boiler industry.
- No new information on cell degradation was presented.
- Half-Integrated Laboratory System module was tested.
- Performed initial Integrated Laboratory System-single module test series (240 cells).
- Completed economic analysis for high temperature electrolysis using H2A methodology.
- Completed CFD analysis of multiple-cell stack geometry.
- Too high area-specific resistance; The hydrogen production rate decayed very fast within first 100 hours.
- Corrosion was a big issue last year, but nothing was mentioned about it in today's presentation.
- Total voltage for electrolysis was 1.3V, only about 0.2V better than for room temperature, conventional electrolysis. Durability improvements, if any, were not presented. Economic assessment details were not presented, and overall price of hydrogen projected did not look like the researchers had correctly accounted for the cost of electricity or safety or high temperature materials. It was not clear that the cost of hydrogen made this way won't be higher than for conventional electrolysis at room temperature. Corrosion problems noted last year had not been addressed.
- Lab scale tests are important to the project development.
- The SOEC stack lifetime needs to be improved. Discussion on the work in this area is necessary.
- They should consider engaging SECA for additional insights on the solid oxide electrode materials they are using.
- The H2A cost seems higher than expect, it is recommended that they engage Tiax, DTI, or others intimately familiar with H2A to review their analysis.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.8** for technology transfer and collaboration.

- Massachusetts Institute of Technology and University of Nevada Las Vegas were listed as collaborators but their roles were never explained.
- This team needs more industrial partners to execute the work plan and less academic involvement.
- Collaborating with Ceramatec, Argonne National Laboratory, Massachusetts Institute of Technology, and University of Nevada Las Vegas.
- Good to see they have evaluated a cell made by another fuel cell manufacturer.
- There seems to be adequate communication between the partners.
- Good collaboration group. Information did not seem to flow well between members.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.5** for proposed future work.

- Proposed future work is meaningless if team cannot execute planned FY08 work plan.
- This team should not be allowed to scale-up this technology and it should be transferred to an industrial partner as soon as possible.
- The project end date is FY 2015. Slide #18 gives plans for 2008 but nothing for 2009-2011 periods. Plans jump from 2008 to 2012.
- Use quantitative rather than qualitative terms for future plans. Just saying "we will continue to investigate cell degradation" is not enough. Need to be more specific about what exactly will be done.
- No plans presented to address the high area-specific resistance that is seen in the results presented today. It is important to reduce the area-specific resistance.
- Why is the corrosion issue dropped from the future plan?
- Parallel approach seems reasonable.

- Since the stack is the critical component, its development should receive more attention and resources.
- Vague - generally sounds like going in right direction regarding durability, but would prefer to see plans for scale-up shelved until durability problems solved. Ideally, would prefer to see a better economic assessment at this stage, plus plans for accelerated aging tests to show 5000 hours of electrolyzer operation with minimal degradation at a temperature that would be at least 100 degrees Celsius higher than the target operation temperature.

Strengths and weaknesses

Strengths
- Good team with solid oxide fuel cell experience.
- They are pursuing a technology that has the highest potential efficiency of all of the high temperature thermochemical water splitting technologies.
- The team seems adequate.
- They are well funded.
- Good group of researchers. Product made more hydrogen than any of the other thermal cycles presented today.

Weaknesses
- Team lacks leadership and cohesion. FY08 is 75% over and most of the key FY08 R&D issues have not been initiated.
- Lack of coordination of results. Lessons learned from prior work are not used/implemented in the on-going work.
- For example, what was learned in the assessment of degradation in long-duration test cells that was completed in 2006? How is that result used in the work going on since 2007? It is not clear to this reviewer how the results are being analyzed and used for future research.
- I think this project is going tangentially into other areas — why integrate nuclear energy and fossil/biomass sources for hydrocarbon synthesis. Focus should be on hydrogen production.
- Stack component development needs increased resources. It is the critical path.
- Durability seems like a show-stopper, economic value seemed unclear. General sense that this is not something you would want attached to a nuclear reactor.

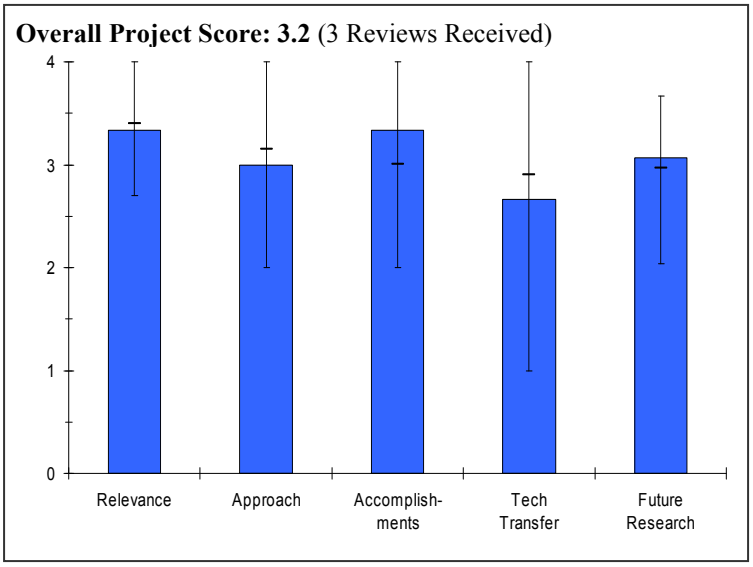
Specific recommendations and additions or deletions to the work scope

- PI should come up with a detailed research plan for 2009 and 2010.
- Delete the co-electrolysis of carbon dioxide and steam to carbon monoxide and hydrogen. Focus on steam electrolysis for hydrogen production.
- Is there a timeline to end the research on understanding the cell degradation phenomena?
- Carbon dioxide processing will only divert attention from the hydrogen production goals of the process and should be removed.
- They should have an outside company help them with their H2A analysis.
- Concentrate on improved durability and less effort on scale-up. Would prefer to see durability addressed at this scale before scaling up. Would prefer accelerated aging test that shows 5000 hours with minimal degradation at higher temperature.

Project # PD-28: Alternative Thermochemical Cycles
Michelle Lewis; ANL

Brief Summary of Project

The objectives of this project are to 1) develop a commercially viable process for producing hydrogen based on a thermochemical cycle that meets the Department of Energy cost and efficiency targets; and 2) coordinate university evaluation of alternative cycles considered in the literature as promising and down select to the most promising cycle. Selection criteria were chemical viability, engineering feasibility, projected efficiency and hydrogen production cost, and the Department of Energy-NE's timeline for an integrated laboratory-scale demonstration.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- Thermochemical water splitting for hydrogen production supports the Hydrogen Fuel Initiative.
- Work on interesting previously little studied confined thermochemical/ electrochemical cycle.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- Approach seems reasonable.
- The cycle is low temperature which enables it to integrate with solar or nuclear.
- Electrolyzer efficiency will be a critical component.
- For this "Copper-Chlorine" cycle the focus has been on improving the $CuCl_2$ to CU_2OCl_2 and electrolysis process.
- While the relatively low temperature for oxygen generation (530 degrees Celsius) has process advantages, it is limiting the energy efficiency in terms of a carrot(?) cycle analysis - need to understand this better.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.3** based on accomplishments.

- It appears that progress has been made on understanding the chemistry for all the reactions other than the electrochemical ones.
- Progress on the electrolysis is difficult to assess since only sparse data was reported.
- Overall very good work toward the development of this "Copper-Chlorine" cycle. It's not clear what the yields and selectivities were for the engineering lab scale hydrolysis reactor.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.7** for technology transfer and collaboration.

- The AEC member does not seem to be a "team player".
- Other than the electrolyzer work, there seems to be appropriate levels of interaction between the team members.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.1** for proposed future work.

- More details on the electrolysis reactor need to be reported before review on that critical component can be made.
- This project is in the early stages and significant development in each of the components and in understanding the chemistry is needed.
- Performing the proposed continuing process development research would be assisted from a better understanding of fundamentals of the underlying chemistries, particularly the operative thermodynamics.

Strengths and weaknesses

Strengths
- The cycle selected operates at relatively low temperatures making it acceptable for use in nuclear as well as solar driven systems.
- There appears to be the needed expertise on the team to address the critical issues.
- The apparently clean oxygen release at 530 is quite remarkable - a process asset.

Weaknesses
- It is not clear when this method compares with normal electrolysis with the use of excess heat use.
- Further understanding is needed on the electrolyzer operation and performance.
- Significant work will be needed on developing a durable system.
- Breaking the azeotrope and maintaining an efficient system will be difficult.
- Use of inert carrier gases will increase the operating costs significantly.

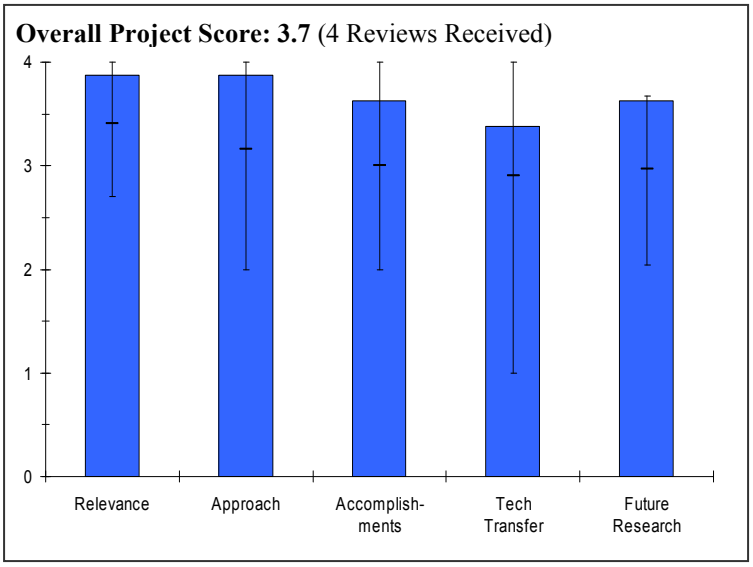
Specific recommendations and additions or deletions to the work scope

- None.

Project # PD-29: Indirectly Heated Biomass Gasification
Richard Bain; NREL

Brief Summary of Project

The objective of this project is to experimentally update the technical and economic performance of an integrated biomass gasification-based hydrogen production process based on steam gasification. The expected key outcomes are 1) production of clean syngas; 2) production of high purity hydrogen; 3) development of updated yield and gas quality correlations; and 4) development of updated technoeconomic model.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.9** for its relevance to DOE objectives.

- They have addressed issue associated with 2012 and 2017 targets of gge for hydrogen production from biomass gasification.
- The project is evaluating the production of hydrogen from biomass-steam gasification. This is a key goal of the Hydrogen Program and the work is directly supporting this objective. The work is being conducted at a scale that will provide solid data to extrapolate the costs of a larger scale system. The results will be used to determine if the Department of Energy cost target can be obtained - and based on information provided at the presentation - preliminary analysis indicates that this process can achieve the Department of Energy cost targets.
- Project milestones and targets fully supports Department of Energy RD&D objectives.
- $1.60/gge hydrogen in 2012 and $1.10 gge hydrogen in 2017 both at the plant gate are identified as the achievable project targets.
- This approach to renewable hydrogen is one of the least-costly and most ready-to-use.

Question 2: Approach to performing the research and development

This project was rated **3.9** on its approach.

- They have utilized an integrated approach for analysis that incorporated technical data, process modeling, and economic modeling which is both thorough and fundamental.
- Identified and correlated new sets of variables for analysis of gasification and reforming data.
- The work consists of a comprehensive test program at a reasonable scale (20 g/hr biomass feed).The work is evaluating all aspects of the process including gasification, hydrocarbon reforming, clean up and hydrogen separation. In addition, the work is considering process intensification - combining methane reforming and heavy hydrocarbon reforming at the same time (which is typically not done together).The work is using an existing facility that is capable of generating a large amount of useful data. The work is providing large amounts of information on all the system components.
- Objectives and milestones clearly addressed technical barriers for biomass gasification for hydrogen production to achieve Department of Energy cost targets.
- Approach is well focused on obtaining data needed to understand the barriers.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.6** based on accomplishments.

- They have completed an evaluation of gasification and tar reforming.
- They have identified and correlated new sets of variables for analysis of gasification and reforming data.
- The work is about 1/3 complete and has already generated a significant amount of data - in particular detailed composition of the syngas stream from hardwood biomass - including the higher hydrocarbons. This is valuable information for future work on biomass gasification.
- National Renewable Energy Laboratory has tested their reforming catalyst and provided extremely encouraging results. The reactor is operated as a fluid bed and can be recycled numerous times with little decrease in activity. This is a novel approach, in that the reforming is typically carried out in a fixed bed reactor.
- The work is using steam rather than oxygen gasification. This reduces the cost and helps to reach the Department of Energy cost target.
- The results are demonstrating good conversions and overall hydrogen yield.
- Completed one gasifier/reformer campaign and initial update of gasifier correlation.
- On target with 2008 milestones timeline.
- Very good approach along plan… but how far it has come to address the barriers will not be clear until the system level modeling is completed.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.4** for technology transfer and collaboration.

- The technical application of the work is clear and will benefit the refinement of this as a viable industrial process. Not clear how the PI will institute this.
- The results of the work will be published as have the results obtained previously. The work is producing detailed data that will be valuable to future research.
- National Renewable Energy Laboratory should consider involving an industrial partner - mainly just to validate the results being obtained and to get some independent input for the direction of the project.
- Project update suggests that there is good coordination with Department of Energy Biomass Program-sponsored research at National Renewable Energy Laboratory related to Gasification and tar reforming work.
- Not evident in presentation, but technology transfer axis could be very important if/when industry is ready to commercialize.
- Coordination around development of reforming catalyst might be increased.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.6** for proposed future work.

- The PI will move forward to complete gasification, reformers, and shift reactor testing.
- Evaluation of technical models and H2A economic evaluation will be completed.
- They will include an additional parameter not included in their initial parameterization - the role of the catalyst.
- The work is on schedule and the future plans are appropriate. The work will evaluate a biomass softwood feed that will provide a good comparison between two different biomass feedstocks.
- The data will allow for a good cost analysis using H2A.
- Plans include critical tasks to complete the technical work and modeling work.
- Future work includes economic analysis using H2A model and making Go/No-Go decision.
- Plans are excellent but very short term (not a criticism, I understand this is a short term program).

Strengths and weaknesses

Strengths
- This project has a strong integration of technical evaluation, process modeling, and economic modeling.
- Excellent and comprehensive project to develop detailed data and information on several important processes in the production of hydrogen from biomass feedstocks.
- Good project plan with technical and economic targets clearly identified.

- Good execution of the project plan.
- Well executed short term program to obtain data about gasification of biomass.

Weaknesses

- As it stands, the project has not dealt with the role of catalyst in product distribution (which must surely affect the downstream modeling). It seems though that this aspect will be incorporated in future work.
- None identified.

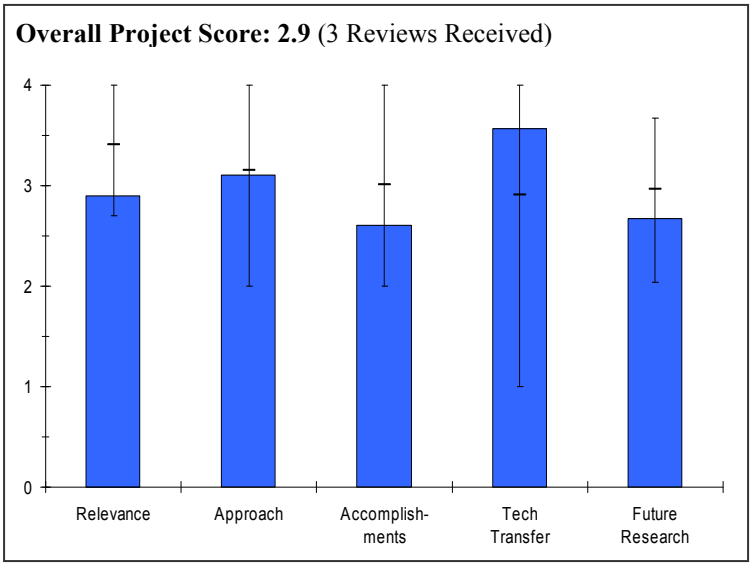
Specific recommendations and additions or deletions to the work scope

- No changes are required in the project work scope.
- It is a well organized, planned and executed project.
- This could be an important user facility if/when industry is ready to commercialize.
- Continued or occasional operation might be warranted to further improve reforming catalyst as well as processes ancillary to the gasifier, such as the separations and shift, etc.

Project # PD-30: One Step Biomass Gas Reforming-Shift Separation Membrane Reactor
Michael Roberts; GTI

Brief Summary of Project

The long-term objective of this project is to determine the technical and economic feasibility of using the gasification membrane reactor to produce hydrogen from biomass. The first year goal was to select an initial candidate membrane material that can be fabricated into a module for testing with the bench scale gasifier by evaluating ceramic, metallic, composite and glass ceramic membranes.



Question 1: Relevance to overall DOE objectives

This project earned a score of **2.9** for its relevance to DOE objectives.

- Removal of hydrogen in the gasifier should favor hydrocarbon and carbon monoxide conversion after initial gasification reactions.
- Potential for fouling of membrane by ash, tars, and/or carbon deposition. The latter becomes more likely with hydrogen removal.
- If the membrane is in the cyclone at 1500°F where there is no heat source, only the water-gas-shift conversion will be benefited. The bulk of the hydrogen will still remain with the hydrocarbons.
- They have addressed issues associated with 2012 targets of gge for hydrogen production from biomass gasification.
- They have taken on a challenging problem for which the benefits appear to be great and are in line with stated Department of Energy goals.
- Goal is to facilitate hydrogen production from biomass gasification, which is nominally aligned with Department of Energy RD&D objectives.
- The approach - of adding to the gasifier a membrane for hydrogen removal - does not clearly improve gasification. It could easily increase cost (due to added components) or decrease yield of hydrogen (because hydrogen and carbon monoxide that does not go through the membrane are downgraded to local fuel), or both.
- This can only really help with gasifier yield if it is actually deployed inside the gasifier, where the exotherm of shift can be used to supplement gasifier energy. Deploying right after the cyclone may enable use of a high temperature membrane, but that does nothing, in itself, to address gasification barriers.

Question 2: Approach to performing the research and development

This project was rated **3.1** on its approach.

- Membrane material development will be key.
- Will the membrane be tested in gasification / pre-gas clean up environment, in the presence of tars and solids (char, ash)?
- Location of membrane will be an important factor, i.e., exposure to constituents.
- Not clear if the oxygen membrane will have sufficient flux to make a reasonably compact gasifier.
- They have adopted a challenge to incorporate membranes directly into gasifier and the benefits of this approach appear to be great (calculated at 40% improvement in hydrogen production with this approach).
- Since this technology must be inside the gasifier to add value, there should be more analysis of critical barriers related to membrane survival in the gasifier environment… i.e. what materials issues are raised by exposure to ash, sulfur, etc.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.6** based on accomplishments.

- A hydrogen-membrane has been selected. Not clear if its flux is sufficient to meet their reactor size targets.
- Good sulfur tolerance at 850 °C.
- Permeation tested with syngas. Use of sweep gas improves flux – they expect to use steam as a sweep gas in their final design. How will this additional steam affect the process efficiency?
- 50% flux loss in twenty hours. What is the degradation mechanism?
- They have identified a lead candidate membrane (copper-palladium) material with which to proceed.
- They have demonstrated failure mechanisms (grain boundaries) in existing materials and developed palladium incorporation at grain boundaries in CMAS. The connection between these aspects was not clear from the presentation or whether the high palladium incorporation resulted in increased hydrogen permeability.
- Nice work exploring new approaches to hydrogen membranes, new approaches are needed to reduce or eliminate the unaffordable levels of palladium in current membranes.
- Real barriers will be exposure to gasifier environment, and there has been little progress here.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.6** for technology transfer and collaboration.

- Good team of collaborators.
- The integration of academic research with national lab and industry partners is a powerful combination.
- Good coordination among subcontractors.
- Not clear (not discussed) how much program draws best membrane ideas from broader institutions.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.7** for proposed future work.

- Membrane material development is planned. Flux goals are not mentioned.
- It is not clear why they are making thin membranes before confirming a material with high permeance and durability.
- They will continue to evaluate new materials with enhanced properties for hydrogen permeability and catalysis.
- They will expand the palladium-glass materials synthesis on larger scale.
- They will fabricate parts for hydrogen permeation studies.
- Plans are well designed to incrementally improve palladium membrane, and provide proof of concept for ceramic and glass membranes.
- It is not clear that any membrane success, applied as proposed, would address the gasifier barriers described, how actual membrane barriers will relate to exposure to gasifier environment, and the plans get to proof of concept on that feature proceed much too slowly.

Strengths and weaknesses

Strengths
- Initial focus on membrane material development is good.
- They have identified a lead candidate membrane material with which to proceed with the project while at the same time continuing to evaluate new materials for enhanced performance.
- Multiple (3) membrane approaches.

Weaknesses
- Locating membrane in cyclone where there is no catalyst or heat source is not very promising.
- Data interpretation is difficult when all experimental information is not provided.

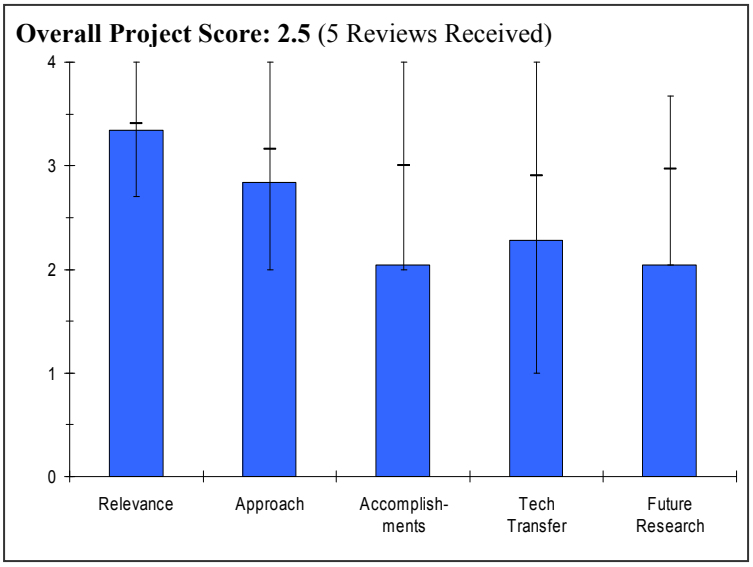
- While hydrogen in this scheme is potentially recovered through the membrane with great benefits, there is the potential that not all the hydrogen will be recovered this way. In that case the PSA will presumably have to be re-introduced thus diminishing the overall cost-benefit.
- Lack of materials exposure to gasifier environment (does not need to be a functioning membrane, even coupon exposure would allow evaluation of impact of exposure).
- The reviewer thinks this concept will really struggle to be economically advantageous. A techno-economic analysis is needed.

Specific recommendations and additions or deletions to the work scope

- Membrane testing should be conducted at conditions closer to anticipated environment - presence of tar, high hydrogen removal across membrane, etc.
- Define criterion for selecting membrane material to proceed to testing in biomass reactor.
- Better quantify the potential advantages.
- Find some way to "coupon test" prospective materials in a gasifier.

Project # PD-31: A Novel Slurry Based Biomass Reforming Process
Thomas Vanderspurt; UTRC

Brief Summary of Project



The objectives of this project are to 1) illustrate through an initial feasibility analysis on a 2000 ton/day (dry) biomass plant design that there is a viable technico-economical path towards the Department of Energy's (DOE's) 2012 efficiency target (43% lower heating value) and assess the requirements for meeting the DOE's cost target ($1.60/kg hydrogen); 2) demonstrate through preliminary results that an acid tolerant model sugar solution reforming catalyst with acceptable kinetics has been synthesized and that a viable technical path for scale up (mass production) of this catalyst in a cost-effective way exists; 3) identify hydrolysis conditions for a simulated biomass system and viable techno-economic path towards the achievement of the hydrolysis of the real biomass system; and 4) demonstrate through extensive test results an acid tolerant, long life, cost-effective biomass hydrolysis product reforming catalyst.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- They have addressed Department of Energy target goals for hydrogen production costs and lower heating value.
- Their model systems are both relevant and feasible and as such, are in line with the Department of Energy objectives.
- The work, as originally proposed, directly supports Department of Energy's objective of producing hydrogen from biomass.
- Project with its overall objectives supports the hydrogen vision and Department of Energy RD&D objectives.
- Key features outlined in the Project Progress Report propose steps toward 54.2% lower heating value energy efficiency.
- Project targets hydrogen production cost of $1.60/Kg hydrogen when biomass is obtained at $25/Ton
- Novel slurry based biomass reforming is a great concept.
- The project addresses an important aspect of the Department of Energy Program involving production of hydrogen from biomass.

Question 2: Approach to performing the research and development

This project was rated **2.8** on its approach.

- Good process concept.
- They have utilized an integrated approach for analysis that incorporated both technical and economic feasibility of using a gasification membrane for hydrogen production from biomass.
- They have tackled an important problem, and developed a nice conceptual design-synthesis-modeling approach to catalyst design.
- The original approach was to utilize molecular modeling and basic chemical principles to design and prepare effective catalysts for the proposed conversion. This is a reasonable approach, and United Technologies Research Center (UTRC) has had success with this approach in the past.

- However, based on the current technical results - this approach does not appear to be working in this project. This may be due to the fact that conversion is extremely complicated - but UTRC is having little success even with one model compound (glycerol). Conversion rates and hydrogen yields are extremely low and tend to indicate that continuing with the current approach will not lead to success.
- Project plan is addressing biomass gasification efficiency barrier.
- Project, at the present, is not addressing feedstock cost and availability barrier.
- Technical work is focused on catalyst selection and testing to improve hydrogen production in the reformer.
- Project uses mainly sugar and sugar alcohols for test cases and planning for simulated biomass system for future work.
- Good analysis of the catalyst work was provided.
- The project is well aligned with addressing the barriers listed. A "one pot" method to produce hydrogen from raw biomass is a noble goal.
- This is a very difficult project given all that must be accomplished. It is not clear that at the end of the day it would not be better to separate some of the key unit operations.
- Some important details were not clearly presented. For example, how would one separate out the lignin, ash, and protein at the end of the process?
- It is not clear that the quantum mechanical approach used by UTRC to design the water-gas-shift catalyst could simply be extended to this much more complex catalyst system with such a complex feed, especially in the absence of any mechanistic information to determine what is needed. At the end of the day, a previously developed catalyst was used.
- The HYSYS simulation demonstrating possible 54% efficiency is not helpful unless many of the assumptions that went into that model are spelled out.
- Might it be better to neutralize the acid function and then proceed?

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.0** based on accomplishments.

- Systematic progress, nicely reported. Unfortunately, results are discouraging.
- What is the hydrogen productivity expressed as mol of hydrogen produced compared to maximum achievable in the Annual Program Review? At what level do they need to be for the $1.60 target?
- Addition of $KHSO_4$ shuts down hydrogen production.
- They have achieved 50% lower heating value and production costs of $1.60/kg (although the data showing this was from last year and not presented here - it would have been nice to see).
- They have solved their problems of reproducibility by switching to stirred Zirconium autoclave reactor.
- They have solved catalyst issues by switching to a platinum/CeZrO system which has stable performance below 190º.
- To date - the project has limited technical accomplishments and progress.
- Reaction rates and hydrogen production, even with the model reactions (glycerol) is minimal. The actual feedstock will be considerable more complex. Moreover, UTRC was unable to provide any suggestions on the actual reaction mechanism for the conversion.
- Tests conducted in the autoclave indicate some hydrogen production, but UTRC could not provide any quantitative information. These tests were evidently conducted with actual biomass (sawdust) samples.
- It is not clear that UTRC was able to produce the identified catalyst structures. During the presentation, UTRC could not provide any technical or analytical information to indicate that the proposed structures were actually prepared.
- With the project approximately 50% complete, UTRC has obtained minimal (to none) positive technical results.
- Based on the current results – it is unlikely that any of the current catalysts could meet the Department of Energy cost target for hydrogen production.
- The progress report summarizes catalyst test results for several bio-based liquids, primarily glycerol. They also tested one wood sample.
- Project was started in May 2005 and three years later reported accomplishments suggest that progress has been slow. PI stated that this is partly due to funding interruptions.
- Work to date so far provided some key directional results for further future catalyst tests.

- Addition of milestones with Go/No-Go decision point for the success of catalyst in terms of both technical and economic performance will be critically important for the project.
- It is unclear why glycerol was selected as the model compound for the complex sugar solutions.
- The poisoning effect of sulfur, both by computation and by experiments with $NaHSO_4$ raised questions how this problem would be addressed.
- A statement of measured vs. required rates of hydrogen production would have been helpful to know how much greater activity must be achieved.
- Was the addition of $KHSO_4$ meant to simulate the possible effect of acid on catalyst performance? Or was it sulfur stability, or both? It was not clear how the possible negative effect of the acid function used for the hydrolysis was addressed in the test protocol.
- What level of feed conversion was achieved in Slide 15?

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.3** for technology transfer and collaboration.

- Collaborating with UND. What is their role?
- Their catalyst systems have been outsourced for synthesis, which is a good indication of the maturity and 'transferability' of that aspect of the technology.
- Tech transfer and external collaboration appears to be minimal.
- Other than the Annual EERE Hydrogen Review, only one other presentation at an American Chemical Society meeting is identified. No publications or other means of tech transfer are identified.
- The summary slide indicates some collaboration with UNDEERC - but it is not clear what this collaboration involves.
- Project report suggests that some coordination exists. It is not clear what part of the project is conducted by University Of North Dakota
- The extent of collaboration with North Dakota was not apparent.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.0** for proposed future work.

- No new catalyst strategies were discussed.
- They will show cost effectiveness of the catalyst system and identify hydrolysis conditions to optimize biomass reforming.
- They will scale-up to a 2-L autoclave to build on current successes and the planned scale-up of reaction to a 1kW demonstration scale will be an excellent validation of the technology
- There have been few technical accomplishments in this project. UTRC and Department of Energy need to come to a mutual agreement on the future work scope and redefine the future research direction.
- Project management will be more effective with inclusion of key milestones for technical and economic feasibility with Go/No-Go decision points.
- Future work suggests more catalyst testing.
- Future plans need to focus on overcoming barriers, feedstock availability and cost and efficiency of gasification.
- The future work was rather broadly defined with no specific detail. Greater discussion of the vision of the entire process would be helpful to the reviewer, and which specific tasks would be taken on in what order.
- The term "viable path" appears to be rather loosely used.

Strengths and weaknesses

Strengths
- Good process strategy to convert biomass to hydrogen.
- They have tackled an important problem, and developed a nice conceptual design-synthesis-modeling approach to catalyst design.

- The work attempts to develop active catalytic materials based on basic molecular principles. This is a reasonable approach for catalyst development (however, the current results are not supporting initial assumptions).
- Catalyst design and catalyst testing.
- Good technical team, smart people.

Weaknesses

- Result to date is not great. New catalyst approaches may be needed.
- It is not clear what the final catalyst will be in the final scale-up demonstration of the technology and whether or not they will continue the effort to develop new catalyst systems (it is not part of future plans).
- According to the summary slide - this project is approximately 50% complete and there are no solid results to suggest that UTRC should continue with the current approach.
- At the current time, this project appears to lack any clear sense of technical direction. During the presentation, UTRC indicated that they would continue to produce more catalyst materials with different metals and compositions - but there does not appear to be any clear plan for what these compositions will be.
- Based on the presentation, it is not clear that UTRC has a clear plan to separate the reaction products and the remaining unreacted solids (which could be a complex mixture).
- Milestones and Go/No-Go decisions addressing both technical and economical feasibility.
- Cost analysis.
- Lack of more specifics in terms of how the many challenges involved in this project will be addressed and handled, and in what order.

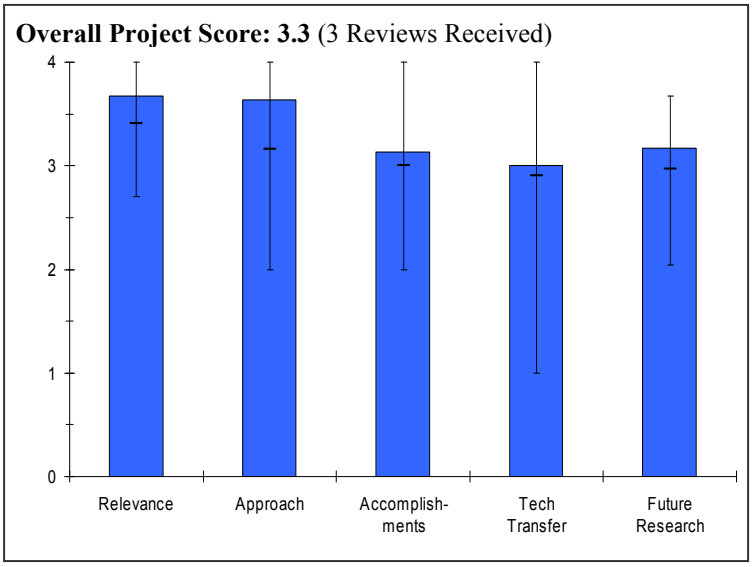
Specific recommendations and additions or deletions to the work scope

- Concentrate on the catalyst and aqueous phase reforming until breakthrough. Proceeding with water-gas-shift can at best be a distraction.
- UTRC needs to provide Department of Energy with a detailed revised work plan to complete the work.
- The work plan needs to contain specific targets, goals and objectives to ensure that the project is making adequate advancements.
- The specific milestones should be based on a semi-annual basis – and mutually reviewed (on the determined completion dates) by Department of Energy and UTRC to ensure they are being met.
- Due to the lack of technical success – Department of Energy should consider a complete revision of the current work scope.
- Addition of milestones with Go/No-Go decision point for the success of catalyst in terms of both technical and economic performance will be important for the project.
- Experimental Tasks to address economic targets in reference to Department of Energy goals.
- Inclusion of feedstock cost and availability.
- Consider some simplifications by perhaps increasing the number of unit operations to reduce problems of reactor type, acid handling, solids removal, etc.

Project # PD-32: Hydrogen From Water in a Recombinant Oxygen-Tolerant Cyanobacteria System
Qing Xu; J Craig Venter Institute

Brief Summary of Project

The objective of this project is to develop an oxygen tolerant cyanobacterial system for continuous light-driven hydrogen production from water. The approach is to transfer oxygen tolerant hydrogenases into cyanobacteria to overcome the hydrogenase oxygen sensitivity issue. Environmental DNA encoding hydrogenase was converted into a functional hydrogenase with both hydrogen evolution and uptake activities.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.7** for its relevance to DOE objectives.

- The project goals are well-aligned with Department of Energy program targets for novel biologically-derived catalysts for hydrogen production.
- The focus on identification of novel hydrogenases is good.
- The focus on increasing the level of hydrogen production from the heterologous system is good.
- Obtaining oxygen sensitive hydrogenase and developing molecular biology-based techniques to manipulate the enzyme is absolutely critical to the initiative.
- It seems relevant. However, explanation was very complex, making it difficult to assess relevance.

Question 2: Approach to performing the research and development

This project was rated **3.6** on its approach.

- The metagenomic approach for identification of novel hydrogenase-related sequences is logical, and builds upon progress in the investigators' lab.
- The focus on construction of new molecular biology toolkits for introducing hydrogenase-related gene cassettes into heterologous host strains is appropriate.
- The control experiments have been carefully designed to increase confidence in the experimental results with the heterologous expression studies.
- The use of retrogenomes as sources of hydrogen genes is very exciting. The approaches are appropriate, although it is not clear why they choose the genes that they did.
- Approach seems reasonable, however hard to assess in given presentation.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.1** based on accomplishments.

- The progress towards goals was excellent, with reconstruction and identification of a novel environmental nickel-iron hydrogenase and stable expression in a heterologous host.
- Demonstration of hydrogen production from the novel nickel-iron hydrogenase was good.
- There was good progress in demonstrating the correct maturation and targeting to membrane fraction of the Thiocapsa hydrogenase in the heterologous Synechococcus host.
- There was good progress towards introducing other hydrogenase genes into different heterologous cyanobacterial hosts (e.g. Synechocystic 6803).

- It is important that catalytically active enzymes were not obtained but it is clear that the PIs are very close to achieving their goal

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- Good evidence was presented for coordination with other university investigators, including some not formally listed as co-investigators on the project (Michigan State University).
- Good partnerships/MTA with international entities for global ocean survey genome mining project.
- The J. Craig Venter Institute and National Renewable Energy Laboratory components seem quite distinct and parallel, displaying little synergy.
- The two institutions bring enormous expertise in molecular biology and the growth and physiology of anaerobes and hydrogenase biochemistry. However, the interactions between the PIs need to be developed further to obtain the achieved enzyme.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.2** for proposed future work.

- Future goals of stable hydrogenase subunit expression in industrial "workhorse" E. coli strains are good.
- Introduction of different environmental hydrogenases into various heterologous expression host strains is logical and appropriate.
- This was not as usefully described as it might have been. The resources of the PI and JVCI in bringing high throughput assays to this project should be a priority.

Strengths and weaknesses

Strengths
- The investigators' knowledge of canonical hydrogenases and structure-function relationships is very robust.
- The investigators' track record of novel gene identification and development of synthetic biology toolkits is very strong.
- The multi-pronged use of different combinations of known hydrogenases, novel hydrogenases, different maturation cassettes, and different heterologous hosts ensures casting a wide net for knowledge of optimizing hydrogenase activity.
- The experiences of the PIs and their inhibitors, the unlimited "molecular" resources in terms of the metrogenomes and the overall project goals.

Weaknesses
- The project has not identified contingencies for identification of novel, noncanonical hydrogenases. Although screening experiments have been proposed, it is not clear how the screens will be designed to discriminate between low level of protein expression or stability but extremely high activity vs. high level of protein expression or stability with modest hydrogenase activity. Some more defined metrics would have been preferred.
- The project has not demonstrated hydrogenase activity in the catalytic subunit expressed in the heterologous E. coli host
- The project has not identified contingencies for co-evolution of novel hydrogenases; perhaps targeting the catalytic subunit is not the target with the highest return—what if testing accessory genes from environmental samples will provide a new way to protect the existing hydrogenases from destruction?
- It is a pity that the active enzymes were not obtained but this is only a matter of time.
- All of the pieces are in place for the PIs to be successful.

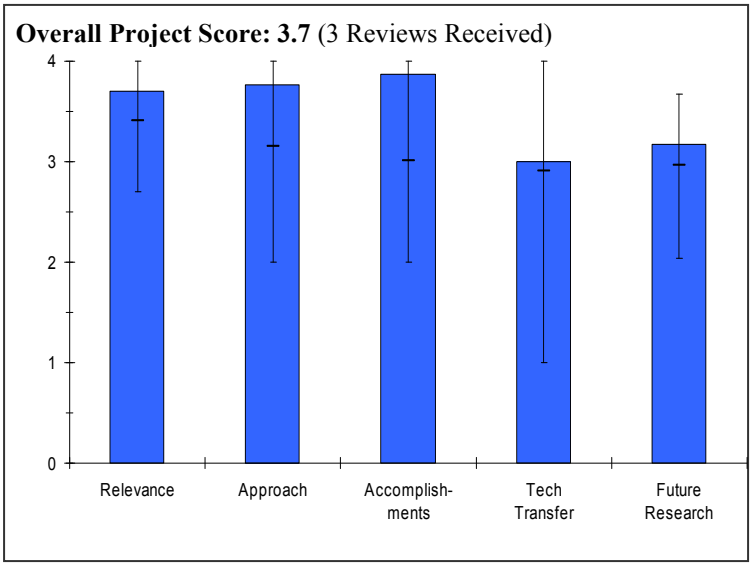
Specific recommendations and additions or deletions to the work scope

- None.

Project # PD-33: Maximizing Light Utilization Efficiency and Hydrogen Production in Microalgal Cultures
Tasios Melis; UC Berkeley

Brief Summary of Project

The objectives of this project are to 1) minimize the chlorophyll antenna size of photosynthesis to maximize solar conversion efficiency in green algae; 2) identify and characterize genes that regulate the Chl antenna size in the model green alga *Chlamydomonas reinhardtii*; and 3) apply these genes to other green algae as needed. The approach is to 1) interfere with the molecular mechanism for the regulation of the chlorophyll antenna size; and 2) employ DNA insertional mutagenesis and high-throughput screening to isolate tagged green algae with a smaller Chl antenna size.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.7** for its relevance to DOE objectives.

- The project goals are well-aligned with Department of Energy program targets for maximizing efficiency of biologically-derived hydrogen production.
- The focus on construction of a minimal photosynthetic antenna complex is good.
- Increasing solar conversion efficiency in algae is a fundamental priority.
- Very relevant for biological production.

Question 2: Approach to performing the research and development

This project was rated **3.8** on its approach.

- The discovery-driven approach for screening of efficient hydrogen production from reduced antenna is appropriately conducted.
- The focus on usage of molecular biology toolkits for introducing altered hydrogenase-related gene cassettes into heterologous or homologous host strains is appropriate.
- Not well described but the results speak for themselves.
- Strong emphasis on outcome - good!
- Good explanation of how this is working and how it will work.
- Clear representation of complex issues.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.9** based on accomplishments.

- The progress towards goals was excellent, with efficiency targets achieved ahead of schedule.
- Dramatic improvement over the last four years. Excellent progress.
- Have already completed 2010 milestones.
- Fascinating correlation of Tla1 gene in other species.

PRODUCTION AND DELIVERY

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- Specific transfer of technology via licensing to a start-up algal biofuels company is excellent
- This is a weakness of the project. The PI need to collaborate with groups involved in engineering hydrogen production. This area needs to put 2+2 together to make 4.
- This is a sole source project.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.2** for proposed future work.

- Future goals of quantification of photosynthetic yields in tla mutants are well-defined.
- Advanced biophysical analyses of tlaX and tlaNew mutant seem unnecessary in view of the achievement of target volumetric goals.
- With great success this project need to move to the next level and involve hydrogen production.
- Clear track on tlaX and tlaNew research.

Strengths and weaknesses

Strengths
- The investigators' knowledge of photosynthetic systems is very robust.
- The investigators have demonstrated superior progress towards defined goals.
- The identification of a novel gene regulating antenna size is interesting and unique.
- Accomplishments to date are impressive.
- The main researcher gives mush strength to this project.

Weaknesses
- The project has not completed comparative genomic analyses to determine biological function of tla1 (and its alleles). If this gene is present in a variety of organisms ranging from microbes to humans, there ought to be more information known about its role in those other organisms, perhaps relevant to what it is doing in algae.
- Are tlaX and tlaNew alleles of tla1? Do they represent different genes with redundant functions? Do the represent members of a gene family?
- Are there synergistic or pleiotropic effects of tla that might shed light on its role in antenna size?
- The investigators have not demonstrated hydrogen production, merely vigorous gas production.
- It is unclear how full-scale molecular genetic, biochemical, physiological characterization of tlaX and tlaNew strains will be conducted and thus actually shed knowledge on potentially pleiotropic effects on antenna size. A systems biology approach might be fruitful to decipher regulatory effects.
- Lack of collaborations to involve hydrogen aspect.

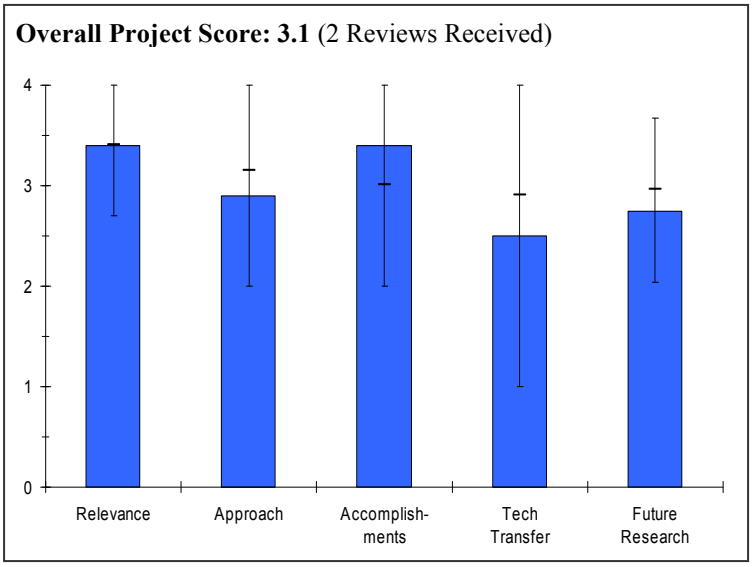
Specific recommendations and additions or deletions to the work scope

- Keep going!

Project # PD-34: Use of Biological Materials and Biologically Inspired Materials for Hydrogen Catalysts
Trevor Douglas; Montana State University

Brief Summary of Project

The objectives of this project are to 1) optimize the hydrogenase stability and electron transfer; 2) optimize the semiconductor nano-particle photocatalysis, oxygen scavenging and electron transfer properties of protein nano-cages; 3) perform gel/matrix immobilization and composite formulation of nano-materials and hydrogenase; and 4) perform device fabrication for hydrogen production. Montana State will incorporate hydrogenase and mimetics into stabilizing matrices as well as into electroactive poly (viologen matrices).



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.4** for its relevance to DOE objectives.

- The project goals are well-aligned with Department of Energy program targets for novel biologically-derived catalysts for hydrogen production.
- The focus on improvement of hydrogenase stability is good.
- The focus on improvements of enzymes and catalyst supports is good.
- Obtaining stable catalyst and comparing the biological and inorganic versions side by side is very worthy.

Question 2: Approach to performing the research and development

This project was rated **2.9** on its approach.

- The approach for targeting the nickel-iron hydrogenase is logical, and builds upon progress in the investigators' lab.
- The focus on encapsulation of purified hydrogenase within the sol-gel is interesting, and has demonstrated success in increased stability at room temperatures.
- The platinum cluster encapsulated within protein cages is clever and represents a good target for achieving improved catalyst activity with corresponding palladium encapsulated nanoparticles.
- The approach demonstrates a good synergism between enzymology and protein structure-function with materials composite synthesis and design.
- Overall theme was appealing but the goals were not specific.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.4** based on accomplishments.

- The progress towards goals was difficult to ascertain, and had to be specifically drawn out of the oral presentation. The target goal of improved fold stability (80% as stated) was not easily related to the information presented on protection from external protease action vs. activity enhancement due to sustained protection from oxygen inactivation.
- Encapsulation of active hydrogenase and recovery of activity encapsulated in Sol-Gel showed very good progress.

- There was good progress in demonstrating the linear relationship between activity and platinum cluster size.
- Unfocused presentation. It was not clear just what has been achieved, how the different aspects related to each other, and where each would go in the future.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.5** for technology transfer and collaboration.

- Effective collaboration with industrial partners was demonstrated, with the use of specialized photochromic and thermochromic films.
- Does not appear to be at the stage to take to the next level.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.8** for proposed future work.

- Future goals of incorporation of stable and active catalysts into polyviologen matrices were good.
- Full implementation and testing of the prototype device is a logical and feasible goal.
- Only very general plans with specific milestone.

Strengths and weaknesses

Strengths
- Project strengths are the investigators' knowledge of nickel-iron hydrogenases and structure-function relationships.
- Strong biological experiences and background of the PIs.

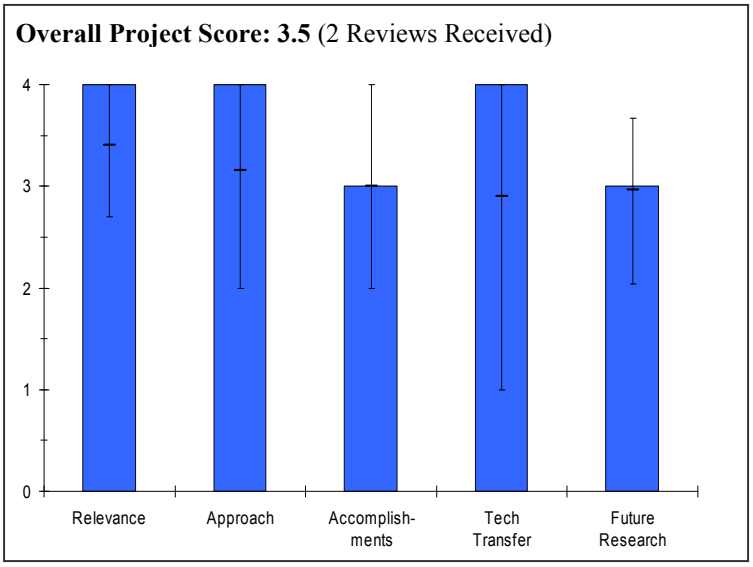
Weaknesses
- The project did not clearly define its benchmarks for hydrogen production, with respect to improvements in enzyme stability, enzyme activity, or metrics for sol-gel encapsulants or supported/caged matrices.
- Underdefined and unfocused research plan.

Specific recommendations and additions or deletions to the work scope

- None.

Project # PD-35: Photoelectrochemical Hydrogen Production: UNLV-SHGR Program Subtask
Eric Miller; MV Systems

Brief Summary of Project



The primary objective of the Department of Energy (DOE) Photoelectrochemical (PEC) Working Group is to develop practical solar hydrogen-producing technology using innovative semiconductor materials and devices research and development to foster the needed scientific breakthroughs. The objectives of the DOE-SHGR PEC are to 1) identify and develop PEC thin-film materials systems compatible with high-efficiency, low cost hydrogen production devices; 2) demonstrate a functional multi-junction device incorporating best-available PEC film materials; 3) develop collaborative avenues (national and international) integrating the best theoretical, synthesis and analytical techniques, for optimizing future PEC materials and devices; and 4) explore avenues toward manufacture-scaled devices and systems.

Question 1: Relevance to overall DOE objectives

This project earned a score of **4.0** for its relevance to DOE objectives.

- Focused on key issues of solar to hydrogen using photoelectrochemical.
- Concern about cost issues.
- Set goal to out-perform photovoltaics + electrolysis.
- Realistic understanding of the barriers to practical success.
- The photoelectrochemical working group is an important effort aimed at coordinating research from a dozen institutions. The University of Nevada, Las Vegas-SHGP program is an effort to discover new photoelectrochemical hydrogen materials using theory, synthesis and analysis.
- There was almost no original science in this presentation.

Question 2: Approach to performing the research and development

This project was rated **4.0** on its approach.

- Good integration of theory, synthesis, surface science, and electrochemistry.
- Program takes advantage of knowledge base available in solid-state electronics/physics.
- State of the art materials characterization.
- The concept for this project, the development of the photoelectrochemical "tool chest" is sound.
- WO_3 has too large a band gap to be useful in a practical system. N incorporation, as admitted, cannot improve the material.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- Interesting new materials have been identified that demonstrate the power of the integrated approach.
- State of the art (and in-house developed) characterization.

PRODUCTION AND DELIVERY

- Elegant next generation materials have been produced.
- So far, most of the effort in this project has been directed towards assembling "tools". Comparatively little has been accomplished in terms of discovering new materials with improved properties.
- Almost no time in the talk was devoted to any specific technical accomplishments.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **4.0** for technology transfer and collaboration.

- Exceptionally strong collaborations that have leveraged unique abilities.
- Coordination with other institutions is a very strong focus for this project.
- This is almost a subcontract to transfer some program administration to University of Hawaii?!

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- The Program outlined is on-track.
- New materials should continue to be generated and characterized.
- Development of community-wide standardized protocols is critical.
- While interaction with other researchers is fine, this group needs to focus on discovering and characterizing some new classes of photoelectrochemical materials rather than just extending the findings from other groups.
- I didn't see any specific or original research ideas.

Strengths and weaknesses

Strengths
- Important collaborations.
- Important development of a community resource for characterization.
- Access to instrumentation and interactions.
- They seem to be good at networking and facilitation, but not clear on science.

Weaknesses
- None.
- Lack of new ideas about classes of materials to explore.

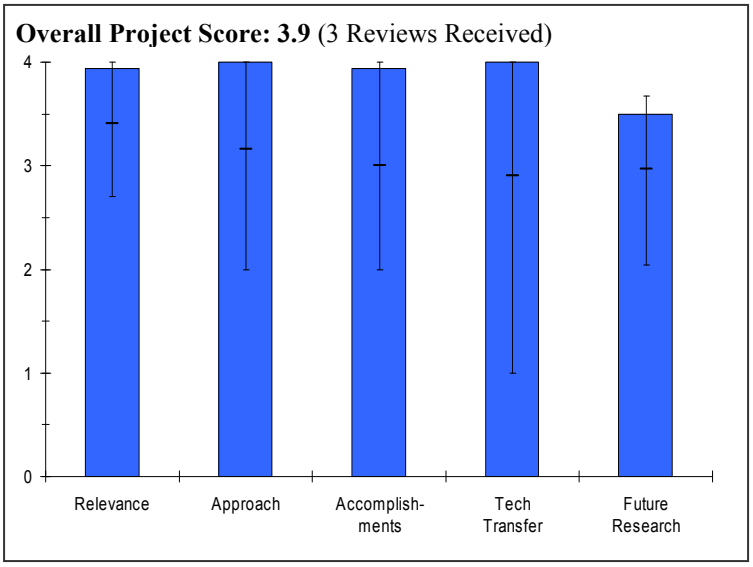
Specific recommendations and additions or deletions to the work scope

- Continue as is.
- Make finding new materials the major focus of research rather than developing tools.

Project # PD-36: Photoelectrochemical Water Splitting
John Turner; NREL

Brief Summary of Project

The objective of this project is to discover and characterize a semiconductor material set or device configuration that 1) splits water into hydrogen and oxygen spontaneously upon illumination; 2) has solar-to-hydrogen efficiency of at least 5% with a clear pathway to a 10% water splitting system; 3) exhibits the possibility of 10 years stability under solar conditions; and 4) can be adapted to volume-manufacturing techniques. The main objective for the past year has been to develop and optimize state-of-the-art materials that we have identified as promising for meeting the Department of Energy's near-term efficiency and durability targets and to develop PEC modeling and analysis efforts.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.9** for its relevance to DOE objectives.

- Development of new materials that will allow pragmatic solar to hydrogen production.
- Realistic goals for conversion efficiency.
- Understanding that photoelectrochemical must compete on all levels with photovoltaics + electrolyzer.
- Turner's group at National Renewable Energy Laboratory has been a consistent bright spot in the photoelectrochemical hydrogen field since 1991. His research program is critical for progress towards Department of Energy goals and objectives.
- Very clear articulation of objectives and relevance.
- Very direct presentation of simultaneous need for efficiency, durability, and energetics.
- Graphic description of max current density/ %IPCE/ eV.
- Good basic science to understand the limitations of various classes of materials.

Question 2: Approach to performing the research and development

This project was rated **4.0** on its approach.

- Use of knowledge base to generate new multi-element materials (alloys?).
- Excellent electrochemical characterization.
- Amazing solid-state synthesis capability.
- Good mix of theory and wet chemistry (important approach – start with a known material, use theory to suggest improvements, make theoretically suggested materials and see what happens).
- Due to his deep understanding of photoelectrochemistry, the PI is able to choose materials that have high potential. His willingness to utilize breakthroughs from the photovoltaics community and to engage theorists have led to technological and conceptual breakthroughs.
- John's oral presentation was direct, clear, and concise.
- Assertion that photon-to-electron conversion efficiency must equal or exceed photovoltaics systems was clear.
- Similarly, the color correlations for the InN/GaN alloys made his correlations to eV transitions very clear.
- Good connection to DFT calculations.

- The PI has knowledge and experience with most all techniques needed to characterize photoelectrochemical materials.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.9** based on accomplishments.

- New GaN+InN= GaInN system (very interesting).
- New low temp synthesis of Cu_xSe_y thin films.
- New SiN systems.
- New ZnO+N (nice interaction of theory and experiment).
- Despite recent budgetary issues, this group had produced many new results on photoelectrochemical materials. Experimental and theoretical results on InGaN, $CuGaSe_2$, SiN, CoFeAl oxide were all new and interesting.
- Systematic presentation of key points by examples: mixed metal oxides, GaN/InN alloys (band gaps and transitions correlations), $CuGaSe_2$ thin film studies.
- Connections to theory.
- The nitrides are interesting but are still very inefficient.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **4.0** for technology transfer and collaboration.

- A historical record (which continues) of collaboration with universities and industry.
- Virtually all of the other photoelectrochemical hydrogen presenters acknowledged significant interactions with the Turner/National Renewable Energy Laboratory project.
- Well-documented collaborations with: DFT group, other National Renewable Energy Laboratory teams (photovoltaics), CSM.
- Good interaction between experiments and theory.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.5** for proposed future work.

- Program is ending since it is not a Department of Energy funding priority.
- I was VERY disappointed to learn that Department of Energy is not planning to continue funding for this program. What a ridiculous decision.
- Builds on the GaN/InN materials and extrapolates to other III-V nitrides.
- Continues photoelectrochemical WG collaborations.
- Turner knows enough and has enough experience to make good decisions about projects and paths.

Strengths and weaknesses

Strengths
- This program has powered the hydrogen Program photoelectrochemical work since its beginning.
- Excellent science.
- Excellent collaboration.
- Innovative ideas, solid results on a variety of new materials, expertise of PI and other National Renewable Energy Laboratory researchers associated with the project.
- Well-presented and systematic articulation of key principles.
- Well defended series of exploratory work with correlation to theory.
- PI has a vast experience in photoelectrochemistry. Many students are getting exposure to and trained in photoelectrochemical techniques at NREL.

Weaknesses

- None.
- None, other than lack of adequate Department of Energy funding.
- Needs more computing power to calculate more band structures to identify materials trends.

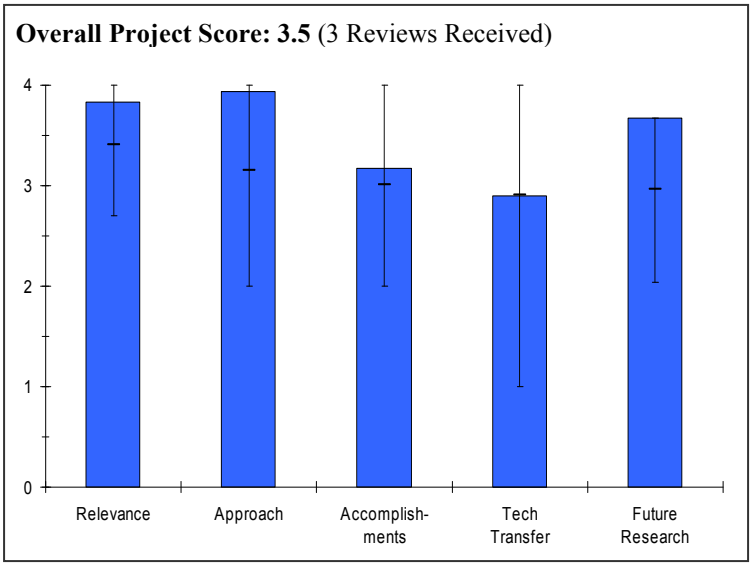
Specific recommendations and additions or deletions to the work scope

- Although money is limited and hard decisions have to be made, I believe discontinuation of this program represents a critical path error.
- Provide adequate funding so that work in this important area, and by this group, can continue.
- Keep up the good work and the collaborations (and the strong summary of findings).
- Provide more computation resources.

Project # PD-37: Critical Research for Cost-Effective Photoelectrochemical Production of Hydrogen
Liwei Xu; Midwest Optoelectronics

Brief Summary of Project

The objectives of this project are to 1) develop critical technologies, including transparent, conducting, and corrosion resistant coatings and photoactive semiconductor materials, required for cost-effective production of hydrogen from sunlight and water using thin film-Si based photoelectrodes; and 2) develop and demonstrate at the end of the three-year project, tf-Si based photoelectrochemical photoelectrodes and device designs with the potential to achieve systems with 8% solar-to-hydrogen efficiency with a durability of 1,000 hours by 2013.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.8** for its relevance to DOE objectives.

- Follows Department of Energy proposed standards for photoelectrochemical solar to hydrogen.
- Silicon-based systems.
- Aimed at real world stability.
- This project provides a good balance with respect to other material - discovery oriented projects. The project addressed a number of important applied issues associated with development of photoelectrochemical-hydrogen technology.
- While not clearly a photoelectrochemical project, this "almost" commercial system shows a functional, practical approach to hydrogen production with sunlight.
- Two approaches - immersion cell and substrate cell also illustrates two practical time-lines (mid-term and long-term) toward commercialization. The Department of Energy needs more such "market transformational" projects.
- This project is largely engineering, but as engineering projects in this area go, this one shows some promise of producing an actual prototype.

Question 2: Approach to performing the research and development

This project was rated **3.9** on its approach.

- Two viable approaches.
- In situ photoelectrochemical.
- Integrated photovoltaics-cell.
- New corrosion resistant front surface junction materials (alloyed ZnO).
- Tunable multijunction photovoltaics to match water splitting energetic needs.
- Philosophy: use materials that have low technology barriers.
- The project leverages Midwest's expertise in manufacture of multi-junction thin film photovoltaics devices. Two distinct approaches are being developed for photoelectrochemical water-splitting cells (immersion-type and substrate type). Both approaches are worth exploring.
- It is good to have "practical" projects than just the traditional "support the labs-type" basic research.
- The approaches here recognize practical engineering challenges and the focus on TCCR materials is methodical with clear Go/No-go decision points - Bravo!

- The concept is just a solar cell immersed in an electrolyte. The advantages of this over an external solar cell and an electrolyzer are not clear. An advantage is the adjustable band gap and perhaps cheaper than the separate systems.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.2** based on accomplishments.

- Develop triple junction photoelectrode.
- Develop corrosion resistant oxide layers.
- Large scale electrodes are now available (1x3 feet) but not protected at this time.
- High quality ZnO layers have been made and characterized.
- Demonstrate defect shunting.
- Test large area photoelectrodes 12x12 (some degradation observed with time in outdoor testing - 3% conversion is observed).
- Considerable progress has been made towards the goals of this project; however, most of the results were for existing photovoltaics materials. Despite its importance to the immersion type approach, little information was presented on the TCCR films.
- No earth-shaking basic discoveries, but very solid engineering progress.
- The need for improved TCCR's (for the immersion systems) and for the semi-con/electrolyte junction layer (for the substrate systems is well articulated.
- The technology for large area αSi cells is being developed independently from this project.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.9** for technology transfer and collaboration.

- Good collaborations on underlying science.
- Strongest interactions are with University of Toledo.
- National Renewable Energy Laboratory collaborations well explained; so was the connection to the University of Toledo.
- Not sure about the role of Xunlight.
- Definitely a technology transfer from the lab to a developmental company.
- This project has the possibility of producing a commercial system to "test the water" for photoelectrolysis.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.7** for proposed future work.

- Good materials and chemical strategies.
- Good engineering approaches.
- If this project can be successfully completed, it will constitute an important, practical benchmark for an integrated photoelectrochemical hydrogen system.
- Again, solid engineering considerations for both types of systems.
- No clear exposition of what the next generation oxides or classes of materials are being considered.
- Good direct coupling of solar capture and electrolysis in the substrate-type system.

Strengths and weaknesses

Strengths
- Good engineering.
- Good manufacturing capability already in place.
- Good approach (and collaborations) on materials science.
- Low technology barrier approach is a plus.

PRODUCTION AND DELIVERY

- Existing fabrication expertise at Midwest and commitment to developing systems for solar hydrogen generation.
- Practical demonstration of near-commercial system.
- Very clear presentation of project background and approaches.
- Very solid understanding of engineering design and challenges.
- Will be a good demonstration of photoelectrolysis in an integrated system. There may be some advantages to local hydrogen generation rather than separate electrolyzers other than simply cost.

Weaknesses

- Cells have net efficiency now of 3% even though the photovoltaics works at 12%.
- Work on electrocatalysts is needed.
- Maybe a shortage of publications and presentations, but understandable for a project in a company.
- No indication of economics (capital, operations and management, etc.).
- No attempt to estimate life-times of systems/components, etc.
- I have a feeling that this is a small side interest for the company rather than their major thrust which is to produce αSi solar cells.

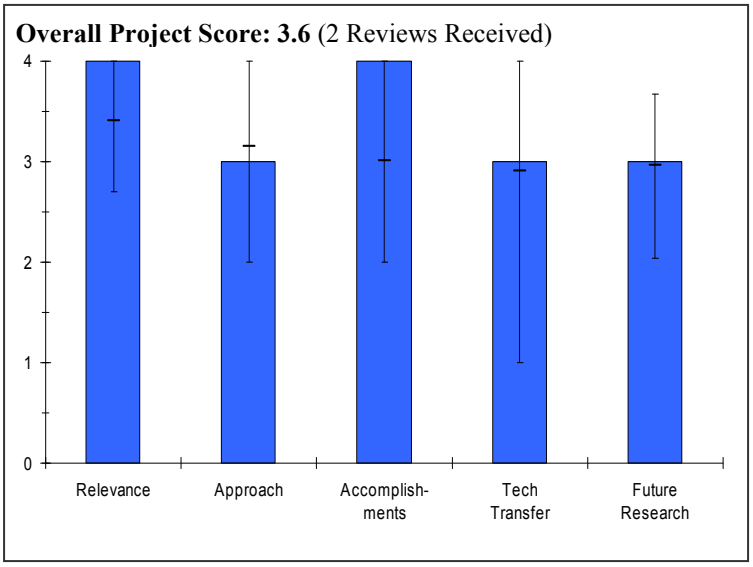
Specific recommendations and additions or deletions to the work scope

- Wonderful program, continue it.
- Plans for future are sound.
- Keep up support of such "near-term commercialization" projects to balance out the multitude of basic, fundamental research.
- Need more support of "engineering" projects, which explore engineering challenges.

Project # PD-38: Development and Optimization of Cost Effective Materials for PEC Hydrogen Production
Eric McFarland; U. of CA Santa Barbara

Brief Summary of Project

The overall project objective is to discover and optimize an efficient, practical and economically sustainable material system for photoelectrochemical (PEC) production of bulk hydrogen using solar light energy as the primary energy input making use of novel syntheses and high throughput experimentation methods. The task objectives of this project are to 1) identify improved materials for solar photon absorption using high throughout methods and exploratory design and synthesis of new mixed metal-oxides; and 2) optimize the morphology of the PEC material system for maximum efficiency.



Question 1: Relevance to overall DOE objectives

This project earned a score of **4.0** for its relevance to DOE objectives.

- Addresses key programmatic issues related to solar to hydrogen via photoelectrochemical production.
- Addresses solar optical response limitations.
- Attempts to incorporate cost issues up front.
- Uses a 10% conversion Go/No Go decision screen.
- This project is advancing many areas of understanding and technology in the area of photoelectrochemical hydrogen production.
- Materials development is important to the goal of efficient photoelectrochemical water splitting. αFe_2O_3 is not a material that can be efficient, but it is a useful prototype system for understanding lower band gap metal oxide photoelectrodes.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- Project has identified key limitations in materials synthesis.
- There is very little understanding developed of the chemical mechanisms that are limiting control over the material.
- Program uses (in combination) many well-known materials approaches.
- Results, while useful, are empirical and thus not producing strong guiding principles. The suggestion that glucose or glycol be used as the oxidant makes no sense (thermodynamics are downhill, i.e. no optical conversion.)
- The PIs tasks #1-5 represent a nice combination of combinational and directed science that is likely to achieve many of the project's objectives. Pursuing tasks #6-9 at this point in time is premature.
- McFarland is an experienced and creative materials scientist. My opinion, however, is that the homogenous (slurry) systems will not be viable.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **4.0** based on accomplishments.

- Synthetically strong program.
- Improved optical response and ICPE of native Fe_2O_3.
- No progress to date on an actual reactor or reactor design.
- Water splitting has been observed at short circuit (very important).
- Some system stability has been observed, but not tested to the extent needed to draw pragmatic conclusions
- Despite some interruptions in funding, the PI and his group have made good progress in improving the ability of Fe_2O_3 and related materials to split water.
- Has made progress in understanding αFe_2O_3 that may be useful when developing other low gap oxide materials or for using αFe_2O_3 in a tandem system.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- Number of publications and presentations are moderate, but PI does interact in significant way with photoelectrochemical community.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- Program is on-track. It should continue as is with a focus on issues of stability and conversion efficiency.
- For the most part, future plans are sound. As indicated in tasks #6-9, PI seems determined to develop a photoelectrochemical structure that mimics a cell, despite the obvious problems with such systems.

Strengths and weaknesses

Strengths
- Strong materials synthesis approach.
- Good real-world evaluation of systems.
- High level of expertise in material synthesis and characterization.

Weaknesses
- Perceived weaknesses may be a result of zero funding last year.
- Issues are: materials stability testing, the use of glucose etc. in place of water oxidation which dramatically decreases solar conversion efficiency (one is adding in an effective combustion component).
- Inclination to "engineer" a complete system before finding an adequate photoelectrochemical material.

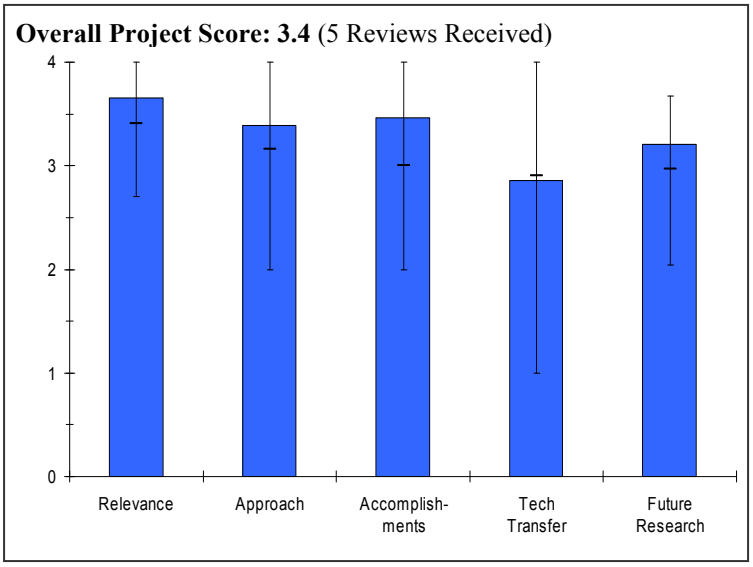
Specific recommendations and additions or deletions to the work scope

- Continue with everything except alternate oxidation reactions.
- Less emphasis on tasks #6-9.

Project # PD-39: Scale-up of Hydrogen Transport Membranes for IGCC and FutureGen Plants
Doug Jack; Eltron Research Inc.

Brief Summary of Project

The overall project objective is to develop a H_2/CO_2 separation system that 1) retains CO_2 at coal gasifier pressures; 2) operates near water-gas shift conditions; 3) tolerates reasonable achievable levels of coal-derived impurities; 4) delivers pure H_2 for use in fuel cells, gas turbines and hydrocarbon processing; and 5) is cost effective compared to alternative technologies for carbon capture.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.7** for its relevance to DOE objectives.

- Economic and practical hydrogen separation/purification is essential to the industry.
- Hydrogen production from coal is one of the goals of the President's Hydrogen Fuel Initiative.
- This project is clearly important to hydrogen production from coal and contributes to achievement of Department of Energy's hydrogen separation goals and the goals of the Fossil Energy office.
- The project may help to enable coal gasification as a hydrogen production option in a carbon-constrained environment.
- Matches well with carbon dioxide sequestration - no pressure drop. However, re-pressurization for hydrogen is required.
- Thermodynamic advantages are favorable.
- Small and large units are possible.

Question 2: Approach to performing the research and development

This project was rated **3.4** on its approach.

- Good approach, as it is focused beyond just membrane material and how to make a working membrane module.
- Comprehensive approach to scale-up/demonstration and incorporating test and evaluation results.
- It seems they could test the membrane separator on a slip stream or simulated feed rather than a H_2/N_2 mix.
- Durability tests should include tolerance to contaminants such as sulfur, trace metals, etc. Understanding the impact of sulfur is a key to success.
- Longer term life tests and / or accelerated life tests are needed.
- The approach appropriately incorporates gradual increases in the scale of hydrogen production to address the technical challenges associated with each scale.
- The stage gate approach is appropriate but Go/No Go decision points with clear criteria should be incorporated to guide direction of the project at the various production scales proposed.
- Self-supporting membrane is very ambitious considering the need for high efficiency (thick membrane).

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.5** based on accomplishments.

- Hydrogen transport resistance model is a good tool.
- Early phase work shows that membrane material performance will meet Department of Energy goals.

- Good progress and a great value for the budget. Strong characterization work.
- Researchers have begun lifecycle tests, but longer tests or accelerated lifecycle tests are required.
- The PI has made significant progress – initial hydrogen flux results are encouraging – toward developing membranes that meet the Department of Energy goals and targets.
- Model development is supported by experimental data.
- Milestones were explained in detail.
- Results explained in a qualitative fashion. Difficult to evaluate progress made-due to the lack of quantitative data.
- No discussion on membrane material impact on performance.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.9** for technology transfer and collaboration.

- Partners have dropped out and technology transfer plans are unclear. Team needs to acquire test site partners and should work with industrial gas companies to gain industrial insights into practical operational challenges. Inclusion of Praxair (an industrial gas supplier) should ensure ease of technology transfer beyond the host site that is now being sought.
- Collaborations with test and evaluation systems and sites important-need more specifics.
- They have a solid team, but team responsibilities and interactions were not clearly identified, so it is difficult to assess their collaboration.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.2** for proposed future work.

- Membrane thickness and configuration (tube vs. disc) are critical to reaching Department of Energy goals. Project should concentrate on techniques for producing and testing long 500 micron wall, catalyst coated tubes and incorporating these tubes into modules (tube sheets) for testing.
- The costs of life cycle use were not clearly addressed.
- Future work seems appropriate.
- They need to add tests on real syngas streams to assess contaminant tolerance. Tests should also be conducted at higher temperatures and lower partial pressures to assess hydrogen flux at these levels.
- Future plans are appropriate and adequate and focused on the barriers.
- Manufacturing costs reductions should be included.

Strengths and weaknesses

Strengths
- Good membrane development based on projected performance and costs.
- Very frank and open presentation.
- They are well funded and have a solid team.
- Good progress (flux, etc.) is being made toward meeting the Department of Energy separations membrane targets.
- Non-palladium based membranes are cheaper.

Weaknesses
- 500 micron just meets the Department of Energy goal when lab tested. "Real" gas streams are likely to significantly lower this rate (impact the catalyst layer). Team needs to show understanding and plan to compensate/control membrane module performance.
- Tube manufacturing, catalyst coating, tube sheet system will all impact performance and more importantly costs. The degree of impact needs to be accessed.
- Testing on real gas streams is needed.

- They should consider operation at higher temperatures (up to 600 degrees Celsius) and lower partial pressure.
- Life of membrane is less than one year. Needs to be improved.

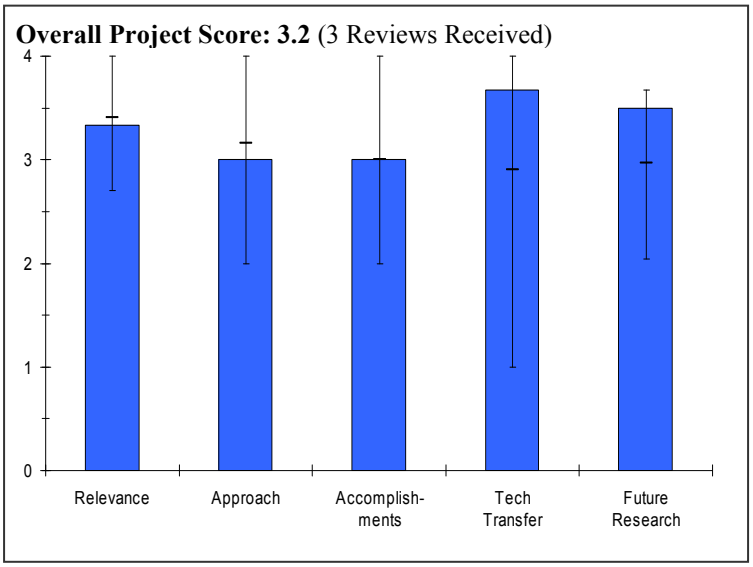
Specific recommendations and additions or deletions to the work scope

- The very thin tube wall combined with the economic need for long tubes dictates that knowledge about tube strength/stresses under pressure (including quick ramp-up and ramp-down) and pressure cycling: plus double sided catalyst surface adherence/wear (will tubes flex against each other); plus tube sheet connections... all be evaluated in detail.
- Suggest accelerating and expanding the project.
- Include Go/No Go decisions with clear criteria to guide future research.
- Tests that include all contaminants and measure the rates/cumulative effects.

Project # PD-40: Cost-Effective Method for Producing Self-Supporting Pd Alloy Membrane for Use in the Efficient Production of Coal-Derived Hydrogen
Kent Coulter; Southwest Research Institute

Brief Summary of Project

The overall project objective is to develop technologies that effectively and economically separate hydrogen from mixed gas streams that would be produced by goal gasification. The objectives of this project are to 1) develop a process methodology for the cost-effective manufacturing of thin, dense, self-supporting palladium alloy membranes for hydrogen separation from the mixed gas streams of coal gasification processes; and 2) reduce Pd membrane thickness >50% over current state-of-art and show potential to meet the Department of Energy 2010 technical targets.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- Project fully supports Department of Energy RD&D goals.
- Department of Energy hydrogen flux targets are surpassed.
- Membranes are essential to hydrogen process flows/purity.
- The use of palladium-based membranes may find limited use because of cost and scale-up, although the use of thin membranes appears to be the right way to go with such an expensive metal.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- Project providing innovative technology and product development for thin film (3-10 Micron) membrane with high hydrogen flux (more than Department of Energy levels are achievable).
- Generated depth in production of membranes using variety of binary and ternary palladium alloys.
- Membrane is not self supporting and they have challenges to overcome in construction of membrane modules.
- The experimental approach is adequate but suggest that the PI conduct additional background literature research on palladium alloy behavior to avoid duplication of previous efforts.
- The first part of the talk described work that was completed. An effective way to produce thin unsupported membrane films appears to have been demonstrated. Implementing these films in an operating device appears to be difficult. The second portion of the presentation focused on a new project examining ternary compositions, starting first with computational work and then followed up by experiment. This is a reasonable approach assuming that the density functional theory (DFT) computations give reliable results that can be validated with experiment.
- It is likely that it will prove difficult to produce materials that are as well formed as designed theoretically. Phase segregation or surface enrichment could occur that would not be predicted by modeling.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- Successful results with hydrogen flux surpassing program goals.
- Team plans for more work with membrane assembly. Issues are identified and they plan to fine tune annealing process to eliminate surface defects.
- Pinholes at the edges of foil on the supporting material occur. Steps to overcome the issues with modularization are in progress.
- The testing conducted on prototype membranes seems logical but some concern that the research activity duplicated previous efforts by past DOE projects.
- Technical accomplishments from the previous program seem reasonable.
- The recent work using the DFT calculations shows promise and the fact that the work has been submitted for publication (if accepted) speaks well of the work.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.7** for technology transfer and collaboration.

- Excellent cooperation and teamwork between collaborators.
- The project appears to have done well in seeking collaborations with others. Each has a specific role to play. It does not appear that potential collaborations have been well defined with possible commercialization partners. IdaTech is a possible commercial partner, but the relationship appears to be less strong based on recently described issues. This project appears to be mostly in the research stage.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.5** for proposed future work.

- Clearly identified steps to eliminate issues related to membrane fabrication and to carry out modularization work.
- Future plan includes the cost estimate work for production of membranes.
- Suggest as part of future work that the PI perform a literature review of past DOE projects on behavior of palladium alloys for hydrogen sensors to help guide future research.
- The proposed forward plan is reasonable and appears to be on track.
- With the proposed future fabrication of several new membrane compositions, it would be good to see that the plan would include some science into the analysis of the materials, either as produced or following testing. Detailed surface and bulk analysis of some of the best materials might be in order. Otherwise the Program sound like a fairly simple make and test without a lot of insights gained.

Strengths and weaknesses

Strengths
- Well-defined, timely and successful execution of the project plan and alignment with targets.
- Successful teamwork and partnerships.
- Good progress made on creative membrane technology and membrane production. Estimates look promising for low-cost production of thin film membranes.

Weaknesses
- Did not address the broad knowledge base on palladium embrittlement for hydrogen sensors as it applies to this project. Concern that the PI is re-discovering existing knowledge.
- The difficulties of the actual implementation of the free-standing membranes are left somewhat unresolved. Understand that other partners will be approached, but it is not clear whether the problem is with IdaTech or with the membrane materials themselves.

PRODUCTION AND DELIVERY

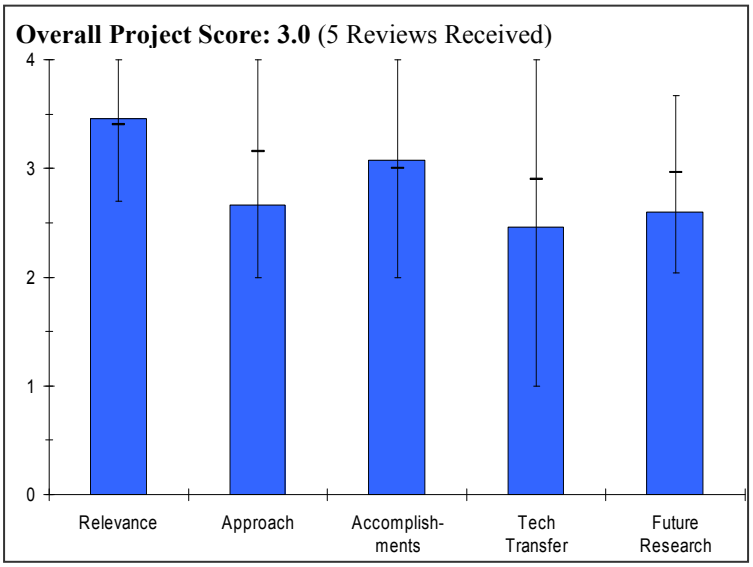
Specific recommendations and additions or deletions to the work scope

- Very good project. Film technology and thin film membrane might have other key application areas.
- Suggest a comparison of the knowledge gained in this project to past DOE efforts on palladium alloy work for hydrogen sensors.
- Add more science and characterizations to the materials, and seek to understand the strengths and limitations of the DFT computational method applied to this problem.

Project # PD-41: Experimental Demonstration of Advanced Palladium Membrane Separators for Central High-Purity Hydrogen Production
Sean Emerson; United Technologies

Brief Summary of Project

The objectives of this project are to 1) confirm the high stability and resistance of a PdCu trimetallic alloy to carbon and carbide formation and, in addition, resistance to sulfur, halides and ammonia; 2) develop a sulfur, halide and ammonia resistant alloy membrane with a projected hydrogen permeance of 25 $m^3m^{-2}atm^{-0.5}h^{-1}$ at 400°C and capable of operating at pressures of 12.1 MPa; and 3) construct and experimentally validate the performance of 0.1 kg/day H_2 PdCu trimetallic alloy membrane separators at feed pressures of 2 MPa in the presence of H_2S, NH_3 and HCl.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- Membranes are essential for hydrogen separation/purification for both central and distributed hydrogen production.
- The project helps with development of hydrogen infrastructure.
- Power+Energy (P+E) and United Technologies Research Center (UTRC) alloy separators can meet or exceed DOE targets.

Question 2: Approach to performing the research and development

This project was rated **2.7** on its approach.

- Did not clearly address the engineering issues associated with heated membranes. The technical plan is narrow but well-equipped. Combination of low pressure screening, high pressure with poisons, and modeling is good. Standardized testing approach is good for reproducibility and reliable screening.
- UTRC has good capability for membrane material and tube development.
- The strategy for making membranes tolerant to the three poisons needs to be more clearly defined.
- Materials alloy construction should incorporate the information learned from the extensive characterization being done. Little information presented on how material alloys are being defined.
- Use of thermodynamic solubility data and modeling tool is a good approach, but project researchers should use existing data to make better decisions in the modeling approach.
- Fundamental understanding of the issues of membrane durability, impurities, hydrogen selectivity, and flux.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.1** based on accomplishments.

- Conducted a logical experimental program and made significant progress in its first year.
- UTRC and P+E possess capability to make state of the art Pd membranes.
- Constructed and tested 10 membrane materials and quantified effect of CO, CO_2, N_2, and H_2O on hydrogen permeability. None of the membrane materials have been tested with any of the poisons yet (H_2S, etc.).

- High degree of characterization (XRD, XPS, EBSD) helps fundamental understanding of material properties and changes.
- Modeling projections estimate that the flux target will be met at 500+°C.
- Model calibration data good.
- Not enough data on membrane configuration for performance estimates.
- Evaluated performance of first fcc-PdCu separator.
- Produced five separators with UTRC ternary composition.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.5** for technology transfer and collaboration.

- Collaboration between membrane fabricator, characterization, and system integrator is good.
- Partners are well qualified and roles defined: (P+E for membrane separator fabrication and Metal Hydride Technologies for hydrogen solubility measurements).
- No technology transfer plan included.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.6** for proposed future work.

- There is a narrow test program planned that should be completed under current project.
- Suggest as part of future work that the PI perform a literature review of past DOE projects on behavior of palladium alloys for hydrogen sensors to help guide future research.
- Testing with poisons is planned.
- Future work seems limited to testing next set of approximately five materials.
- Test plan is well organized and consistent with objectives.
- Contaminant tolerance improvement details are not adequate.

Strengths and weaknesses

Strengths
- UTRC's experimental and research capabilities are very good. Project strength appears to be testing capability and modeling of test results.
- The team has a very good history of producing Pd membranes.

Weaknesses
- Did not address the broad knowledge base on palladium embrittlement for hydrogen sensors as it applies to this project. Concern that the PI is re-discovering existing knowledge.
- None of the membranes have been tested with any of the poisons.
- Materials testing is limited due to length of time required to test materials.
- Ag addition is considered beneficial, but not pursued here.

Specific recommendations and additions or deletions to the work scope

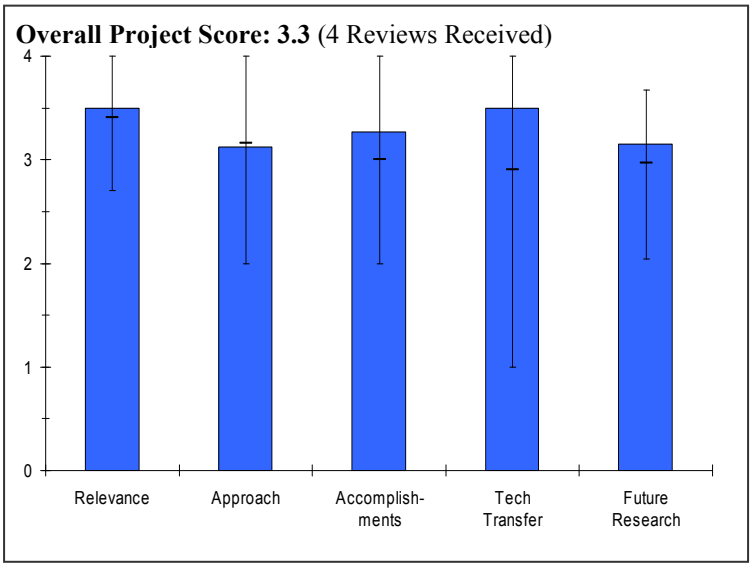
- Suggest a comparison of the knowledge gained in this project to past DOE efforts on palladium alloy work for hydrogen sensors.
- Deal with materials that can tolerate the poisons before refining them to meet the flux targets. Effect of sulfur on carbon-deposition as hydrogen is removed should be considered.
- Need to develop an accelerated stress test to speed the testing portion of the Program.
- Need to incorporate thermal cycling stability tests.
- Need a more detailed cost estimation and relate to the DOE hydrogen production targets.
- Materials alloy construction should incorporate the information learned from the extensive characterization being done.

Project # PD-42: Integration of a Structural Water Gas Shift Catalyst with a Vanadium Alloy Hydrogen Transport Device

Thomas Barton; Western Res. Ins. & U of Wyoming Res. Corp.

Brief Summary of Project

The 2007 objective of this project is to integrate the water-gas shift (WGS) catalyst and metallic membranes into a device and test under gasifier conditions. The 2008 objective of this project is to build a modular WGS/membrane integrated device capable of producing 10,000 L/day hydrogen from coal-derived syngas. The ceramic catalysts developed are superior to commercially available WGS materials with respect to survival in a pressurized device. Two different viable integrated device designs using vanadium membranes are under fabrication that should meet scalability issues and performance criteria.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- Combination of water-gas shift (WGS) and hydrogen membrane separation is an attractive option. The project appears to be well focused on addressing the two tasks of reducing WGS costs capital costs and membrane costs by integrating the two unit operations together.
- Development of a non-Pd membrane is a necessary technology need for lowering cost.
- Water gas shift (WGS) catalyst does not contain precious metals. WGS catalyst monolith will help enable low-cost high-efficiency integrated gasification combined cycle (IGCC) designs.

Question 2: Approach to performing the research and development

This project was rated **3.1** on its approach.

- Focus on non-precious metal WGS catalyst is good.
- The approach described is clear but fairly minimalist. There is no indication of where challenges might exist and how specific focus might be put to address these challenges.
- Vanadium-based membrane has been very good potential.
- WGS catalyst-based on aluminum-ceria monolith is a logical support.
- Fundamental understanding of the barriers for hydrogen separation and purification, namely WGS capital costs and hydrogen transport membrane costs.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.3** based on accomplishments.

- Effects of catalyst formulations and synthesis techniques on performance have been investigated.
- Significant progress is being made. Fe-Al-Cr-Cu-Ce system catalysts have been tested by impregnation into porous mullite substrates. Highest activity and stability has been shown for 75Fe-15Al-8Cr-2Cu. Small additions of CeO_2 look promising.

- Reaction rate has diminished by 50 percent within 100 hours which leads to several questions. Is there an acceptable rate that must be maintained? What is the deactivation mechanism? Does the activity correlate with surface area or is there something special about the catalyst compositions? Understanding why the catalyst has deactivated could be very important in scaleup work or predicting long term behavior of the system.
- The water gas shift work appears to be mostly a make it and test it approach. From a catalyst perspective there may have been interesting materials and properties, but there is no characterization of the materials.
- Although it is outside of the apparent scope, some measurement of the kinetics of the system would be helpful on scale-up and predicting performance as a function of temperature, pressure, and feed composition away from the specifically tested parameters.
- It was not clear why one would operate the membrane in series rather than parallel. It was claimed that either option appears possible.
- Good activity; however, stability improvement are needed.
- Multi-pass HEX design is quite scalable.
- Does ceramic adhere well to the vanadium? They may not have to be physically connected.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.5** for technology transfer and collaboration.

- Good, experienced collaborative team of University of Wyoming, Chart Energy and Chemicals, REB Research and Consulting, DOE Ames Laboratory.
- The interaction with Chart and REB is a very good one. The microchannel-type device is attractive if it can avoid excessive weight issues, and a reasonably low cost method to fabricate can be identified.
- WGS catalyst commercialization is a good idea.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.1** for proposed future work.

- Catalyst will be supported on honeycombs within a heat exchange reactor.
- The reactor should be modeled to show expected temperature and concentration profiles, with outlet compositions matching design point.
- The future plan is clear and scale-up design is well planned. Tests under gasifier conditions will be useful.
- Commercialization of the water gas shift catalyst monolith will be pursued with the assistance of a catalyst manufacturer.
- Successful testing of the two scaled integrated devices will be followed by design of a 10x assembly based on the economic and performance data for testing under coal gasification conditions. Ceria is expensive and use has to be limited.

Strengths and weaknesses

Strengths
- Focus is on non-precious metal materials.
- Good progress, plan, collaborators, path toward possible commercialization.
- Integrated WGS-membrane reactor is an attractive option.
- Presence of gasifier facility is very good.

Weaknesses
- Catalyst is still deactivating rapidly after 100 hours.
- Better understanding of the WGS aspect of the device would seem appropriate, in order to interpret future results and troubleshoot as necessary.
- Effect of high humidity and low hydrogen in presence of sulfur and the exit of the reactor needs to be understood (ceria stability and poisoning). Appears as if future testing will help address these issues.

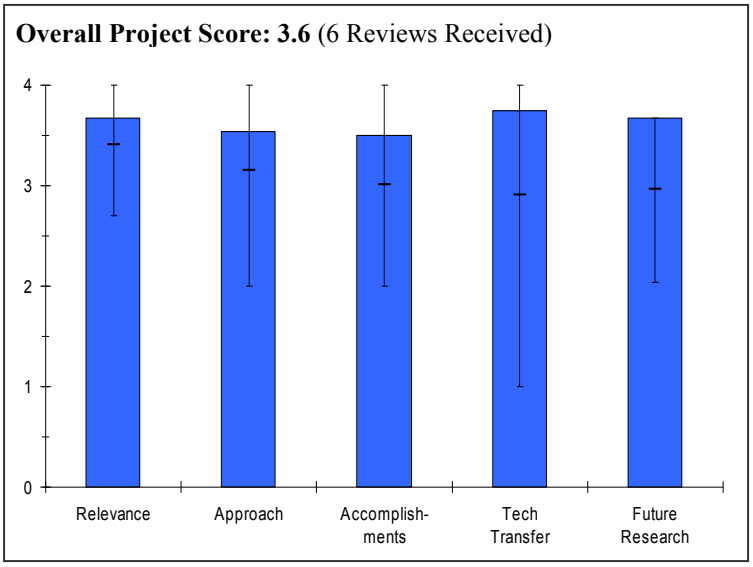
Specific recommendations and additions or deletions to the work scope

- Need to establish the rate at which the catalyst can be expected to maintain reaction rate, before proceeding to reactor scale-up.
- Need to understand vanadium membrane fabrication issues at large scale.

Project # PD-43: High Flux Metallic Membranes for Hydrogen Recovery and Membrane Reactors
Robert Buxbaum; REB Research & Consulting

Brief Summary of Project

The objective of this project is to find a base metal replacement for palladium ($470/oz) and for REB's own sandwich membranes for use in hydrogen purifiers and membrane reactors. The 2008 milestones are 1) good manufacturing capabilities; 2) to repeat the demonstration of long life tests; and 3) to manufacture reactor purifier discs.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.7** for its relevance to DOE objectives.

- Project attempts to lower the hydrogen production cost by significantly lowering the cost of hydrogen permeation membranes through reduction/replacement of Pd with base metal alloys.
- Successful project will fully support DOE research, development and deployment objectives and meet DOE targets.
- Project is targeting lowering the hydrogen production cost by significantly lowering the cost of hydrogen permeation membranes.
- The project appears to have a single task to reduce membrane cost. The project seems to be well focused on this.
- Low cost hydrogen using cheaper membranes with 15 years life is focused in the right direction.

Question 2: Approach to performing the research and development

This project was rated **3.5** on its approach.

- Producing hydrogen from coal gas would be good. Cleaning of the coal gas can raise the cost significantly. Since zero impurities would be difficult to achieve, the membranes should be tested/demonstrated for impurity tolerance.
- PI has fundamental understanding of the goal and provided good discussion of technical approach to select new membrane material.
- Initial results are achieving significant cost reduction in hydrogen production.
- Creative membrane design using B_2 intermetallic structure sandwiched between very thin Pd layers to reduce cost and extend life. Achieving 100 percent selectivity like Pd using cheap B_2 metal.
- Lower pressure drop is required.
- This approach is logical and seems to be based on many years work and experience by PI in this field. PI provides the competency base for producing the unique membrane with high flux.
- It seems that implementation of these materials is finally coming to fruition. The basic concepts for the potential attractiveness of non-Pd membranes have been known for some time.
- Well organized team member with assigned tasks.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.5** based on accomplishments.

- Project investigators achieved majority of their targets. Based on the technical accomplishments slides, good progress has been made on achieving flux targets and cost.
- The principal investigator reports that technical accomplishments are at a level that they are ready for market study.
- Concepts appear ready for manufacturing.
- Some of their alloys produced were brittle. They researched about 260 alloys and narrow down to a few which work properly.
- There is the potential for much scientific understanding to be gained through the synthesis and testing of several different alloy membranes. One hopes that some of the scientific information gained will make it into the published literature at some point.
- There is room for some type of combinatorial/high throughput testing of candidate membranes. The one-at-a-time approach appears to have been reasonably effective but there may be better ways to synthesize and characterize materials using the new developments in high throughput capabilities, including data management.
- It is not clear what maximum size of membranes can be produced. How the membrane assemblies are envisioned (flux per unit and # units) would be helpful.
- B_2 alloys are promising however need to improve fabricability; may affect overall cost advantages.
- Significant progress. Lowered the cost/flux hydrogen permeation membranes to lower the cost of hydrogen. Replaced palladium with base metals having $100/ft^2 vs. $3000/ft^2 – 100 percent selectivity like Pd – 50 scfh/ft^2 UHP H_2 at ΔP=200psi – 15+year life projected – low embrittlement. Alloys not identified.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.8** for technology transfer and collaboration.

- Good collaboration and distribution of tasks. Iowa State University helps pick alloys, x-rays; Ames Laboratory makes alloy samples; LANL coats, welds alloys, some tests; NETL conducts permeation and life tests; G&S Titanium Co. fabricates membranes; and REB Research manages and assembles.
- Close well-coordinated collaboration between all of the team members. Team members' responsibilities and their work and part in the team clearly described.
- The project appears to have a good set of collaborators, and a path to commercialization through REB.
- Good team, excellent work scope assignment.
- Already got a side-benefit for nuclear material applications.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.7** for proposed future work.

- Impurity tolerance should be conducted early during material selection. Evaluate trade-off between flux and impurity tolerance.
- Economic analysis to show DOE hydrogen production target costs are addressed.
- The proposed plan appears to be a reasonable continuation of work done thus far.
- Excellent comparison with previous year's future work.
- Willingness to make corrective action on a timely basis is very good.
- Logical and straightforward planned work. Make larger non-porous membranes (Great Western, REB). Higher pressure tests, sulfur tests with current, tweaked alloy (NETL). Test membranes, purifier w/coal gas (REB, WRI). Continue life tests with new tweaked alloy (LANL). Make disc-membrane membrane reactor with new alloy membranes (REB). Confirm that behavior matches flux, cost, and durability goals (REB, ISU).

Strengths and weaknesses

Strengths
- Good collaborative team and technical approach.
- Capability in making commercial membrane reactors.
- Building high performing cost effective hydrogen permeation membranes.

PRODUCTION AND DELIVERY

- Good work plan with specific targets with specific timelines.
- Excellent team work.
- A lot of experience and familiarity with this area of research and materials. A good collaborating team.

Weaknesses

- Membranes appear to be limited to sulfur-free fuels. Need to expand on this area further.
- This project might benefit from some computational work, not just in gaining new insights or possible leads, but also in providing information in the other direction to assist the computational projects dealing with such materials. Where do the models fail or what important aspects are not included in the models? There appears to have been a lot of data generated, additions to the science-based are to be encouraged.
- Test with WRI gasifier may be beneficial.

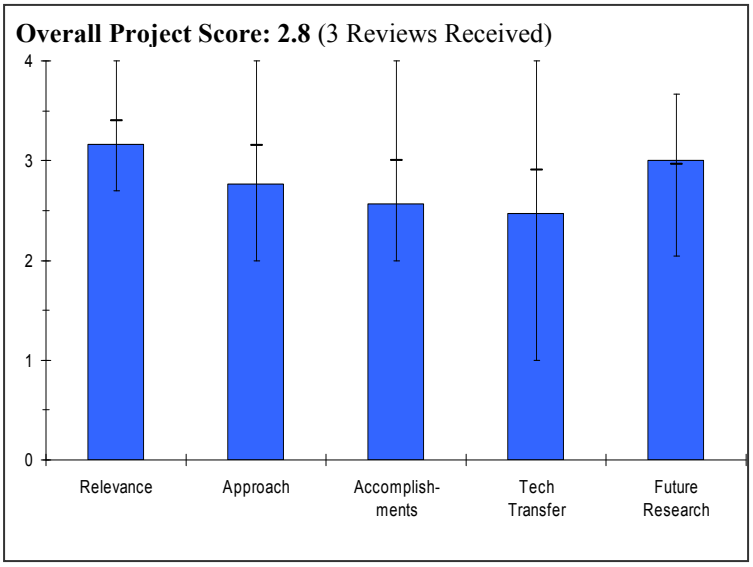
Specific recommendations and additions or deletions to the work scope

- Place high priority on impurity tolerance.
- Inclusion of discussion how project cost targets specifically contributing to achieve DOE hydrogen production cost targets.

Project # PDP-01: Fundamentals of a Solar-Thermal Mn_2O_3/MnO Thermochemical Cycle to Split Water
Al Weimer; CU

Brief Summary of Project

The objective of this project is to research and develop a cost effective Mn_2O_3/MnO solar-thermal thermochemical cycle through theoretical and experimental investigation. Additionally, based on the previous, the University of Colorado will develop a process flow diagram and carry out an economic analysis of the best process option. A reaction mechanism has been hypothesized for Mn_2O_3 dissociation. Mixed manganese oxides have been shown to improve the product recovery steps. Experimental investigation using a mixed manganese oxide is ongoing.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.2** for its relevance to DOE objectives.

- Project aligns with needs of DOE Production Subprogram.
- This project's objective is to research and develop a cost effective solar-thermal thermochemical cycle through theoretical and experimental investigation.
- Based on the above study, a process flow diagram and economic model will be developed.
- Project objective is solar powered hydrogen generator on a large scale.

Question 2: Approach to performing the research and development

This project was rated **2.8** on its approach.

- Approach is very good; however, efficiency and energy balance should be the initial part of any cycle analysis and should be described on a poster presentation.
- Thermodynamic assessment of Mn_2O_3/MnO cycle will be carried out.
- Mn_2O_3 dissociation will be experimentally investigated.
- NaOH recovery is an important step for this cycle to work and this project is investigating this issue.
- It is not clear why this cycle should be better than so many other cycles that are investigated for a very long time.
- It is not clear that this is a closed cycle - it may be an irreversible process. The values of [ΔH, ΔS, $Q + \Delta G$] have not been calculated for most steps, nor have the value of rate constants for key steps. No way to ascertain likely equipment designs or efficiencies.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.6** based on accomplishments.

- $ZnMn_2O_3$ needs to be evaluated in an effusions cell to determine Zn vapor pressure. Zn tends to show high vapor pressure as low as 1,000°C and could lead to short term materials degradation and cycle inefficiencies.
- Found a probable mechanism for decomposition of manganese oxide (using TGA & Aerosol flow reactor).
- Used mixed manganese oxide to study NaOH recovery & hydrogen production. NaOH is a critical step in the production of hydrogen by this cycle. Good to see progress made in this area.

- Initial PFD work has been done.
- Mixed manganese oxide has been prepared and the synthesis route is scalable for manufacturing large quantities.
- Conversion ranged from 50 to 75 percent and conversion increased with temperature and gas flow rates.
- More than half the money has been spent without clear results in any area. Design seems to presume a spray system with solid manganese oxides whose oxygen leaves instantaneously at 1,500°C but where zinc remains trapped in the manganese and the manganese-zinc-sodium undergoes no destructive reactions.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.5** for technology transfer and collaboration.

- Collaborations could be strengthened to greatly improve this project and to identify issues with the cycle.
- Collaborating with University of Nevada, Las Vegas and Swiss Federal Institute of Technology.
- It would be good to establish collaboration with other groups working on thermochemical cycles for hydrogen production (General Atomics, SRNL, INL, etc.).
- Many groups were involved, but not a sign of clear integration of their work.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- Good research plan. NaOH recovery is important step in this process. The principal investigator has identified that mixed manganese oxide is better than manganese oxide and have synthesized the mixed oxide. The next step is to investigate its dissociation mechanism.
- Should Evaluate hydrogen production rate using mixed manganese oxides and compare it with the conventional manganese oxide cycle.
- Update the process flow chart using the mixed manganese oxide cycle and re-evaluate the economics of hydrogen production.
- Researchers' main objective at this time seems to be to show that the cycles close, when, in fact, it is likely that they do not.

Strengths and weaknesses

Strengths
- Strong background/knowledge in chemistry.
- Lot of results obtained with small amount of funding. This is possible only in an university — definitely not possible in any of the DOE laboratories.
- Good international collaboration with the Swiss institute.
- Innovative and politically useful cycle.

Weaknesses
- Overall process efficiency is low at 32 percent while heat required is exceptionally high (1,500°C) and may present materials development issues.
- Initial reaction of Mn_2O_4 to MnO will not proceed to 100 percent completion and no results where shown on if the initial reaction of the mixed metal systems have higher conversions than the pure Mn_2O_3 base case.
- Recycling of the mixed oxide might be a problem. The temperatures are very high and therefore I suspect Zn will be lost.
- Any reason why Zn-mixed oxide is better than Fe-mixed oxide?
- High temperature materials are an issue for this thermochemical cycle to work.
- The researchers seem unaware of all the project weaknesses, and seem to have no systematic way of addressing those they do recognize. Then again, it may be only poor presentation.

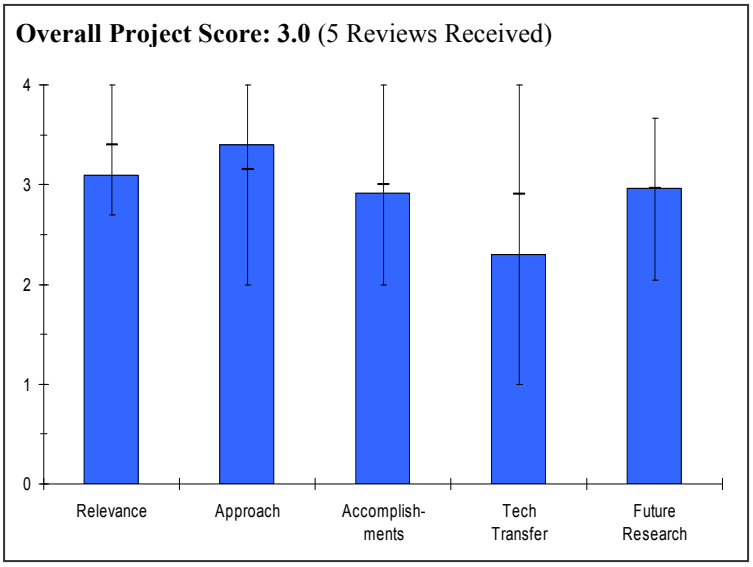
Specific recommendations and additions or deletions to the work scope

- Perform H2A analysis for this process.
- Work should be focused on mixed manganese oxide cycle only. No more work on straight manganese oxide system.
- Perform research to understand why Zn-mixed oxides are better than Fe-mixed oxides. Determine what will be the ultimate mixed-oxide system.
- Need thermodynamic analysis of cycle, and estimate of parasitic loss at pumps, sprays, heat-exchangers
- Need cost analysis of cycle, temperatures, materials, vessel size.
- Need a plan that moves project forward to go/no-go decision points.

Project # PDP-02: Novel Low-Temperature Proton Transport Membranes
Andrew Payzant; ORNL

Brief Summary of Project

The objective of this project is to develop a novel ceramic proton conductor based on $La_2Mo_2O_9$ for use as a hydrogen separation membrane. The objective will be achieved through 1) compositional development; 2) characterization of the electrical properties, chemical stability, hydrogen flux and thermo-mechanical properties; 3) neutron diffraction analysis of selected materials to better understand the hydrogen transport properties; and 4) evaluation of surface exchange catalysts. The goal will be to synthesize this asymmetric membrane from candidate materials with and without exchange catalysts for additional flux testing to determine the range of flux possible in these materials.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.1** for its relevance to DOE objectives.

- Development of non-Pd based hydrogen membrane is a good option/pathway for hydrogen production.
- CO_2, H_2O tolerant-separation membrane for 300 to 500°C operation. It is likely to be hydrogen tolerant as well. Quite relevant.
- Energy efficient and economic hydrogen separations provide not only separation/purification opportunities, but also can be used to advantageously alter reactor kinetics.
- This project explores a unique crystal structure that is apparently permeable to hydrogen, and might have utility for the separation of hydrogen from other gaseous species. If successful, this research could provide an improved method for hydrogen purification, and subsequent utilization as a fuel or chemical reactant.
- The project is evaluating a high risk alternative for hydrogen separation. The technique utilizes a solid oxide membrane that will selectively separate hydrogen from any gas mixture. This is a fundamental, long term research effort that will not meet any of the near term DOE targets (2015), but may provide information for future hydrogen separation membrane techniques.

Question 2: Approach to performing the research and development

This project was rated **3.4** on its approach.

- Tasks 3 and 4 are good strategies for improving material formulations.
- Task 1 contributes toward fabrication methods. This work (making thinner membranes) can also be done when the project moves toward commercialization.
- Task 2 can be avoided since the flux that is to be reported under this research and development activity is supposed to be normalized with respect to pressure differential (20 psi?) anyway.
- Innovative proton-conducting ceramic, low cost.
- The project is based on a material whose beta phase was identified as an oxygen ion conductor in 1999/2000 and in 2003/2004 identified as a proton conductor when in the alpha phase. The material structure and chemistry appear to be very stable in H_2 and CO_2.

- The project team is in the very initial stages of taking a material and producing a useful membrane. Initial flux measurements are very low on thick 3-mm samples. The project team has identified the barriers to increasing flux greater than four orders of magnitude and is working towards that goal.
- The approach is to prepare a series of lanthanum molybdenate compounds and then test these materials hydrogen transport. Such transport might be permeation along grain boundaries and other micro fissures, or it could be dissociative absorption and then dissolution of atomic hydrogen. One goal is to determine the transport mechanism. Another goal is to maximize the rate of hydrogen transfer, and another goal is to evaluate the system to determine poisons that might interfere with the transport step.
- The work is examining a technique that has been researched in the past - solid oxide proton membrane separation. However, the unique aspect of this work is the attempt to develop materials that will operate at low temperatures (200 - 500°C), rather than approximately 850°C. This could be a big advancement for these materials; however, achieving high flux levels will be a major barrier.
- This is a fundamental research effort to identify and test new transport materials. No commercial materials will be developed in the near future. This is an appropriate long term fundamental research project for a National Laboratory as long as funding is maintained at the current levels (approximately $200K per year).
- The work is considering a different family of compounds (non-perovskite) that have not been examined in the past.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.9** based on accomplishments.

- Good material characterization work, includes flux, conductivity, XRD, expansion.
- Pr doping does not seem promising, but the researchers should not lose heart. This is the nature of such research and development.
- Weakness: Some plots do not have the y-axes!
- Flux is still low and mechanism still not understood, but they've made thinner membrane, done basic experiments, made key measurements.
- They have solved membranes-sealing problem
- Thin (10-20 micron) supported membranes have been made. Team has a good match between the membrane thermal expansion and potential substrate material. Full membrane density is required, but not yet achieved.
- High Temperature tests completed indicate very stable material in H_2 and CO_2
- This activity was initially funded by the Department of Energy's Fossil Energy, and then transferred to the Office of Energy Efficiency and Renewable Energy. The work had just begun when funding was withdrawn and just now new funding is available to restart the project. There is no significant progress to date, but a well thought through technical plan was developed.
- Hydrogen flux levels are extremely poor at this time - well below 1 $cm^3/cm^2/min$.This is barely at detectable levels. If increases are not obtained within the next year - DOE should consider ending this work.
- Leaks do not appear to be a significant problem with these membranes, which is probably due to the lower temperatures being used for this separation. However, current tests are being conducted with thick membrane disks (3 mm) which may be easier to seal.
- The project has had some success with materials development. The work has been able to produce defect free, thin layers (10 micron) of the membranes on a zirconia support. Thin membranes will be required to achieve high flux levels – probably on the order of 3 - 5 microns.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.3** for technology transfer and collaboration.

- Some collaboration with the University of Cincinnati.
- Suggest the principal investigator also consider collaboration with organization with similar material expertise.
- Oak Ridge National Laboratory and the University of Cincinnati will want broader collaboration on the project progress if there is to be any commercial product.
- One university partner is involved in membrane characterization.

- This is very early stage work (and wider coordination probably has IP concerns). Industrial partners, (experienced with commercial production of the substrate and potential end users) however, could accelerate this development.
- Technology transfer is minimal and there does not appear to be any external collaboration. The work is being conducted 100 % at ORNL. No publications have been produced from this work. This work has been ongoing since 2004 and there should have been some technical publications by this time.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- See comments in Approach.
- Weakness: Incorporating Pd goes back to precious metals again.
- Trying to understand mechanisms. Adding pressure and catalyst.
- Production and flux testing of numerous thin fully dense supported membranes is needed to demonstrate the practicality of producing and using this membrane. Demonstrate that the approaches to improving flux are doable and practical.
- The proposed research will evaluate the feasibility of using this material for hydrogen purification.
- Future work will just continue materials development to reduce membrane thickness and increase flux. This is an acceptable approach for this stage of the research.
- The project needs to meet some pre-determined yearly targets and goals - in particular a reasonable flux rate.

Strengths and weaknesses

Strengths
- It investigates hydrogen transport in non-PM membranes.
- They have a good approach.
- It is a well run and worthwhile project.
- New/novel dense film separation materials are being developed that opens up new opportunities.
- Alpha phase should permeate very high purity hydrogen.
- Material shows H_2 and CO_2 stability.
- The PI is highly competent and knowledgeable in solid state transport.

Weaknesses
- Results to date are not great, but the problem is challenging.
- Hydrogen flux is very low.
- Many performance metrics are unknown. This is a result of hydrogen permeation being a very new use for this material and limited work has been done or reported. However, structure and chemistry suggest performance could be similar to other dense ceramic/cermet membranes
- Limited flux testing has been done.

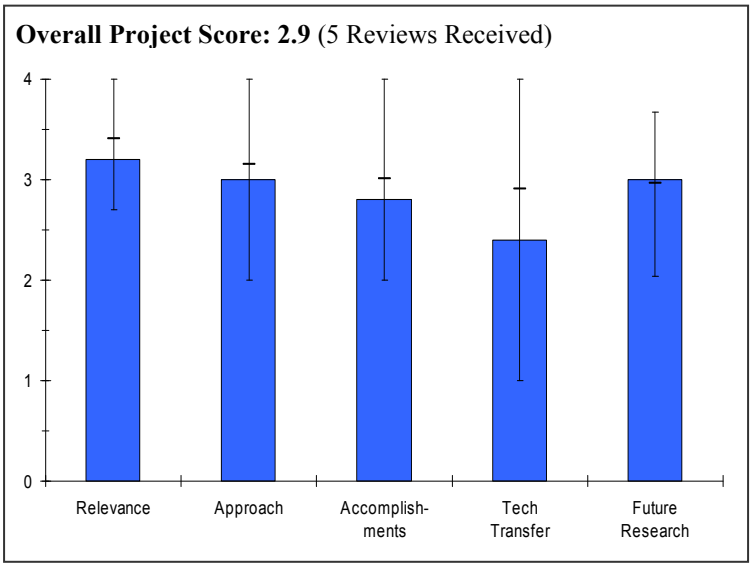
Specific recommendations and additions or deletions to the work scope

- This project can be categorized as a high risk/reward activity. The researchers should be encouraged to continue the focus on non-PM materials.
- Incorporate sensitivity to H_2S, CO_x in material characterizations.
- Modify substrate so that can use thinner membrane coats or so that membrane can be used as solid oxide fuel cell.
- Focus on the production of fully-dense very-thin supported membranes before exploring surface treatments to promote hydrogen dissociation.
- Develop back of the envelope projections for metrics.
- DOE needs to define some yearly technical targets/milestones for this project. The work is simply continuing with no clear goals or direction. The targets should be mutually determined by DOE and the Oak Ridge National Laboratory; and if the yearly targets are not met, the work should be discontinued. DOE should support these fundamental, high risk research efforts – but needs to be able to terminate these projects when no technical achievements are being produced.

Project # PDP-03: Ultra-Thin Proton Conduction Membranes for H_2 Stream Purification with Protective Getter Coatings
Margaret Welk; SNL

Brief Summary of Project

The objectives of this project are to 1) provide a functional support that will protect membranes from corrosive species in reformate gas stream; and 2) synthesize an "ultra-thin" dense ceramic proton conducting membrane to increase hydrogen flux over existing membranes. Dense membranes, whether metallic or ceramic, are especially vulnerable to sulfur attack. Sandia was successful in the deposition of titania and recently SrO. The deposition of ZnO was also successful.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.2** for its relevance to DOE objectives.

- Sulfur tolerant membrane for hydrogen extraction.
- Project objectives deal with hydrogen stream purification through innovative membrane production.
- Project needs to address its targets in terms of DOE cost targets for hydrogen production.
- Overall project objectives and technical plan are provided; however it seems to be quite appropriate for potentially significant cost reduction for hydrogen production toward achieving DOE's cost goal.
- Dense membranes, whether metallic or ceramic especially are vulnerable to sulfur attack. The functional support will protect membranes from corrosive species in reformate gas stream.
- The PI will synthesize an "ultra-thin" dense ceramic proton conducting membrane to increase hydrogen flux over existing membranes.
- Project is responsive to DOE's 2012 Target.
- System Cost \$/kg H_2 \$0.70 (\$400/kW).
- Electricity Cost \$/kg H_2 \$2.00.
- O&M Cost \$/kg H_2 \$0.60.
- Excellent understanding of markets and cost.
- Developing a membrane that could lead to cost, operability and footprint advantages over PSA is in line with DOE's goal.
- Removal of sulfur post water gas shift is perhaps not as critical since sulfur must be removed before shift and in some cases before SMR catalyst due to negative effect of sulfur on the catalysts.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- Project is only 25 percent done. Some basic technologies are complete-on schedule. Their approach is reasonable.
- Project approach addresses several technical barriers for Hydrogen Production identified under Hydrogen Separations.
- Researching for functional support to protect against corrosive species such as sulfur.
- Investigating synthesis of an ultra thin dense ceramic proton conducting membrane to increase hydrogen flux.

- Formation of ultra thin membranes (atomic scale) $SrTiO_2$ could improve flux. Coating of supports with ZnO could getter materials.
- Not clear whether alumina or silicate will be used as the support or both.
- Approach is sound and logical to complete objectives. They will: 1) Define market and requirements. 2) Conduct an industrial users survey. 3) Design and build pressurized electrolyzer stack. 4) Develop plastic stack technology demonstrate electrolyzer performance and capital costs, perform testing.
- Coming up with a membrane that can handle real life, post shift, reformate conditions is the right approach. Especially if the membrane can show clear advantages over well-proven PSA system.
- Again, removal of sulfur post water gas shift is perhaps not as necessary since sulfur must be removed before shift and in some cases before SMR catalyst due to negative effect of sulfur on the catalysts. The sulfur getter might have to be a separate part of the membrane to allow for installing in the feed stream to reforming system to trap out sulfur species.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.8** based on accomplishments.

- Project is only 25 percent done. Some basic tech complete. On schedule. It would be nice if the membrane were gas tight.
- Successful results reported for the deposition of TiO_2 toward synthesizing an ultra thin proton conducting membrane.
- Work on SrO deposition has just been completed. Thus they are able to successfully deposit $SrTiO_3$ on the ceramic surface. Following tightly deposited $SrTiO_3$ thin film they plan to start conducting hydrogen flux experiments.
- They reported success for building support with fine pore structure to enable synthesis of ultra thin proton conducting membrane. They are successful in adjusting the pore size to desired levels.
- They reported successful ZnO deposition within the pore structure of Al_2O_3 mesoporous disc support. They showed good results in sulfur scavenging and regenerating ZnO.
- Regeneration of ZnO will enable this technology to achieve continuous operation when two alternating units are used.
- Only limited progress has been made.
- Good progress has been made. A stack has been completed. 1 kg H_2 / hr production rate is currently being upgraded to 15 bar pressure capability.
- Would like to see data of membrane performance on either simulated reformate stream (with steam) or real reformate from a reformer system.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.4** for technology transfer and collaboration.

- Plan is okay. It is too early in project to expect much.
- No partners at the present. The principal investigator is considering appropriate potential partners since they are now successful with building the ultra-thin proton conduction membrane.
- Although a score of 1.0 is given according to the criteria, this score in reality should be N/A and should not affect the overall score.
- The principal investigator is looking at ultra-thin $SrTiO_3$ deposition work to be successfully accomplished before bringing in new collaborators to the project. Successful results gave a “go” for this milestone.
- Collaboration is planned with Eltron and Pall.
- Collaboration is strong and effective with General Electric and the National Renewable Energy Laboratory.
- Perhaps too early at this stage partly due the progress of the project, but the membrane will need to be tested under real life or close to real life conditions (to be accomplished by working with projects working on reforming).

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- Main future research is making membranes gas tight and measuring flux.
- They addressed critical steps to overcome technical hurdles faced in the first year.
- Technical future work plan seems to be sound.
- Inclusion of cost analysis in their fiscal year 2008 work plan will be valuable. The technical targets may be addressed in terms of hydrogen production cost targets toward achieving DOE goal of reducing the cost of hydrogen to $2.00 - $3.00/gge delivered.
- The project needs to continue work to get the $SrTiO_3$ on the support.
- System testing at ambient and 15 bar pressure is planned.
- Operation and management cost assessment will be completed. System design will be done. This will complete project objectives.
- Perhaps need to establish some near term intermediate goals to better evaluate progress and future funding decision.

Strengths and weaknesses

Strengths
- It is a reasonable project.
- Technical objectives are planned appropriately and they successfully executed the planned work in the first year.
- Technical progress seems to be in line with their proposed timeline.
- Future technical work plan outlines tasks appropriately to achieve targeted technical results.
- Technical work plan and successful execution within the planned timeline are strengths for the project.

Weaknesses
- Concentration polarization or seals may doom project.
- Economic feasibility study will strengthen the project.
- Critical go/no-go decision points are needed.
- Plasma assisted atomic layer deposition (ALD) while one can control fine control thickness, depth of penetration, stoichiometry, etc. may not be an economical process. This needs to be investigated.

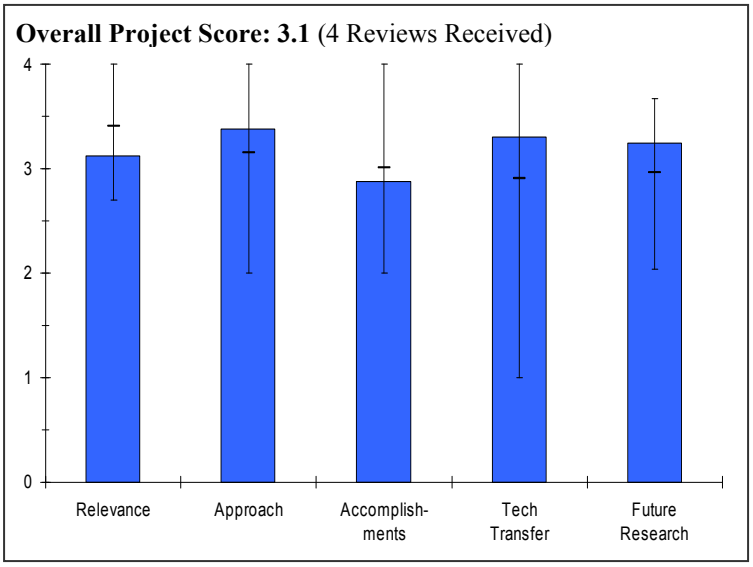
Specific recommendations and additions or deletions to the work scope

- Keep on going.
- Build go/no-go decision points into the work plan with regard to both technical and economic targets.
- Economic feasibility study with critical cost analyses to validate that the technical success will result in cost reduction for Hydrogen production to meet DOE goals.
- Do not need to look at removing sulfur post water gas shift. Might need to decouple the getter from the membrane and have it put in front of the system to remove sulfur in feed stream prior to SR reactor.

Project # PDP-04: Renewable Electrolysis Integrated System Development and Testing
Kevin Harrison; NREL

Brief Summary of Project

The objectives of this project are to 1) characterize electrolyzer performance with variable input power; 2) design, build and test shared power electronics; 3) identify opportunities for system cost reduction and optimization; and 4) test, evaluate and model the renewable electrolysis system. The National Renewable Energy Laboratory (NREL) has increased energy capture of the second generation wind to stack power electronics. And verified stack voltage efficiency to help meet the Department of Energy milestone. NREL has also integrated grid, wind and photovoltaic functionality into single power electronics module to reduce capital cost.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.1** for its relevance to DOE objectives.

- The project supports the hydrogen vision and research, development and deployment objectives to an extent. The principal investigator did complete the contractual tasks successfully. Although theoretically possible, the key technology challenges to practical deployment of distributed small-scale PEM electrolyzers integrated with renewable electricity generation is not addressed to the comprehension of the reader or reviewer.
- Very good. Clear and distinct objective which matches up well with the DOE program.
- For electrolyzers to be a cost effective pathway, capital cost must be reduced and efficiency boosted.
- Project directly addresses these two required developments.
- Performance evaluation is essential to the Program.
- Effective use of renewable energy is a key component of an energy transition to carbon-free energy.
- Electrolyzer performance is essential to renewable electrical energy utilization for a hydrogen economy.

Question 2: Approach to performing the research and development

This project was rated **3.4** on its approach.

- The identified, listed barriers are not new or unknown. (Most presenters on the subject listed the same three, common-sense barriers.)
- Difficult to figure out what new info the project has unfolded; seemed more like routine data collection rather than research and development.
- Presentation of the activity description and conceptual integration schemes by the principal investigator was impressive, but this does not develop a commercially viable, workable system; what new and different approach the principal investigator plans to take to overcome the known barriers should be addressed in the presentations. The stability of sulfonated tetrafluorethylene copolymer for long-term use, the use, recyclability, cost of noble metal or any other material electrodes, overall efficiency including compressor parasitic load, etc., issues the presenter should be prepared to discuss.
- Very good. Would have hoped that this section would have been more detailed.
- Project shows technical feasibility by actually constructing and testing devices.
- Approach is sound: analytical modeling alone would not conclusively prove feasibility.
- Methodical approach is a strength.

- Broad choice of energy sources is a strength.
- Good analytics.
- Using a standard performance protocol is a good approach - based on published international drafts of related work.
- Broad choice of electrolyzer types and manufacturers is a strength.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.9** based on accomplishments.

- Phased approach to overcoming barriers and accomplishing DOE cost and performance targets.
- However, since the key technology challenges are not unknown, and difficult, the PI did not clarify what new approach the PI will take to achieve the DOE targets.
- Very good - project appears to be where it should be at this point in the schedule.
- Gen 2 energy capture improvement is substantial.
- Project is still in progress, with continuing work and future work to follow.
- Operation of such a system is complicated and challenging. The project is to be commended for accomplishing this effort and keeping this complicated system operating.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.3** for technology transfer and collaboration.

- Several partner's names are listed; but the roles and responsibilities of each or any of the partners are not discussed.
- Outstanding for collaboration.
- While it is hard to gauge the quality of the interactions, there are a large number of partner companies and even larger number of companies providing feedback. Overall, I judge the level of interaction to be much above average.
- Manufacturer feedback is included, as strength.
- Publication of the protocol, as an international standard, is encouraged.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.3** for proposed future work.

- Rational follow-on work scope.
- Very good - sound engineering approach.
- Funding may stop and this work is too important to allow this to happen.
- Continuing work to evaluate new electrolyzer designs would be a strength.
- Publication of the testing protocol would be valuable to the entire industry.

Strengths and weaknesses

Strengths
- Strengths are the collaboration followed by the verification with what appears to be actual, commercially available hardware.
- Good to have actual test data.
- Excellent number of electrolyzer companies involved in project.
- Broad and suitable choice of electrolyzers with manufacturer feedback.
- Broad and suitable choice of energy sources.
- Broad and suitable choice of power conditioning.

Weaknesses

- How does the distributed generation cost become lower than the central generation cost (not including shipment)? This infers that small electrolyzers are more efficient than larger units.
- It is not clear why efficiency drops off with current density. Electrolyzer efficiency should be higher at part load.
- Graphical representation of Gen 2 energy capture is good but I'd also like to see a numerical evaluation (e.g., X percent of energy captured at speeds under 30mph).
- Power electronics capital cost reductions by combining functionality and eliminating redundant components seems logical and feasible but question is "by how much?" I don't see any quantification of cost reduction or description of a costing methodology.
- Presentation showed results of optimization, but did not include description of how exactly improvements were made.
- Possible lack of future funding.
- Performance protocol has not been published as a standard.

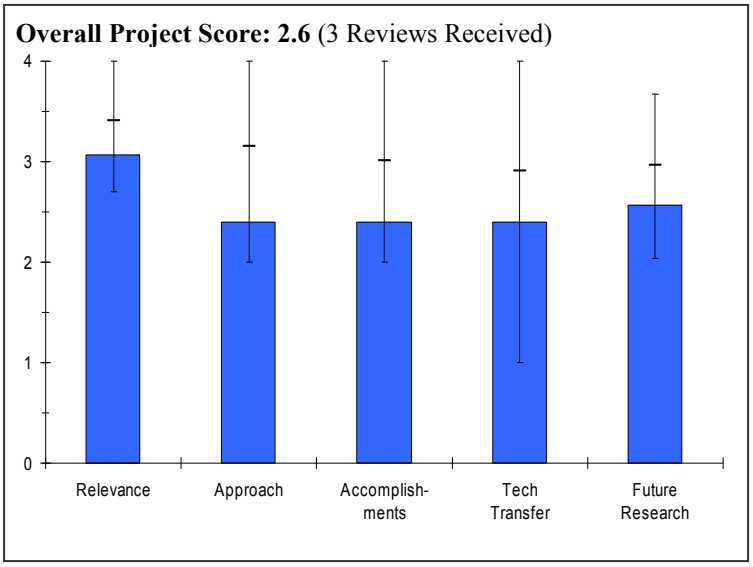
Specific recommendations and additions or deletions to the work scope

- Continue the good work.
- Publication of the testing protocol as an international standard would add credibility to the project, support the international efforts on the same topic and give credit to the laboratory.

Project # PDP-07: Photobiological Hydrogen Research
George Philippidis; Florida International University

Brief Summary of Project

The overall objective of this project is to identify which structural and active site maturation genes of the O_2-tolerant NiFe-hydrogenase from the photosynthetic bacterium *Rubrivivax gelatinosus CBS* are critical to optimal expression of the enzyme in *E. coli*. Expression in *E. coli* will facilitate eventual expression of the hydrogenase in cyanobacteria at the National Renewable Energy Laboratory. The 2007-2008 objectives of this project are to 1) clone the largest structural gene cooM of the hydrogenase into duet expression vectors under the T7 promoter; and 2) detect and purify the fully efficient (recombinant) hydrogenase in *E. coli*.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.1** for its relevance to DOE objectives.

- Although still somewhat in its infancy, this work has great potential for numerous applications.
- This is an essential but very difficult problem that several other projects also seem to be involved with.
- The project goal of constructing molecular biology cassettes of hydrogenase genes is well-aligned with the Program goal of understanding and optimizing biological hydrogen production.

Question 2: Approach to performing the research and development

This project was rated **2.4** on its approach.

- Standard non-innovative approach.
- The cloning strategy for construction of hydrogenase cassettes seems straightforward.
- The "top-down" approach of reconstructing a functional hydrogen-producing gene cassette in a heterologous host is not particularly innovative but seems feasible.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.4** based on accomplishments.

- Clear methodology and roadmap activities accomplished.
- Not yet achieved the goal of obtaining an active enzyme and it isn't clear why.
- The progress towards goals was good, with some specific milestones achieved in a timely fashion.
- The progress on several tasks (3.0 and 4.0) is weak and behind schedule.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.4** for technology transfer and collaboration.

- Working with the National Renewable Energy Laboratory, the pathways overlap, appears to be good communication.

- It was not clear what would be done once the main enzyme was obtained by the collaborator.
- The partnership between a university and national lab is good.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.6** for proposed future work.

- The future work proposed is in line with DOE mission.
- Plan and direction completed for future work, sounds like funding is the unknown.
- What will be done if this product is successful?
- Future tasks are well defined.
- Future plans to finish cassette construction and optimize hydrogenase expression levels are logical.

Strengths and weaknesses

Strengths
- Molecular experience of PI and overall goal of obtaining an active enzyme.
- The investigators' prior record of collaboration is very strong.
- The investigators have demonstrated good progress towards defined goals.

Weaknesses
- Overall goal. What is the next step?
- The project plan is "brute-force" construction of known components. It is unclear that reconstruction of a functional hydrogenase cassette will necessarily lead to determination of the "minimum number" of hydrogenase genes required for fully efficient hydrogenase expression. There may be nonlinearity in terms of specific maturation elements that are not reflected in stoichiometric combinations of gene cassettes.
- The need to purify back the recombinant hydrogenase enzyme from the heterologous host is not clearly articulated.
- The techniques for testing successful transformation are somewhat old-fashioned and laborious. Why can't the investigators use PCR to look for co-transformation rather than having to grow up mini-preps and run out gels?
- There is no contingency plan for modification of co-expression if induction results in little or no activity (likely due to formation of insoluble or inactive inclusion bodies, etc.).

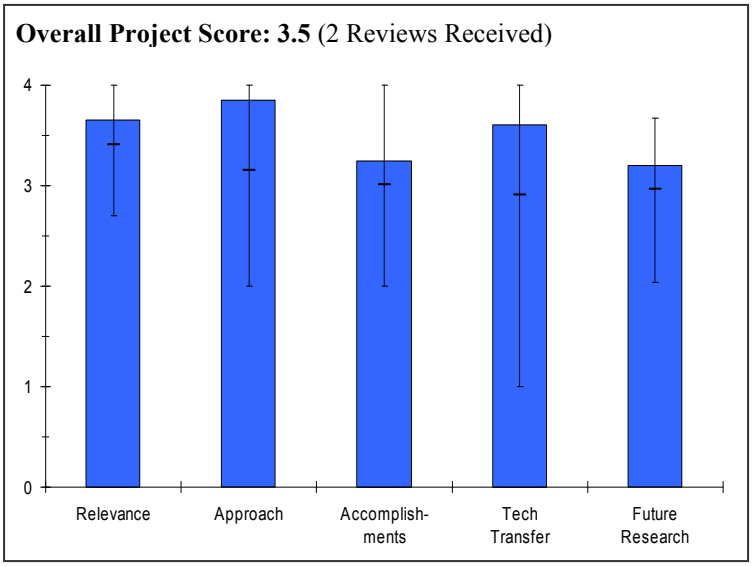
Specific recommendations and additions or deletions to the work scope

- None.

Project # PDP-11: Enabling Hydrogen Embrittlement Modeling of Structural Steels
Brian Somerday; SNL

Brief Summary of Project

The objectives of this project are to 1) enable application of structural integrity models to steel hydrogen pipelines; and 2) enable development of micromechanics models of hydrogen embrittlement in pipeline steels. Models can demonstrate that hydrogen embrittlement can be accommodated and pipeline safety margins can be quantified. Micromechanics model are essential for understanding the fundamentals of hydrogen transport and embrittlement in steels.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.7** for its relevance to DOE objectives.

- Understanding hydrogen embrittlement is essential to mass distribution and storage of hydrogen.
- This project promises to improve understanding of failure mechanisms of steel pipelines carrying hydrogen.
- This project supports achievement of DOE's targets for reliability/integrity and hydrogen leakage of hydrogen pipelines.
- It is not clear that this project will lead to capital cost reductions for H_2 pipelines.

Question 2: Approach to performing the research and development

This project was rated **3.9** on its approach.

- Approach seems to be right on target.
- The approach is effective and is focused on meeting the needs of ASME code.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.3** based on accomplishments.

- Good progress has been made in the basic understanding of embrittlement but obviously more is needed before methods of overcoming the barriers can be suggested.
- Project is making progress in measuring the properties of pipeline steels in high-pressure hydrogen gas using fracture mechanics methods.
- Barriers to further progress are being appropriately addressed.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.6** for technology transfer and collaboration.

- The list of collaborators and the fact that Sandia is dependant on others for test data and material samples indicates that collaboration is excellent.
- Sandia National Laboratories (SNL) is a member of the Pipeline Working Group, which allows them to share information with a number of other organizations doing pipeline research, as well as stakeholders.

- It does not appear that any universities are involved in the working group. University participation should be considered if they offer any capabilities that SNL does not already possess.
- Modeling does not appear to be included in SNL's scope. The anticipated modelers should be collaborators in the project.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.2** for proposed future work.

- The future indicates a continuation of efforts but should start to propose methods of overcoming the barriers.
- Proposed research is appropriate.

Strengths and weaknesses

Strengths
- Good coordination with others.
- Solid technical capabilities.
- This project promises to improve understanding of failure mechanisms of steel pipelines carrying hydrogen.
- Collaborations with the Pipeline Working Group will lead to effective information-sharing.

Weaknesses

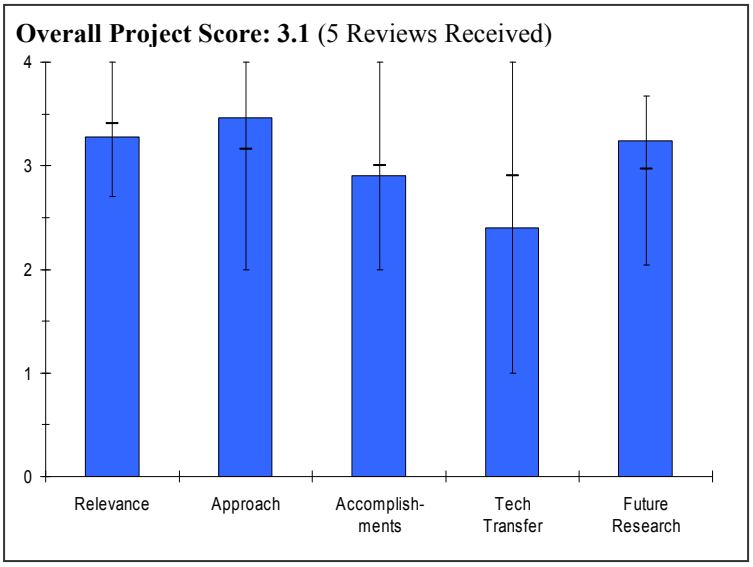
Specific recommendations and additions or deletions to the work scope

- Start to focus on screening methods for identification for acceptable materials.
- Consider including structural integrity and micromechanics modelers as partners/collaborators.

Project # PDP-14: Advanced Alkaline Electrolysis
Dana Swalla; GE Global Res.

Brief Summary of Project

The objective of this project is to study the feasibility of using alkaline electrolysis technology with current-generation nuclear power for large scale hydrogen production. The approach of the project is to 1) define market and requirements; 2) design and build a pressurized electrolyzer; 3) conduct plastic oxidation life test; 4) demonstrate electrolyzer performance and capital costs; 5) conduct system operation testing; 6) create industrial-scale system conceptual design; and 7) create 1-kg per second demonstration system conceptual design.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- This project has potential to produce hydrogen on site at reasonable costs.
- The project is working toward several DOE goals including lowering hydrogen production costs and increasing efficiency.
- Electrolysis is certainly one of the most viable options for near-term hydrogen production.
- This electrolysis work can be applicable to any electricity generating technology not just nuclear.
- Reducing the capital cost of electrolyzers would be a key step towards overall DOE goals.
- While the objectives are relevant, this is mostly an attempt to bring General Electric up to the state-of-the-art.
- Project is focused on reducing the cost of electrolysis and in deploying a system that can be used for many different applications of value to the hydrogen economy transition as well as to stationary and portable power sources that potentially have more immediate commercial applications.

Question 2: Approach to performing the research and development

This project was rated **3.5** on its approach.

- The project has a systematic and methodical approach.
- This project is focused on leveraging viable electrolysis technology with nuclear power and GE's advanced manufacturing to lower both the cost of electricity and capital costs which are two of the major hurdles for hydrogen via electrolysis.
- Good background work to identify existing hydrogen customers to bridge the gap to the eventual transportation sector demand for hydrogen.
- Design of stack for lower cost seems well engineered and thoughtfully conducted.
- The approach tries to bring GE up to the state of the art, but does not appear to be advancing it.
- The costs of current alkaline stack modules seem too high relative to existing commercial products.
- PI is focused on major technical improvements to achieve cost reduction and has followed a well designed plan.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.9** based on accomplishments.

- Good progress with electrocatalysis/electrode design.
- Why does the performance curve not show the current density (x-axis)?
- The project has demonstrated increased electrodes performance leading to a lower cost per unit area and higher efficiencies.
- Stacks have been successfully assembled using their plastic stack construction design.
- While these stacks have been constructed, they have yet to be tested.
- More experimental data would be expected at this point in the project especially since it is set to end on September 30, 2008.
- Similar to last year, they have yet to test the potential plastic degradation resulting from the plastic stacks being exposed to an alkaline electrolyte.
- Good concept definition of stack design.
- Electrodeposition seems to yield good performance, but would like to see more detailed performance comparisons with alternative methods.
- Completed market study for distributed hydrogen applications.
- Progress to date does not demonstrate any advancement of the technology or manufacturing techniques to significantly overcome any barriers. The costs of the stacks still seem high.
- All advancements are suggested as promising, but are not demonstrated on a large enough scale to be believable.
- Project is 70 percent complete and the results show significant progress toward the cost target. Technical innovation has resulted in significant improvement in cost on the order of 50 percent reduction.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.4** for technology transfer and collaboration.

- Not explained in the poster.
- The project has obtained useful real-world data from Entergy Nuclear to benchmark the system costs.
- The project has worked with the National Renewable Energy Laboratory to benchmark the cost of hydrogen via electrolysis based on the H2A model.
- Very little outside collaboration on the research and development aspects of the project.
- It is not clear there was much (if any) technology transfer or collaboration. However, it's not clear that any was needed.
- While there seems to be collaborations about market conditions, etc., there is nothing to suggest any collaboration with others in the electrolysis technology community.
- There is little collaboration with external organizations at this point, but the project is being successfully executed by resources and knowledge bases available from within the principal investigator's institution.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.2** for proposed future work.

- Future work planned is sound.
- The proposed future work to test the system at ambient and 15 bar is good.
- The operation and management cost assessment is important.
- It seems as if the project still has significant barriers to address in a very short time to ensure a successful project.
- Overall, the plan builds on their past progress and it focused on potential barriers.
- System testing at pressure is key.
- The future work suggested seems to be more of the same without indications of advancement.
- Future work to conduct system testing and complete the operation and management cost assessment builds upon the significant progress to date and will bring the project to a successful conclusion.

Strengths and weaknesses

Strengths

- The use of plastic components.
- Strong emphasis on materials durability.
- The overall technology has the potential to lower stack costs and provide for large scale hydrogen production.
- A strong research and development/engineering project conducted professionally.
- There is obvious technical capability in the General Electric organization.
- If cost targets are met following the systems testing phase, the technology has potential to be commercialized for various fuel cell applications as well as mid to small industrial hydrogen uses. The inventions made in the course of the work will facilitate differentiating this technology for commercial applications.

Weaknesses

- Stack testing must ramp up to successfully demonstrate the approach and the technology.
- Market projections are important and necessary, but I hope they didn't spend a lot of money on it. Seems like General Electric should have had a pretty good handle on the market from Day 1 of the project.
- Plastic joining method is poorly described.
- No linkage showing how stack costs combine with BOP costs to yield target $400/kW.
- If market demand study is for distributed generation, why are nuclear plants being considered?
- Bill of materials for system is not provided.
- Would like to see a fuller cost projection and more detailed system level definition.
- There is a lack of practical field experience in the organization.
- They have not addressed scale up, life, or mass production issues.
- There are no project weaknesses thus far; however, the principal investigator must report a final cost that shows the degree to which the target costs have been met.

Specific recommendations and additions or deletions to the work scope

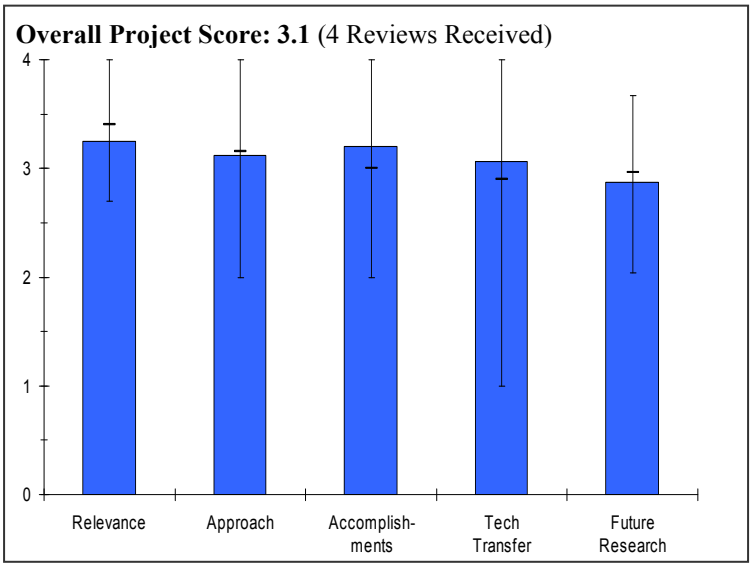
- Would it be possible to use an alkaline exchange membrane?
- Project should be expanded to include existing electrolysis manufacturers or deleted.

Project # PDP-15: Photoelectrochemical Generation of Hydrogen Using Heterostructural Titania Nanotube Arrays

Mano Misra; U of Nev. Reno

Brief Summary of Project

The overall objective of this project is to develop high efficiency hybrid-semiconductor materials for hydrogen generation by water splitting. The 2007-2008 objectives were to 1) develop organic-inorganic hybrid photoanodes; 2) develop combinatorial approach to synthesize hybrid photo-anodes having multiple semiconductors in a single photo-anode; and 3) develop cost-effective cathode materials. The 2008-2009 objectives are to 1) develop mixed metal oxide nanotubular photoanodes; 2) develop multi-junction photoanodes; and 3) design photoelectrochemical systems for on-field testing under real solar irradiation.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- Even optimization of TiO_2 as a hydrogen producing photoelectrode will not result in a useful system since it has too large a band gap to use much of the solar spectrum.
- A well constructed program aimed at building novel metal oxide/ metal sulfide macroscopic structures capable of photoelectrochemical water splitting.
- This program provides a good mix of basic science, system design, and engineering.
- Quite relevant as this research theme has the potential to be a contributing technology in decades to come.
- Long term, high risk research is exactly what should be funded.
- Photoelectrolysis concepts and subsequent funding are well aligned with the long term energy solutions.
- Most aspects of this project are aligned with the important goal of improving the efficiency of direct solar water-splitting.

Question 2: Approach to performing the research and development

This project was rated **3.1** on its approach.

- The principal investigators have developed a good level of expertise in the area of synthesizing TiO_2 nanotube arrays and related structures. Unfortunately, the principal investigators are committed to the idea that they can empirically find a way to lower the band gap of TiO_2 through doping or alloying, despite the numerous unsuccessful attempts to do this over the past 30 years. Similarly, their ideas about sensitization of TiO_2 are not novel.
- TiO_2 nanotubes are being produced and studied by at least a dozen groups (and with more success in many groups) and so there is no novelty in this project. CdS will be unstable in a non-sacrificial system and still will not extend the spectral response enough to make this useful. A strong materials science approach is employed coupled with good electrochemical support.
- The project is focused and productive.
- The materials approach is creative and sound.
- Use of nanotubes and variations of titania is pointing in the right direction. The approach is good and will lead to new and other novel materials.

- Approach and execution of the work is good - the key elements of the materials science are being addressed.
- New combinations of nanotubes, titania, and other relevant tunable band gap materials will emerge - leading to other potentially interesting combinations and thereby increasing the stability and efficiency.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.2** based on accomplishments.

- Most of the approaches being explored in this project have been tried before and have little chance of success. Some of the "accomplishments" are trivial or misleading. Shining light on both sides of a porous electrode to achieve a 6 percent solar to hydrogen conversion efficiency with their TiO_2/CdS system - they are using a sacrificial donor (sulfide) and not splitting water.
- Much of what is being done was well known 20 years ago, so it is difficult to call any of it progress.
- Synthesize high quality anatase rod structures.
- Introduce a carbon component to reduce the band gap.
- Generate TiO_2 rod/CdS particle mixed structures.
- Carried out PEC characterization of indicated materials.
- Demonstration photo-induced hydrogen production from TiO_2 rod/CdS particle mixed structures in the presence of an aqueous sulfide electrolyte. (System stability is uncertain.)
- All research goals are being met.
- The accomplishments with respect to stability are positive yet additional testing needs to be performed to assess if stability is maintained beyond a "few" hours.
- Result is very clear and presentation is very understandable.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.1** for technology transfer and collaboration.

- It is a good sign that the principal investigators have been active in publishing and presenting their work. However, some of their ideas about how photoelectrochemical devices work are not physically sound.
- The appropriate collaborative relationships are in place, especially with the National Renewable Energy Laboratory.
- This project seems to be in communication with other projects.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.9** for proposed future work.

- The proposed future work in not well focused. The basic idea seems to be to keep trying things a hope for a miracle.
- See former comments, but in summary, even perfecting a TiO_2 system will not produce a useful system or device.
- The success of this project rests on understanding the oxidative component. If the semiconductor is being oxidized the system is not viable. Thus, it is appropriate that the researchers are focused on this issue.
- Continued materials development is well defined and appropriately focused.
- The proposed work will attempt to drill down into the mechanisms and materials science. All appropriate for this stage as it is nearing the end of the effort.
- Longer term testing to assess stability under real sunlight conditions will be valuable.
- Newer compositions/configurations should be looked at.
- Please accelerate as much as possible and discuss with engineers to build more realistic design of the reactor.

PRODUCTION AND DELIVERY

Strengths and weaknesses

Strengths
- A strong track record of materials development.
- Interesting heterostructures mixing metal oxide and metal sulfide functionalities.
- A good mix of materials science, electrochemistry, and photoelectrochemistry.
- Strong technical team and partners.
- Materials science and facilities and capabilities.

Weaknesses
- Photoelectrochemistry is not well developed.
- The oxidation process may lead to a major materials instability.
- Weak understanding of photoelectrochemical principles and literature. Willingness to believe that ideas that have been tried and failed in the past will work in this project.
- Not novel and will not produce a useful or stable device and is also not producing any new fundamental information.

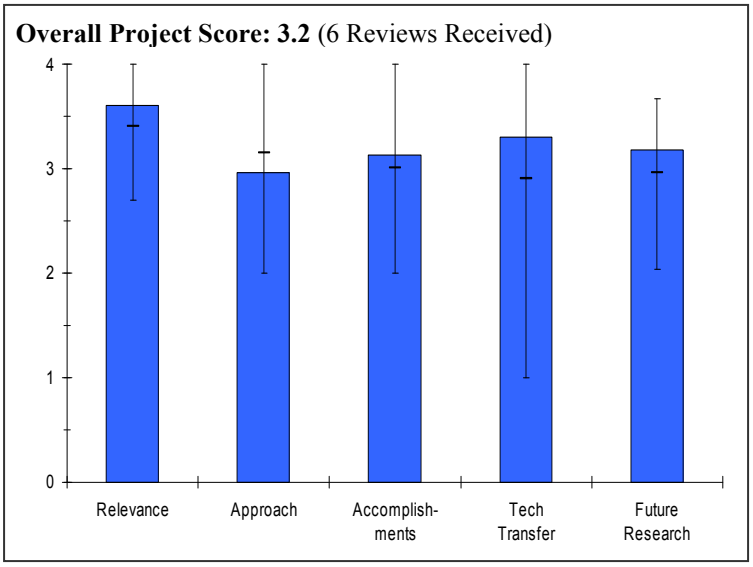
Specific recommendations and additions or deletions to the work scope

- There are some good aspects of this project. But the idea that this technology is ready for scale-up or commercialization (UNR easy H2 PEC cell) is absurd.
- Redirect project.
- The work plan is well supported. Continue as is.

Project # PDP-16: Distributed Bio-Oil Reforming
Bob Evans; NREL

Brief Summary of Project

The overall objective of this project is to develop the necessary understanding of the process chemistry, compositional effects, catalyst chemistry, deactivation and regeneration strategy as a basis for process definition for automated distributed reforming. The fiscal year 2008 objectives are to 1) improve bio-oil atomization with less MeOH addition; 2) conduct a study of partial oxidation at 650C; 3) demonstrate catalytic conversion consistent with $3.80/kg hydrogen; and 4) design, build and operate a bench scale unit capable of long duration runs (8 hours/cycle) with better material balances.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.6** for its relevance to DOE objectives.

- Hydrogen generation from bio-oils has the potential to be a key source of renewable hydrogen in the future.
- This project specifically supports key milestones related to the cost reduction of distributed hydrogen production from renewable liquids.
- The work is evaluating a process to convert biomass derived liquids to hydrogen. This is a goal of the Hydrogen Program and the work directly supports this objective.
- This project is important to the stated goal of hydrogen production from renewable biomass.
- The conversion of whole bio-oil is an important area of investigation because it can serve to minimize unit operations.
- Excellent project of clear relevance because biomass conversion into syn-gas allows for greater flexibility than simply a hydrogen target (e.g., it could go to higher value products, as needed).
- Use of pyrolysis product (bio-oil) is a solid idea.
- Poster was not quite clear; but the presenter's explanations were very helpful!
- Project is responsive to production of reformable fuels for production of hydrogen, etc. Supports 2012 Targets: $3.80/gallon gasoline equivalent, 72% energy efficiency (bio-oil to hydrogen).
- The object to produce hydrogen from renewable sources is in line with the overall goals and objectives.
- Due to the undesirable properties of bio-oils, it might not be best suited for reforming route.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- Initial energy efficiency estimates have been made with Aspen Modeling and more are planned in the future.
- Good approach addressing the key issues related to biomass pyrolysis including a parallel modeling effort.
- The project is attempting to convert a complex biomass liquid to hydrogen. Instead of simply considering ethanol (for example), the project is considering a pyrolysis derived liquid. The liquid contains a variety of compounds, including high molecular weight aromatics. This is a complex mixture to convert and the approach is unique. The process is relatively simple and, if successful, the cost to scale up the process would be reasonable.

- Although several barriers are identified, it appears that feedstock cost is the primary barrier being addressed; secondarily operation and maintenance. Fuel processor cost may be too early to address or at least it does not appear to be addressed yet.
- The project appears to be appropriately focused on developing methods of producing hydrogen from bio-oil, taking into account the complexity of the fuel, its difficulty in handling, etc.
- The interaction with Lanny Schmidt at the University of Minnesota appears to be a good step toward identifying possible catalytic approaches to processing these complex materials.
- Sound approach to developing "basic" chemical engineering understanding.
- Good understanding of unit ops in an integrated reaction concept.
- Volatilizing approaches could be better researched; but choice of ultrasonic system is "good enough" initially.
- Good use of secondary air flow to control surface reactions at the catalyst bed.
- Approach is sound and logical to complete objectives. High conversion of bio-oil in non-catalytic step leads to significant yield of CO at 650°C.
- Lower methanol levels (less than 30 percent) have yet to be demonstrated due to technical problems with the new system.
- Rhodium catalyst can be used to attain equilibrium levels of hydrogen with and without added steam.
- Feedstock effects are under study.
- Experimental results were used as a guideline for ASPEN simulations.
- Again due to properties of bio-oils, significant fraction of methanol has to be used to break down the bio-oil. This approach might not be ideal due to toxic nature of methanol which can pose safety/storage issue for forecourt application.
- The majority of the focus for this project should be on the elimination or minimization of Rh catalyst. This could be a show stopper should the others barriers are resolved/overcome.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.1** based on accomplishments.

- The new nozzle designed to improve bio-oil volatilization was not utilized due to a component failure. This seems to have set back some of the oxidation, catalyst, and reduced methanol work.
- Initial Aspen mass and energy balance modeling has been completed.
- The project has achieved good conversions of the bio-liquid. Near equilibrium levels of hydrogen are being obtained.
- There is formation of some coke on the water-gas shift (WGS) catalyst, but this is to be expected due to the presence of the high molecular weight compounds. However, the catalyst can be regenerated and activity remains high.
- Some benzene remains in the products and this will have to be addressed.
- The need for large amounts of methanol solvent is the key drawback to the process. At best, it appears that about 30 percent methanol will be necessary. This problem needs to be further addressed. This may be overcome by designing a more effective atomizer.
- The process keeps the water requirement to a minimum.
- It seems that progress has been somewhat slow, driven in part by the need to develop a fuel atomization method.
- There appears to be little other work in this area by others so that it is difficult to assess what is reasonable project progress. DOE might consider funding a second separate project in this area with some alternate ideas.
- A better understanding of the effect of different feedstocks on bio-oil quality and composition is planned and seems to be well-advised. It may be that certain bio crops are better aligned with this technology than others.
- Good collaboration with the Schmidt group regarding catalysts.
- Need to explore other viscosity modifiers (why just CH_3OH?).
- Need to see feedstock spectra (correlations between spectro and cracking products?).
- Reasonable data on oxidative cracking (micro-reactor results only?).
- Good progress has been made. Fiscal year 2006: Bio-oil volatilization method developed; oxidative cracking to CO with minimal CO_2.
- Fiscal year 2007: Demonstrated equilibrium catalytic conversion to syngas at low temperature and low H_2O/C.

- Would have liked to see more results on catalyst performance and effects of impurities in bio-oil.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.3** for technology transfer and collaboration.

- This project benefits from a strong team from industry and academia.
- More interactions with the biomass program at the National Renewable Energy Laboratory may be fruitful.
- Publications and presentations of the work appear very limited.
- The project has a number of participating partners, including Chevron, who would be capable of commercializing the process.
- The collaboration with Lanny Schmidt and with Chevron is good. It seems a bit premature to be talking about technology transfer.
- Good work to collaborate with the University of Minnesota group.
- Not very clear about the CSM contributions and the Chevron people.
- Collaboration is strong and effective CSM and NREL.
- Need more interaction with catalyst developers/manufacturers to address catalyst reduction and effectiveness with presence of impurities.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.2** for proposed future work.

- Additional modeling work with Aspen is underway.
- Plans to lower the percentage of methanol are underway along with long-term testing.
- The future plans are appropriate. In particular, the researchers have recognized the need to reduce the methanol and are working to achieve this objective.
- Additional plans are to scale-up and demonstrate the process at a larger scale.
- The future work aims to reduce methanol concentration but it is unclear how this will be done and whether the use of methanol is a result of the scale of the testing or will be a consideration even at a larger scale.
- Much of the work appears to depend on the proper operation of the atomizer. One needs to ask whether this or some other technology will be applied if and when the process is scaled up. Is the vaporization of the fuel a show stopper at a larger scale, or is it easier?
- Excellent; and I hope you are better funded!
- Need to spell out what you mean by optimization (catalyst search? Or process changes - if so, which variables?)
- Fiscal year 2008 work is proceeding well. PI should: Demonstrate catalyst performance (in progress); design, build, and operate bench scale system (in progress).
- Need to establish clear criteria for go/no-go decision (working with DOE and HPTT).

Strengths and weaknesses

Strengths

- The project is aligned with DOE targets and it provides a potential renewable source of hydrogen.
- This is a good project for NREL. This is a high risk research project involving a difficult conversion process. It is unlikely that industry would be willing to conduct any significant research in this area. NREL has had some good success and generated some very useful information and data.
- Experienced team that is well versed in bio-oil after several years of work.
- Well conceived and laid out.
- Good choice of partners (University of Minnesota and Chevron).
- Appropriate "unitized" reactor; but many need more control points.
- Out-year work well conceived.

Weaknesses

- Little mention about the potential of coke formation and how the project plans to deal with this issue over a long cycle.
- Overall, the project still seems a long way away from being a viable option and the path forward is not obvious especially without an energy cycle analysis.
- The Aspen model is a good step, but it is not obvious that this project has sufficient chemical engineering/reaction engineering help. It seems to be at a research and development stage but perhaps a engineering component could help guide the work, for example what needs to be considered if one were to scale up the process.
- For example, is methanol a requirement at a larger scale, or not? If not, then one needs to revisit how to best carry out the tests to avoid this possible artifact to full scale operation.
- Need greater chemical engineering (process control) inputs.
- Need correlations of bio-oil inputs (spectra) with resulting syn-gas products (any interesting correlations?).

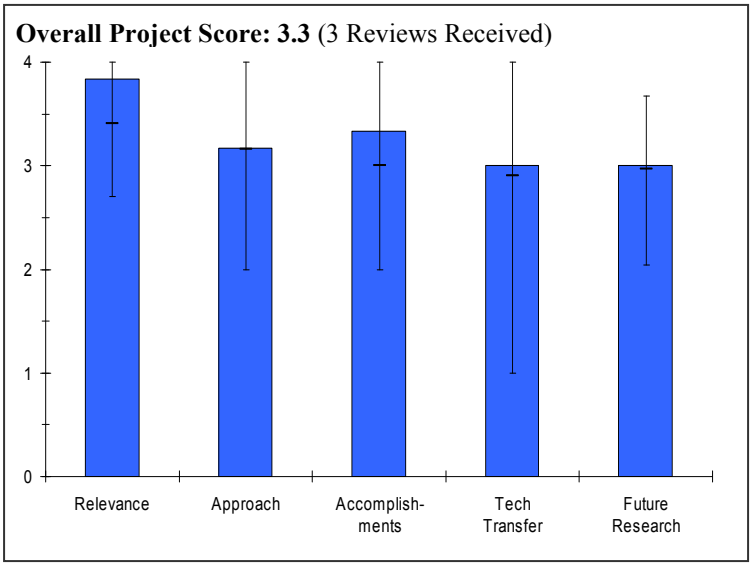
Specific recommendations and additions or deletions to the work scope

- Specifically examine this process of producing hydrogen (from biomass to bio-oil to hydrogen) from an energy standpoint.
- Fiscal year 2008 funding for this project appears extremely high. Yearly funding should be at the prior year levels - approximately $300 to $350K per year.
- Add more capability in reaction engineering and modeling.
- Fund the project more consistently!
- Get more feedstock info (spectra).
- Develop broader steam/C ratios.

Project # PDP-18: Solar Thermochemical Hydrogen (STCH) Production - H2A Analysis
Kurt Roth; TIAX

Brief Summary of Project

The objective of this project is to evaluate which solar-thermochemical hydrogen (STCH) cycles have the potential to meet the Department of Energy central production cost target of $3.00/kg. The tasks for this project are to 1) support cost analysis of STCH cycles carried out by STCH Development Teams using H2A; 2) identify key cost drivers to guide research efforts to improve STCH economics; and 3) ensure meaningful comparisons of hydrogen production cost estimates among cycles to enable the most effective cycle down-select process.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.8** for its relevance to DOE objectives.

- Solar driven thermochemical water splitting is a renewable way to generate hydrogen and is applicable to the DOE objectives.
- There are many solar thermal hydrogen production options available, economic analysis such as this project is key to focusing efforts on the most promising approaches.
- Provided a well informed review and cont-analysis of thermochemical cycles for hydrogen production.

Question 2: Approach to performing the research and development

This project was rated **3.2** on its approach.

- Techno-economic analysis enables DOE to focus their limited resources on the technologies which have the highest probability of meeting their cost targets.
- Providing guidance to the researchers is an important role for Tiax.
- The DOE managers should also be trained so that they can evaluate the H2A spreadsheets on their own after the contract of Tiax is over.
- Approach is sound and logical: use of the H2A cost spreadsheet populated by values suggested by knowledgeable researchers and vetted to assure fair assumptions among the various approaches.
- Close and iterative collaboration with the technology development team.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.3** based on accomplishments.

- They should increase their attention on the operation and maintenance costs which will be significant for this technology.
- The chemicals used are the STCH processes are very toxic, costs should be included for spent chemical disposal.
- They should not include oxygen production credits in their cost analysis. The market is not large enough for the amount of oxygen produced.
- Review and feedback on 11 separate pathways.

- Identified specific items for improvising hydrogen analysis, as well as key issues as on cost of thermal versus thermal energy. Comment: In some solar thermal locations there may be a use for long scale oxygen, as in coal gasification processes for the production of liquid panels.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- They are providing valuable feedback to many different collaborators.
- They need to educate the DOE managers, so when the contract is over, the DOE managers will understand what is in H2A and why.
- Number of cases investigated (11) forces collaboration with multiple groups.
- Extensive collaboration with "customer" partner.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- Collaboration with researchers seems adequate.
- Future plans are obvious: continue analysis to complete full set of cases.
- Continue and refine to present project needs with partners. Said funding for HY 2009 is noted.

Strengths and weaknesses

Strengths
- They are providing valuable feedback to the collaborators to make their H2A analysis more realistic.
- Use of H2A spreadsheet is fundamental to this project.
- Use of a single group to examine full set of STCH approaches ensures commonality of assumptions and validity of relative cost comparisons.
- Listing of "lessons learned" is good.

Weaknesses
- They need to make sure to capture all of the costs for operation and maintenance, diurnal operation, thermal storage (if used), and spent toxic material disposal.
- They need to work with the DOE managers to help the managers understand how to apply H2A to this area.
- Project scope (11 analyses) makes listing of technical and economic assumptions difficult in a poster format. However, presentation of $/kg results without description of assumptions is weak.
- There are no descriptions of the various cases (other than their titles).

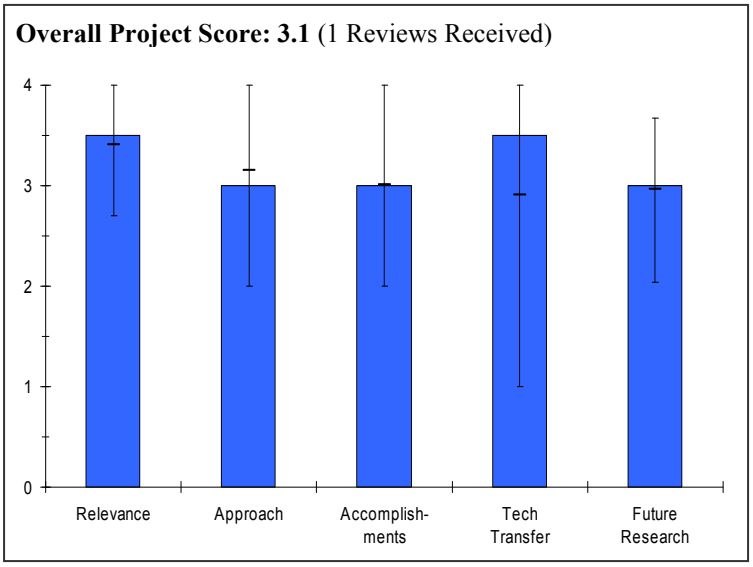
Specific recommendations and additions or deletions to the work scope

- None.

Project # PDP-19: Ocean Thermal Plantships for Production of Ammonia as the Hydrogen Carrier
Chandrakant Panchal; ANL

Brief Summary of Project

The objectives of this project are to evaluate the technical and economic viability of at-sea ocean thermal plantships for production ammonia as the hydrogen carrier to meet the HFCIT cost goal of $2 to $3/gge (delivered, untaxed, 2005$ by 2015); and 2) evaluate the economic impact of co-production of desalinated water. The cost of ammonia as a fertilizer has been significantly impacted by natural gas prices. Ammonia can be an alternate fuel for distributed power generation (combustion turbine or internal combustion engines). Ocean thermal plantships deployed in the Gulf of Mexico can be a source of hydrogen for refineries in the Gulf of Mexico states.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- Economic analysis assumptions and results were presented clearly.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- Project provides analysis of a new technology area for very little funding spent.
- Solid approach that incorporates relevant milestones and go/no-go decision points.
- Go/no-go decision point appeared to be based on funding and not on achieving a quantitative milestone, such as projected hydrogen cost, to show probability of technology success.
- It would have been beneficial to see a summary of comments provided by industrial participants at the September 11th workshop.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.5** for technology transfer and collaboration.

- Project is coordinating with multiple partners.
- Based on the presentation materials, the roles of each partner were not fully defined.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

PRODUCTION AND DELIVERY

- Proposed future development and design work could come at a significant cost. It is unclear what the price tag would be for this work.
- Input on the possible technical challenges that would need to be overcome in future work would be helpful in assessing the likelihood of success of the technology.
- Future work is relevant to the proposed technology.

Strengths and weaknesses

Strengths

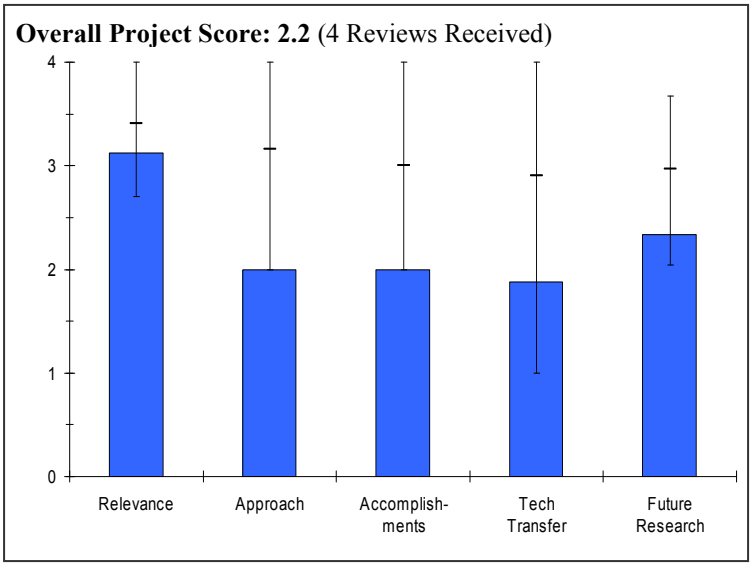
Weaknesses

Specific recommendations and additions or deletions to the work scope

Project # PDP-21: Photoelectrochemical Hydrogen Production
Malay Mazumber; U. Arkansas Little Rock

Brief Summary of Project

The overall objective of this project is to optimize surface properties of anodes for efficient photoelectrochemical (PEC) generation of hydrogen. The objectives of this project are to 1) use plasma surface engineering to control surface states for removing electron traps and improving photo-conversion efficiency; 2) use surface doping for interfacial photo-conversion for hydrogen generation with a minimal change in the bulk for improved durability; 3) correlate surface structures with light absorption and interfacial charge transfer; 4) measure photocurrent density for the test nano-structure TiO_2 electrodes against different bias voltages; and 5) perform comparative efficiency analysis for different photoanodes.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.1** for its relevance to DOE objectives.

- Hydrogen generation by PEC is critical to the presidents Hydrogen Fuel Initiative.
- The object of this project is to use plasma treatments to modify the surface of TiO_2 so that it will absorb more of the visible portion of the solar spectrum and split water. Researchers from around the globe have been working on this system for over 30 years and have achieved very little.
- This project attempts to use plasma treatment of TiO_2 to improve light absorption and photocurrent conversion efficiency.
- Improving semiconductor band gap, conversion process efficiency, and durability is consistent with the DOE goals and objectives.
- Project lacks comparison to DOE goals or system analysis to determine the likelihood that the results of the project will contribute to achievement of the DOE goals for PEC hydrogen production.
- This project supports the long term goal of cost effective renewable production of hydrogen.
- If a useful water photoelectrolysis system is the objective, TiO_2 will not work since its band gap is too large to be efficient. Fundamental science to help understand charge transfer or surface chemistry of oxide semi-conductors will be useful but this project is mainly empirical.

Question 2: Approach to performing the research and development

This project was rated **2.0** on its approach.

- TiO_2 with little modification not novel.
- The PIs assert that plasma treatments provide a mechanism for creating TiO_2 alloys (e.g. w/ N) at the electrode surface, but there was little direct evidence that this has been accomplished. Also, the plasma is supposed to "remove contaminants" from the electrode surface, but under illumination the TiO_2 surface is self-cleaning.
- It is not clear that successful modification of TiO_2 properties will lead to achievement of the DOE goals.
- The project does not incorporate system design to produce hydrogen.
- Approach is focused on removing electron traps and improving photo-conversion efficiency of TiO_2 and improving durability, which are necessary for achieving DOE goals.

- The study utilizes a well thought through systematic study of changes in photocurrent density due to varying anodized Ti samples prepared with and without plasma treatment using several different gases. Good use of XPS to monitor exchange of O_2 for N_2.
- Adding N to TiO_2 to extend the spectral response will not improve performance since: 1) there is a limited solubility of N in TiO_2, 2) it does not absorb much light, 3) it can act as a recombination center (not often reduced band gap response), and 4) it will be unstable to oxidation.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.0** based on accomplishments.

- Not clear that this will absorb visible light.
- So far, plasma treatment has had little or no effect on the ability of TiO_2 to absorb visible photons. There are many possible explanations for the observed increase in photocurrent for plasma-treated electrodes. Very little has been done to distinguish between these possibilities.
- The project has apparently not produced any hydrogen to date from the photocells.
- The project appears to have made progress in increasing the photocurrent density of TiO_2 photoanodes.
- The reduction of the band gap for TiO_2 from 3.32 down to 2.80 due to nitrogen doping provides encouragement that further improvements may be possible through further plasma treatment optimization.
- Much of what has been done was already in the literature 20-30 years ago.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **1.9** for technology transfer and collaboration.

- No industrial collaborations.
- While PIs assert that there is an "active partnership" with Univ. of Reno and Ark. Nanotech Center, it is not at all clear what this partnership entails.
- University of Nevada Reno is testing treated samples.
- There are no industry collaborators; thus, technology transfer is a weak point for this project. A systems engineer should be involved in the project to determine the likelihood that plasma treatment of TiO_2 will contribute to achievement of the DOE PEC hydrogen production goals.
- The Program has ongoing collaboration with University of Nevada Reno and Arkansas Nanotechnology Center.
- There appears to be good communication with other "earmark" projects.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.3** for proposed future work.

- So far, the research in this project has been highly empirical. Future work calls for optimizing the plasma treatment. But since the PI's do not know what the plasma actually does, there is little to optimize. Future work also mentions photocatalytic activity. It is unclear what this is about.
- Future research should include systems engineering as well as continued characterization and optimization of photoanodes.
- The next steps which include further optimization of plasma treatment and systematic study of the impacts of varying catalysts on photoconversion efficiency seem reasonable.
- Again, even perfecting a system based on TiO_2 or even "doped" (actually alloyed) with N will not produce a useful photoelectrolysis system.

Strengths and weaknesses

Strengths

- The principal investigators have set-up a plasma treatment apparatus and a basic photo electrochemistry experiment.
- This project incorporates a seemingly novel approach to TiO_2 surface modification.

- The project supports achievement of DOE's targets for usable semiconductor band gap, chemical conversion process efficiency, and plant durability.
- Clearly demonstrated that there is a cumulative effect of reduced band gap and removal of contaminants.

Weaknesses

- TiO_2 has been studied for many years by many researchers without much promise as a successful PEC material.
- Many. The rationale for this project is weak and the principal investigators lack the instrumentation and experience to correctly interpret what they are doing.
- The project has not conducted systems engineering and analysis to determine the ultimate likelihood of success with respect to meeting the DOE targets.
- The project does not appear to be focused on improving hydrogen production capability, but only improving materials properties.
- Need to design experiments which will further differentiate the impact of reduced band gap versus removal of contaminants on photocurrent density.
- Not original, no new fundamental knowledge, and will not produce a useful device even if all problems with the system are solved.

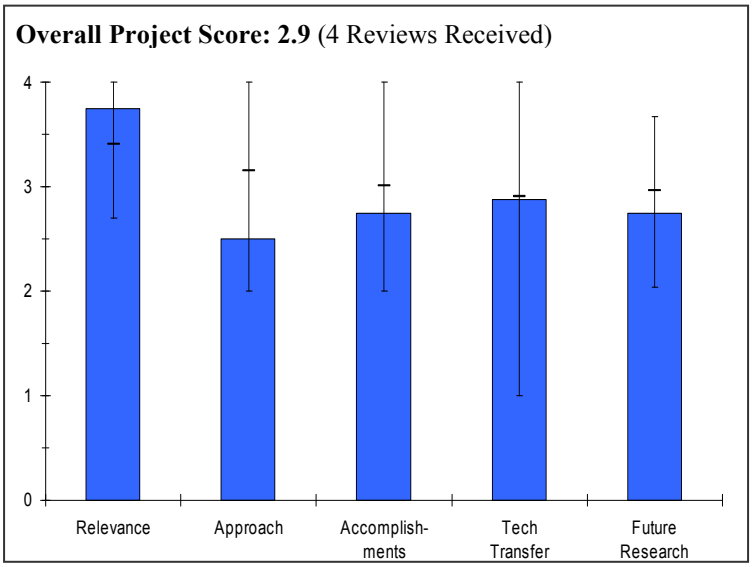
Specific recommendations and additions or deletions to the work scope

- There is little reason to recommend continued funding for this project.
- Add an industrial partner to conduct systems engineering and analysis.

Project # PDP-22: Distributed Reforming of Renewable Liquids via Water Splitting using Oxygen Transport Membrane (OTM)
Balu Balachandran; ANL

Brief Summary of Project

The overall objective of this project is to develop a compact, dense, ceramic membrane reactor that enables efficient and cost-effective production of hydrogen by reforming bio-derived liquid fuels using pure oxygen formed by water splitting and transported by the membrane. The 2008 objective of this project is to optimize the performance of the oxygen transport membrane and demonstrate reforming of ethanol. Membrane technology provides the means to attack barriers to the development of small-scale hydrogen production technology.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.8** for its relevance to DOE objectives.

- Program is aimed at making hydrogen from renewable liquids, which is aligned with DOE's objective.
- Process under investigation is extremely unlikely to be economically competitive for hydrogen production.
- Oxygen transport membrane (OTM) materials are being developed for distributed reforming of renewable liquids via water splitting. Supports 2012 Targets.
- The Program helps to support the DOE objective of using renewable feedstocks (bio-derived liquids) to cost effectively generate hydrogen. Cost reduction goals may be obtained by combining the separation and purification step for oxygen transport to be used to process the bio-liquid. Further the use of one material eliminates concerns about thermal expansion/contraction so likely to add to cost reductions and system reliability. Additionally the PO_x system is an exothermic reaction so energy efficiencies may also be obtained.
- A potentially cost effective, renewable hydrogen process is very relevant to the overall objectives.

Question 2: Approach to performing the research and development

This project was rated **2.5** on its approach.

- I don't believe they have properly identified the barriers.
- Presenter indicated satisfaction with present performance, but cost numbers he provided suggest this performance fall short of capital targets.
- The approach to providing heat for this highly-endothermic reaction (using hot steam) is completely inadequate. A simple heat balance (took me five minutes) indicates that steam/feed ratios over 20 would be needed, and this is simply not competitive.
- Approach is sound and logical to complete objectives. Fuel is reformed using oxygen formed by water splitting and transported by the OTM. Hydrogen is produced on both sides of the OTM. Non-Galvanic. No electrical circuitry or power supply. Single material.
- Given that the project lost funding in 2007 a switch was made from processing natural gas to processing bio-derived liquids the Program is a bit behind but still making significant progress.
- Those working on the project are very experienced in developing transport membranes for other commercial applications and have a very well thought out plan for utilizing existing systems and building on that knowledge to produce more suitable membranes.

- Also initial efforts utilize chemical grade ethanol and builds on those learnings before assessing more challenging fuel grade ethanol.
- Material stability and durability are potential issues due to high temperature operation and presence of reduced and oxidative environments.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.8** based on accomplishments.

- Given the newness of the bio-liquids thrust, team has made good progress on proof of concept experiments.
- However, I don't believe they have a good grasp of the barriers related to flux and heat, and those barriers have been present even in the original configuration of the Program (for CH_4 reforming).
- Good progress has been made despite rapid shifting of work from methane.
- Given that funding was interrupted the progress in membrane fabrication to date is acceptable.
- Lack of actual conditions (no N_2 dilutent) testing and extended testing of the OTM.
- Cost data are based on premature process conditions; need refinement/updates.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.9** for technology transfer and collaboration.

- Appears to have some good collaborations on materials.
- Collaboration is strong and effective. Related membrane R&D is sponsored by Fossil Energy-National Energy Technology Laboratory.
- Fossil Energy-National Energy Technology Laboratory is funding related membrane work at ANL; so potential for technology transfer for a variety of uses.
- Would be helpful to progress this to the point where private industry might have an interest.
- Collaborations with membrane developers and industry partners are needed.
- Have a third independent party such as DTI to conduct the cost analysis.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.8** for proposed future work.

- Plans address certain issues, such as durability and performance at higher conversions and concentrations.
- Plans do not appear to address important barriers of flux and heat management (means to provide heat of reforming).
- Fiscal year2008 work is proceeding well. The principal investigator is optimizing the performance of the oxygen transport membrane (OTM) and demonstrates reforming of ethanol (EtOH).Suggest Pt/Pd thin surface layer as catalyst be explored.
- More tests on membrane stability/durability will be conducted during fiscal year 2009.
- Longer test time and possibility of coking of membrane need to be addressed.
- The next step approaches are reasonable however a lot needs to be accomplished in 2008 including optimization of the membrane thickness and composition in order to get to the full system integration and demonstration phase of ethanol reforming. For instance there is a need to increase membrane flux while also minimizing membrane thickness, increasing porosity and finding the right reaction conditions.
- Again need to have third party to conduct techno-economic analysis of the process.

Strengths and weaknesses

Strengths
- Impressive ability to extrude OTM tubes, nice development of tube morphology to relieve surface limited transport.
- Out-year work well conceived and comprehensive.
- The greatest strength of the project is the experienced scientists who are undertaking the effort.

Weaknesses

- This technology has NO CHANCE of beating simple ethanol steam reforming (ESR).
- It has all the ancillaries of ESR (steam gen, shift, separation), plus a reactor that must be substantially more complex and expensive.
- The overall reaction has stoichiometry (heat and mass balance) that is identical to ethanol steam reforming. There is no justification to splitting the reaction into two parts using the membrane. Splitting the reaction with a membrane adds nothing but complexity and cost, reduces efficiency, and increases the challenge of providing heat of reaction.
- Lack of consistent funding.

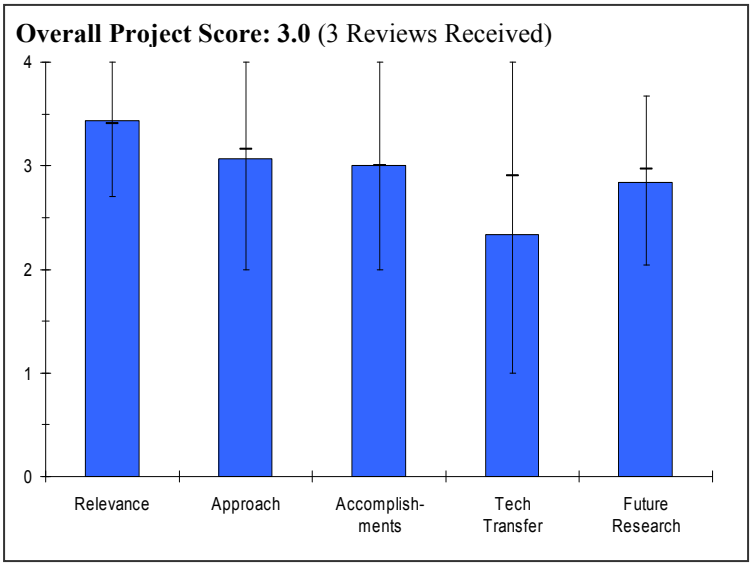
Specific recommendations and additions or deletions to the work scope

- I am a fan of OTM's but this embodiment makes no sense to me.
- I would delete the entire scope of this project.

Project # PDP-25: Carbon Molecular Sieve Membrane as Reactor/Separator for Water Gas Shift Reaction
Paul Liu; Media and Process Technology Inc.

Brief Summary of Project

The objectives of this project are to 1) evaluate a membrane reactor system using existing membranes and catalysts via math simulation; 2) validate membrane and membrane reactor performance and economics; 3) prepare membranes, module and housing for pilot-scale testing; 4) perform pilot scale testing and demonstration; 5) perform economic analysis and technical evaluation; 6) prepare field testing; 7) fabricate membranes and membrane reactors and prepare catalysts; 8) prepare site and install reactor; 9) perform field test; 10) conduct system integration study; and 11) finalize economic analysis and refine performance simulation.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.4** for its relevance to DOE objectives.

- This projects uses (what could be) low cost methods to purify hydrogen for direct stationary PEM systems, or potentially distributed hydrogen production.
- The degree of relevance depends upon comparison with existing technologies, such as PSA.
- A low cost combination water-gas shift (WGS) and membrane unit would be a significant step towards research and development objectives.
- The project focuses on meeting the DOE hydrogen production efficiency and cost goals by combining the LTS and HTS reactions into one and by combining hydrogen purification and separation.

Question 2: Approach to performing the research and development

This project was rated **3.1** on its approach.

- Project uses LTS, membrane separation, followed by regenerable sorption step to purify hydrogen.
- Approach is fundamentally sound but is made difficult to evaluate due in inadequate description of inner device workings.
- The elimination of the extra WGS step and the reduction in PSA beds through use of the HICON process appears to be an approach that will lead to substantial cost reductions and improved efficiency but we still have to wait for the testing of the complete system to know if this is really the case.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- They modeled hydrogen recovery and hydrogen purity.
- PDU unit was being assembled.
- Preliminary H2A analysis was performed.
- Experimental demonstration of Temperature Swing Adsorption (TSA) is good, but would be improved by demonstration at actual expected operating conditions.

- They have analytically shown 90 percent hydrogen recovery at 99 percent purity. Experimental verification is now needed.
- The bench tests of their WGS/MR show that 99.999 percent hydrogen can be produced with 80 percent recovery.
- Elimination of the high temperature shift will help reduce costs and improve efficiency. Still remains to be seen if the efficiency, purity and cost targets can be met once the pilot and field units are assembled and tested.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.3** for technology transfer and collaboration.

- Collaborations with the University of Southern California, Chevron, and Johnson Matthey.
- Unclear what role the partners play and have played (Johnson Matthey is a partner, but stated no catalyst development).
- Little interaction cited.
- Still unclear what the role of Chevron is in this partnership. Do they see this as a viable process?
- What contributions to the project have been made by Johnson Matthey or Chevron?

Question 5: Approach to and relevance of proposed future research

This project was rated **2.8** for proposed future work.

- Project formally ended June 2007, with no cost extension.
- Remainder of project completes the on-going work and demonstrates the technical approach.
- Pilot scale testing and verification of entire process, as they have a plan to do, is the key next step.
- Further economic analysis is necessary: current analysis is weak.
- It looks like the Program will come to an end this year; hence, I am not sure if they will be able to build the pilot and field unit and do sufficient testing and incorporate learnings to produce an optimized system.
- The same concern remains for the H2A analysis; will reliable numbers be generated with out a fully optimized system?

Strengths and weaknesses

Strengths
- Interesting hydrogen purification train for a fuel processing system.
- WGS via a carbon coated membrane is innovative and appears to achieve excellent WGS conversion.
- Modeling appears to achieve low cost and high efficiency.
- Concept of linking a membrane/WGS with a TSA to achieve high CO conversion and very high net hydrogen recovery is clever and sound.
- While membrane unit only achieves 99.5 percent hydrogen purity and thus requires a second purification device (TSA), their argument that all membrane systems (even metal membranes) will require a secondary "guard bed" purifier has some merit. Thus their system is not truly penalized for having a TSA since other system also will have one.
- Tubes (on a ceramic support) are relatively inexpensive, taking some of the burden out of their required high tube surface area.
- Looks like some good collaborative partners; Johnson Matthey, Chevron, and USC.

Weaknesses
- The adsorption 'polishing' step needs careful analysis, especially to understand removal of species such as H_2S to the low concentrations needed for PEM.
- Adsorption step durability needs to be understood and demonstrated especially for gas constituents such as sulfur.
- Inner workings of their unit are poorly/inadequately described.
- Unit has low hydrogen permeance leading to high-required surface area.

- Process flow diagram and heat integration inadequately described. Not clear that unit has sufficient waste heat for SMR endotherm.
- Since you did not do any catalyst development, I am unclear of the role of Johnson Matthey.
- What is the role of Chevron?

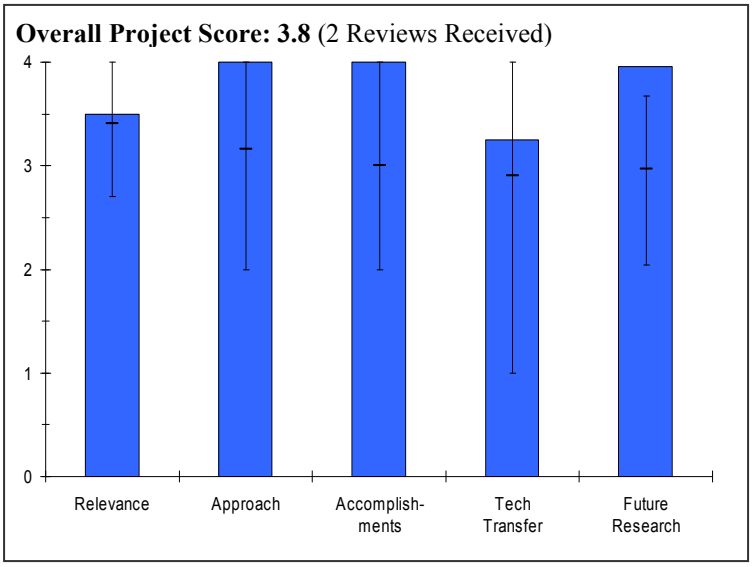
Specific recommendations and additions or deletions to the work scope

- Hydrogen purity analysis needs to measure low-level impurities (H_2S).
- Ninety percent hydrogen recovery seems low to have a high overall hydrogen production efficiency.
- They need to experimentally demonstrate the modeled 90 percent hydrogen recovery and 99 percent purity.
- Economic analysis needs to be completed.

Project # PDP-26: Biological Systems for Hydrogen Photoproduction
Maria Ghirardi; NREL

Brief Summary of Project

The overall objective of this project is to generate an algal strain capable of efficiently producing hydrogen gas from water under atmospheric oxygen concentrations. This goal is pursued by 1) molecular engineering of the algal hydrogenase to limit oxygen access to its catalytic site, and 2) development of a system that iduces culture anaerobiosis and hydrogen production by means of a physiological switch. In addition, NREL is working with other research organizations to develop a system where several biological hydrogen production are integrated into one efficient system. .



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- High priority for the green algae work.
- Highly innovative to bring in photosynthetic bacteria.
- The project goal of optimizing photosynthetic water-splitting biological hydrogen production is well-aligned with program goals for engineering improved biological hydrogen production systems.
- The project goal of increasing catalyst stability and improving oxygen tolerance is also well-aligned with program goals for engineering improved biological hydrogen production systems.

Question 2: Approach to performing the research and development

This project was rated **4.0** on its approach.

- Excellent, cutting edge, molecular and physiological approach.
- The catalyst engineering strategy seems straightforward and feasible, using well-tested site-directed mutagenesis techniques.
- The use of molecular simulations to aid in catalyst re-engineering is appropriate.
- The use of alginate immobilization strategies is a good combination of biological and materials expertise.
- The fermentation and hydrogen production strategies are appropriate.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **4.0** based on accomplishments.

- Virtually all aspects had been taken to the next level. Very impressive.
- The progress towards goals was very good on this project that has only recently secured robust funding.
- The progress on specific milestones is excellent, with most of them on schedule.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.3** for technology transfer and collaboration.

- This is truly a team effort with each member bringing unique attributes and experience.
- The partnership between various universities, an international institution, and a national lab is good.
- The specific mechanisms for coordination between all project partners are not clearly described, although the specific tasks are.

Question 5: Approach to and relevance of proposed future research

This project was rated **4.0** for proposed future work.

- Well thought out.
- The problem in that there are many avenues to go down, and the principal investigator may need to focus in the next area.
- Future tasks are well-defined.
- Future plans to finish reporter gene construction and optimize heterologous hydrogenase expression levels are logical.
- Future plans to improve and stabilize the alginate films are good.
- Future plans to optimize fermentation and performance of different photosynthetic cultures in the stacked bioreactors are logical and systematic.

Strengths and weaknesses

Strengths
- Robust molecular and biological approaches, plenty of strengths on the aspects of enzyme and cellular hydrogen production.
- The investigators' prior record of collaboration is very strong.
- The investigators have demonstrated expertise in the study of hydrogenase enzymes and biophotolytic hydrogen production.
- The project team expertise is balanced and complementary.
- The ability of the investigators to leverage off other federal funding is an advantage.

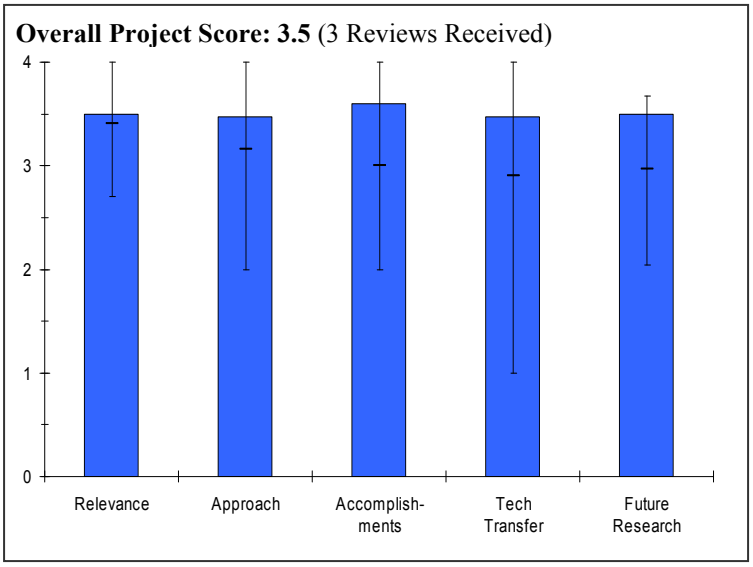
Weaknesses
- Only that there are perhaps too many aspects and focus may be needed.
- The project plan is somewhat diffuse, and it is difficult to determine the necessary sequence of milestones for individual subtasks against the project whole. For example, how does testing of natural samples link to optimizing hydrogen production in heterologous systems?
- The contingency plan for possible failure of heterologous expression is not well-defined.

Specific recommendations and additions or deletions to the work scope

Project # PDP-27: Fermentative and Electrohydrogenic Approaches to Hydrogen Production
Pin-Ching Maness; NREL

Brief Summary of Project

The long-term objective of this project is to develop direct fermentation technologies to convert renewable lignocellulosic biomass resources to hydrogen. The near-term objectives of this project are to 1) optimize bioreactor performance for the cellulose-degrading bacterium *Clostridium thermocellum*; 2) identify key metabolic pathways to guide generic engineering to improve hydrogen molar yield; and 3) integrate microbial electrolysis cell (formerly BEAMR: bio-electrochemically assisted microbial reactor) process to improve hydrogen molar yield.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- The project goals are well-aligned with DOE program targets for maximizing efficiency of biologically-derived hydrogen production via fermentation and electrohydrogenesis.
- The focus on Clostridium thermocellum is good.
- The combination of fermentation and electrohydrogenesis is innovative.
- Very relevant to overall hydrogen.
- High relevance along the lines of biological hydrogen.

Question 2: Approach to performing the research and development

This project was rated **3.5** on its approach.

- The cell growth optimization approach using bioreactors and defined cellulosic substrates is appropriate.
- The pathway inhibition and flux redirection approach is appropriate.
- The microbial electrolysis cell design using optimized fermentation cultures is good.
- Very good approach, particularly the inhibitors, but the approach needs to be complimented by genomics and genetic-based technique, possibly through collaborations.
- Logical and replicable.
- High applicability, pertinent to current biological /energy issues, easy to adapt to current technologies, without much infrastructure changes.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.6** based on accomplishments.

- The progress towards goals was excellent, with pathway engineering targets achieved ahead of schedule.
- The demonstration of robust hydrogen production from corn stover substrates is good.
- The progress has been excellent given the delay in project start.
- Very good progress, particularly with the collaboration to use the bioreactor to utilize non-hydrogen products.
- The microbial energy cell is a brilliant adaptation.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.5** for technology transfer and collaboration.

- The partnership between a university and national lab is good, although any explicit synergy for tech transfer to Bruce Logan's business venture, Ion Power, is not described.
- The new interactions with the University of Manitoba are excellent and add desired project expertise in microbial physiology and pathway engineering.
- The Logan collaboration is outstanding.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.5** for proposed future work.

- Future tasks for each partner institution are well-defined.
- Future plans to scale up fermentation are logical.
- The goal of testing biomass fermentation waste in the MFC/MEC device is logical.
- The future of this project must include molecular and genetic approaches, possibly as outside collaborations.
- A clear plan has been stated.

Strengths and weaknesses

Strengths
- The investigators' expertise in microbial fuel cells is excellent.
- The investigators have demonstrated superior progress towards defined goals.
- The investigators have demonstrated expertise in fermentation testing and quantification.
- The organism is a mainstay of any cellulosic based system and this research will be very valuable.
- Harnessing biological forces will prove themselves in the years to come as overhead costs increase.

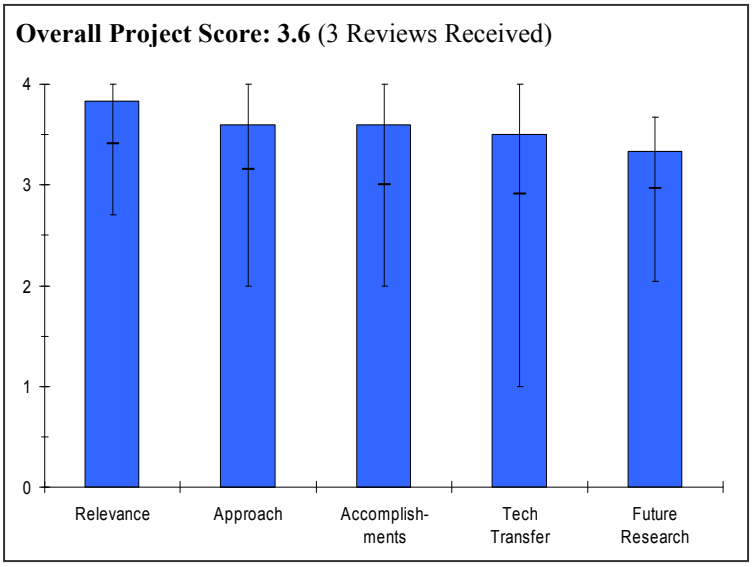
Weaknesses
- There is not a well-described, logical plan to test inhibitors in a systematic way to continue optimization of metabolic pathway flow; this is especially apparent in the plan to test combinations of inhibitors.
- The development of genetic methods for pathway engineering is not described, although the inclusion of the expert collaborator from the University of Manitoba adds necessary expertise.
- The workflow for testing of specific components to the MEC device is not clearly laid out.
- The techniques for metabolite determination have not been clearly described, and the investigators have no prior demonstrated expertise with this experimental component.
- Genetics and DNA arrays need to be applied.
- Need a full scale demonstration or early adopter soon.

Specific recommendations and additions or deletions to the work scope

Project # PDP-34: Theory of Oxides for Photoelectrochemical Hydrogen Production
John Turner; NREL

Brief Summary of Project

The objective of this project is to discover and characterize a semiconductor material set or device configuration that 1) splits water into hydrogen and oxygen spontaneously upon illumination; 2) has solar-to-hydrogen efficiency of at least 5% with a clear pathway to a 10% water splitting system; 3) exhibits the possibility of 10 years stability under solar conditions; and 4) can be adapted to volume-manufacturing techniques. The main objective for the past year has been to develop and optimize state-of-the-art materials that we have identified as promising for meeting the Department of Energy's near-term efficiency and durability targets and to develop PEC modeling and analysis efforts.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.8** for its relevance to DOE objectives.

- An important demonstration of how a clever mix of theory and experiment can be used to design new multi-element semiconductors that move toward the DOE goals for an effective solar water splitter.
- While the work presented here is a nice proof of concept with regard to the experimental approach, it has not, at this point, provided a next generation semiconductor that advances the DOE specs in the area of photoelectrochemistry.
- Finding new materials with improved properties is critical for photoelectrochemical water splitting. This project examines novel materials, not the same materials (e.g. TiO_2) that researchers have looked at for decades.
- Very important "background" project because such theoretical approaches will reduce costs and time for experimental work.
- Once such theories are better correlated to experiments., more such number-crunching pre-work will enable resource use in DOE.
- There is an increasing need to apply modern theoretical approaches to materials that are useful for photoelectrolysis of water.

Question 2: Approach to performing the research and development

This project was rated **3.6** on its approach.

- This project optimizes the beneficial interactions of quantum theory and laboratory experiment.
- A novel semiconductor material is predicted that would not normally be considered. Synthesis of the theoretically predicted system demonstrates that the theoretical predictions are solid.
- The work clearly demonstrates that the search for improved optical response semiconductors that are thermodynamically able to split water can be dramatically enhanced by using a DFT based materials search.
- The approach is demonstrated to provide an important new avenue to discovery materials that have not be experimentally accessible over the past 30 years of PEC research.
- The attempt to shed theoretical light on the materials discovered by Parkinson's combinatorial approach is especially interesting.

- Very solid and clear explanation by the poster presenter (actually, having the poster presenter is essential to the success of this poster - which actually merits an oral presentation!)
- DFT approaches coupled with combinatories (e.g., in the ternary oxides) led to very persuasive conclusions - kudos!
- Isovalent substitution in the Zn-O: N case - inspired.
- Uses state of the art computational methods to explain the behavior of existing materials and to provide guidance for new materials to test for photoelectrolysis activity.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.6** based on accomplishments.

- All technical components are in placed and demonstrated.
- A new alloy type semiconductor photoelectrode material has been theoretically identified and demonstrated to have the predicted properties.
- All project goals are being met in a timely manner.
- No real breakthroughs yet, but the project provided some valuable insight into several complex materials.
- Clearly excellent; but the proof of the pudding, correlation with experimental data, would be a crowning achievement.
- The examples show value of this theoretical predictive too!
- However, is there a tool to go beyond the "band engineering"? Is there a tool to hint at current magnitudes?
- Has been very production since many systems have been calculated and understood.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.5** for technology transfer and collaboration.

- The principal investigators have established useful collaborations with several experimental groups.
- Internal NREL collaborations (theoreticians and experimentalists) are evident; but were there external collaborations?
- Any reach-out to other photo-chemistry interests in other institutions? Purdue? CIT?
- Has worked well with experimentalists providing feedback on known materials and guidance on new materials.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.3** for proposed future work.

- Systems of potential interest have been identified.
- Calculational analyses are being initiated.
- All selected targets are interesting systems that should be pursued.
- This is a well-designed study that is correctly focused and effective.
- The PIs did propose some new systems to examine, but these choices appear to be ad-hoc.
- Good, logical, extensions to experimental projects.
- Not clear as to whether the theoretical structures are readily fabricable or economically manufactured.
- What about stability or meta-stability of the predicted structures?
- Will continue to investigate interesting systems and provide insight into other possible systems that may be the "holy grail" of photoelectrolysis.

Strengths and weaknesses

Strengths
- Researchers have an excellent track record.
- The present study is well constructed and fruitful.
- New, highly complex materials having optimized photoelectrochemical properties are being identified.

PRODUCTION AND DELIVERY

- Developing meaningful and ongoing dialog between theoretical and experimental approaches to discovering materials with improved properties.
- Excellent use of the DFT approximations in developing the ternary oxides and the differentiation between the super-lattice structures and the random alloys.
- Good correlations (albeit only a few) between theory and experiment.
- High quality theoretical work and very productive.

Weaknesses

- NONE.
- None really because this is pioneering work in developing a predictive tool for new studies.
- Not enough computation resources available.

Specific recommendations and additions or deletions to the work scope

- Continue as is.
- Key to this project is having collaborations with experimental groups that can test the theoretical predictions.
- Fund this work to do more band-engineering work!
- Fund the reduction to practice to quickly decide whether the current obtained from these novel studies could be "practical" for scale-up.
- Provide more computation resources.