

2010

Hydrogen Production and Delivery

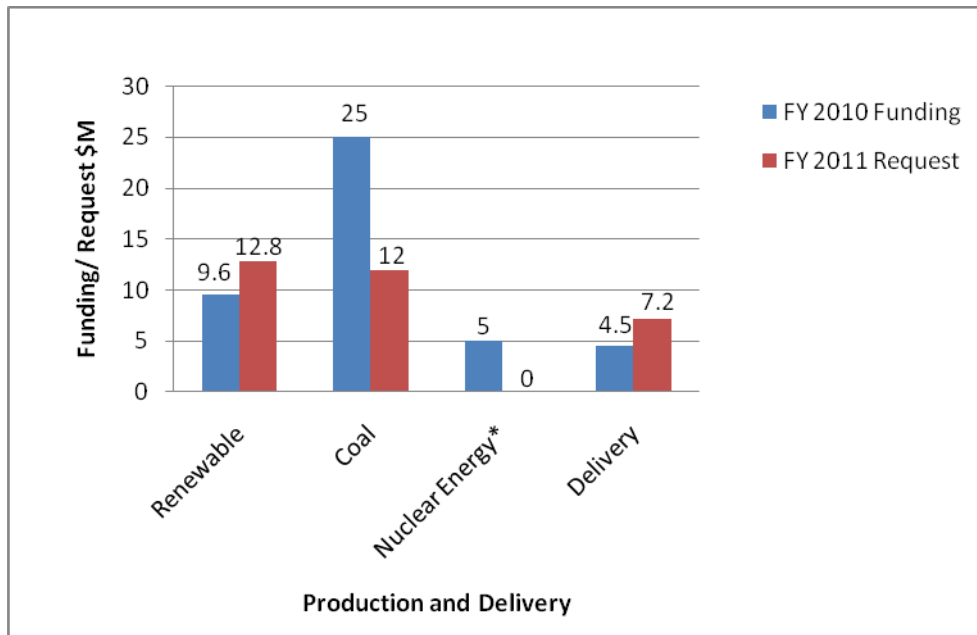
Summary of Annual Merit Review of the Hydrogen Production and Delivery Sub-program

Summary of Reviewer Comments on the Hydrogen Production and Delivery Sub-program:

This review session evaluated hydrogen production and delivery research from all DOE activities in the Fuel Cell Technologies Program (FCT) at EERE and in the Hydrogen and Clean Fuels Program at the Office of Fossil Energy (FE). The production and delivery projects were considered by reviewers to be well aligned with DOE goals and objectives.

The hydrogen production projects reviewed represent a diverse portfolio of technologies to produce hydrogen from renewable-based energy sources, as well as coal with sequestration. Production project sub-categories include water electrolysis, bio-derived renewable liquids reforming, biomass gasification, solar-driven thermochemical cycles, photoelectrochemical direct water splitting, biological hydrogen production, hydrogen production from coal, and separations technologies. The hydrogen delivery projects reviewed included work in key research and development areas such as pipeline embrittlement, new fiber reinforced polymer pipelines and linings, and compressors, in addition to analysis work focused on the next stage of development of the Hydrogen Delivery Scenario Analysis Model. Overall, the production and delivery projects were judged by reviewers to have made considerable progress in reducing both projected capital and operating costs and in improving material properties. Reviewer comments, concerns, and recommendations varied considerably by project and are summarized below.

Hydrogen Production and Delivery Funding by Technology



**The Nuclear Hydrogen initiative concluded at the end of FY 2009. Limited research and development on high temperature electrolysis as a potential end-user application may continue under the Next Generation Nuclear Plant Project.*

Majority of Reviewer Comments and Recommendations:

In general, the reviewer scores for the production and delivery projects were above-average to high, with scores of 3.6, 3.1, and 2.4 for the highest, average, and lowest scores, respectively. The scores are indicative of the technical progress that has been made over the past year. Reviewer feedback, recommendations, and major concerns for each project category are summarized below.

Electrolysis: In general, projects in this area scored favorably and were regarded as well aligned with current program goals and objectives. The projects focused on increasing stack efficiency and decreasing capital cost, along with independent testing and integration with renewable power sources. The reviewers felt that the path forward for PEM electrolysis systems is well laid out and progress is significant. However, it was noted that high pressure operation may not reduce system costs as system complexity is increased and safe gas mixture levels must be maintained. Furthermore, reviewers emphasized that continued independent testing is important to inform the technology area.

Bio-Derived Liquids Reforming: Projects in this topic area included a study focused on increasing mechanistic understanding of hydrogen production from bio-derived liquids, in addition to specific investigations exploring reforming of glycerol, bio-oils, and ethanol. The reviewers noted that much progress has been made in these areas, but stressed the need for further work, including the development of optimized catalysts, investigations into feedstock quality, and demonstration of long-term testing prior to full-scale commercialization. Strengthening collaborations with other researchers and potential end-users was also recommended.

Biomass Gasification: The gasification project reviewed in this topic area focused on developing an initial reactor using a biomass slurry hydrolysis and reforming process for hydrogen production. Reviewers were impressed by the conversions of synthetic and woody biomass feedstocks that have been demonstrated. According to reviewer recommendations, future funding in this area should depend on results of an economic evaluation. Next steps should include investigating effects of variations in feedstock composition and impurities on catalyst performance, use of non-wood flower feedstock, and scale-up to system pilot testing.

Solar-Driven High Temperature Thermochemical Production: The projects reviewed in this topic area were favorably rated for researchers' technical skills and abilities and for collaborative efforts, both domestically and internationally. Reviewers specifically cited strengths in project planning, a focus on key deliverables, and responsiveness to past reviewer suggestions. It was recommended that the primary focus going forward should be on solving critical path issues before scale-up is attempted. Future work should be concentrated on addressing cycle complexity, potentially high capital and maintenance costs, durability under long term cycling, and possible 24/7 operations.

Photoelectrochemical Hydrogen Production: All of the materials R&D projects in this topic area were viewed to be well-aligned with the Program's long-term goals, and reviewers noted that the strong collaborative teaming approach among the projects was effective and necessary for achieving the DOE targets. All projects were cited as having achieved good scientific progress in the range of materials systems under investigation. Reviewers specifically highlighted the new theoretical activities and nano-science approaches as important additions to the research portfolio. It was stressed that further work is needed in evaluating a broader class of material systems, in advancing technology readiness, and in demonstrating technology viability and scalability to large-scale systems.

Biological Hydrogen Production: The projects in this area encompass a portfolio of photobiological and fermentative production methods using various micro-algal, cyanobacterial, and lignocellulosic biomass resources. All projects were highly rated by reviewers. The general consensus was that the researchers are moving toward the DOE goals in this longer-term renewable hydrogen production area. The scientific methods used in the majority of the projects were seen as cutting edge and the collaborations were viewed as effective and productive. Reviewers recommended expanded collaborations, particularly with the DOE Office of Science, and emphasized the need for more feedstock analysis, clearer definition in pathways to technology readiness, and analysis of hydrogen production scalability.

Hydrogen from Coal: The main focus of the six projects evaluated in this topic area was on the development of hydrogen transport and separation membranes for coal-based systems. Reviewers noted progress in all areas and favorably evaluated the projects for their innovation and commitment to meeting DOE targets for flux, sensitivity, cost, and chemical and mechanical robustness. Enhanced collaborations with industrial partners were recommended. The need for further economic analyses was also stressed, particularly since materials cost may be significant in the membrane technologies being developed.

Separations: Projects in this topic area focused on the development and fabrication of several types of hydrogen separation membranes, and according to reviewers, good progress has been made. Projects were generally characterized as innovative, well-designed, and comprehensive in their execution. Reviewers strongly recommended, though, that project teams seek expanded collaborations with metals and materials experts, and with other industry partners that could assist with membrane optimization, economics analyses, and commercialization.

Hydrogen Delivery: Projects reviewed in this area continued to receive high marks from reviewers for the sound progress that has been made, especially in the areas of steel and fiber reinforced composite pipeline technologies. Reviewers complimented teams on their strong technical knowledge and commended the collaboration across industry, national labs, universities, and associations. Specific recommendations were made to better account for cost implications and pressure cycling effects. Reviewers also noted that more work is needed to define real-world, long-term problems that may arise.

Project # PD-02: Biomass-Derived Liquids Distributed (Aqueous Phase) Reforming

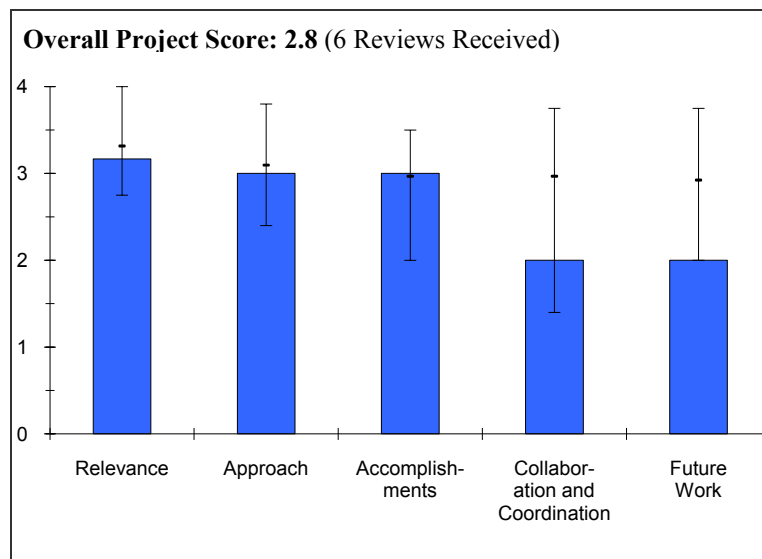
Yong Wang; Pacific Northwest National Laboratory

Brief Summary of Project

The objective of this project is to develop bio-derived liquids aqueous phase reforming (APR) technology for hydrogen production that can meet DOE efficiency and cost targets. Specific objectives are to 1) enhance catalyst performance by increasing catalyst activity and hydrogen selectivity; and 2) develop mechanistic understanding of reaction pathways and means to control product distributions consistent with application end-use.

Question 1: Relevance to overall DOE objectives

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



- The success of this project would support the DOE objectives for the Hydrogen Program by providing an alternate reforming process that utilizes the inherent moisture content of biomass feeds.
- The APR process to produce hydrogen from carbohydrates is a relatively new approach with potential for distributed reforming of biofuels to hydrogen.
- Hydrogen production from biomass-derived fuels is an important objective to DOE.
- This is a very challenging project due to the complex nature of biomass.
- This project has relevance to the DOE objectives. Low (or lower) temperature APR is an interesting pathway to potentially low-cost hydrogen. Catalyst optimization and understanding is critical.
- The idea seems relevant, but production of hydrogen in remote areas with adequate biomass resources presents a strong challenge in transporting hydrogen to areas of final use. The diffuse nature of biomass resources limits production scale, which compounds the transport problem.
- The project objective is to develop a cost-effective hydrogen production process via reforming of bio-derived liquids. If successful, this would meet the DOE goals for distributed hydrogen production from renewable sources. However, the choice of feedstock and catalyst are critical to achieving the objective.

Question 2: Approach to performing the research and development

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

- The research approach for this project is logical and well thought out. The approach addresses the technical barriers and, if successful, it will allow for quantitative comparisons of APR with conventional reforming.
- The APR process operates under comparatively mild conditions that are suitable for distributed biomass processing to hydrogen. The research focuses on the major issues associated with the current APR process, which are insufficient throughput and hydrogen selectivity. The project does focus on the critical barrier in the field.
- The approach is to get a detailed study of platinum-rhenium compared to platinum alone. There is utilization of advanced characterization to understand the role of rhenium. The approach seems successful; however, the addition of a base is necessary to suppress the negative effect of rhenium on the acidity of the catalyst.
- The distribution of products has been greatly improved; however, it is at the expense of a very high residence time.

- Overall, the characterization work is good. The physical characterization work is strong, but chemical characterization (e.g., temperature-programmed reduction (TPR), chemisorption, temperature-programmed desorption (TPD),) is not as strong.
- The balance between characterization and catalyst screening is heavily weighted toward characterization.
- The addition of sorbitol is important for showing process viability.
- The catalyst platform chosen involves noble metal catalysts. For cost-effective large-scale deployment of such a technology, the aim should be to discover and develop cheaper non-noble metal catalysts.
- Much of the work is focused on glycerol and does not address other more relevant feedstocks such as sugars and cellulosic biomass.
- It does not appear that similar work from the University of Wisconsin; Virent Energy and others have been sufficiently leveraged to build on and to advance the APR technology.
- Based on the findings, the work has been appropriately redirected to developing a solid oxide fuel cell (SOFC) application rather than hydrogen production.

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

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

- Substantial progress has been made; however, since this project is nearing completion it appears that there is still much to be accomplished. Perhaps the remaining process and catalyst issues will be completed in a timely manner, but there is some concern that more time will be needed. The economic analyses to date do appear promising, despite the optimistic assumptions.
- The rhenium-incorporated platinum/carbon catalysts developed in this project showed much enhanced catalytic activity compared to the common platinum catalyst, but decreased hydrogen selectivity. The basic findings on the catalytic reaction mechanism in this project may help the further development of high-efficiency APR catalysts for conversion of glycerol and sorbitol and thus contribute to DOE's goal of utilizing renewable biofuels for energy generation. It is a nice piece of scientific work.
- There is great improvement in fundamental mechanistic understanding of reaction pathways and control of products distribution.
- Network analysis is a good start, but investigators should carry out more complete kinetic analysis of the network for reaction rates if they want a "mechanistic understanding of reaction pathways and means to control product distributions consistent with application end-use."
- Good progress has been made toward understanding catalytic reaction mechanisms. However, some similar results have been previously reported.
- The discovery of KOH (potassium hydroxide) addition and its effect on conversion and selectivity is useful and should help overcome some barriers within the framework.
- The results reported are more of academic and scientific nature and do not sufficiently address the stated objective of developing a reforming process for hydrogen production.
- The results clearly suggest that this approach is more suitable for producing synthesis gas for applications such as SOFC rather than for hydrogen production.
- Given the above, the cost of synthesis gas produced needs to be compared with natural gas or other alternatives as fuel.

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

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

- Since this project is nearing completion, additional collaborations with a possible end user are lacking.
- Collaboration only on material characterization by high resolution transmission electron microscopy with Oak Ridge National Laboratory (ORNL). Collaborations (or even consultation) with industry would be very helpful for reliable technical and economical evaluations.
- Thanks to collaboration with Pacific Northwest National Laboratory, Brookhaven National Laboratory, and ORNL, a good understanding of the mechanism could be done.
- The reviewer did not observe any outside collaboration.

HYDROGEN PRODUCTION AND DELIVERY

- The team should partner with a commercial catalyst provider or other entities with experience in practical catalysis.
- Last year, Virent Energy was listed as a collaborator. This year the only collaborator listed is ORNL for some analytical work. It is unclear why the collaboration, and especially the commercialization strategy, is without an industrial partner.
- If the work is redirected as a technology to produce renewable fuel for SOFCs, a corresponding partner in that space would be appropriate for a working relationship.

Question 5: Approach to and relevance of proposed future research

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

- It is unclear what future work will be done.
- Perhaps more attention should be paid to the improvement of hydrogen selectivity. The APR reaction mechanism is very complicated and is affected by many factors which are not fully investigated to an extent allowable by the project scale.
- There was no clear proposed future work.
- The project is 80% complete and the last milestone is to demonstrate full conversion of glucose and sorbitol. However, it is not clear how this is going to be achieved.
- Future plans are not stated, so the approach to and relevance of proposed future research cannot be judged. Answers to reviewers' comments from last year are also missing.

Strengths and weaknesses

Strengths

- A good job has been done on defining the process and developing/characterizing the catalysts to be used.
- The APR process operates under friendlier conditions as compared to the traditional high-temperature reforming technology and thus has the potential for distributed biomass processing to hydrogen. The team presented a nice piece of scientific work. The platinum-rhenium/carbon catalysts developed in this project demonstrated significantly enhanced catalytic activity. The findings on the catalytic mechanism and the role of platinum-rhenium alloying may provide valuable knowledge for the further development of high-efficiency APR catalysts for glycerol and sorbitol.
- This is a low temperature process.
- This method allows for the process of biomass without vaporization of feedstock.
- This method uses waste biomass.
- The project demonstrated an extensive characterization of catalysts.
- The team has a good understanding of the mechanisms and how to control product distribution.
- Collaboration exists with other laboratories and universities for characterization.
- A potential linkage to SOFCs exists.
- Various feedstocks are used.
- The project exhibited a strong physical characterization effort.
- The main strengths occur in the development of catalysts, understanding of catalytic reaction mechanisms, and development of approaches to overcome conversion and selectivity barriers.
- The project demonstrated a detailed analysis and characterization to elucidate reaction pathways.

Weaknesses

- More work needs to be done on the potential feedstocks. For example, will feedstocks for this process compete with food crops? Alternate feedstocks need to be explored, and it would be beneficial if some testing of real feedstocks was conducted.
- Hydrogen selectivity may be more important than reaction rate and conversion rate. This is especially true for distributed production where intensive separation and transportation of gas products are likely to be economically disadvantageous. The very low hydrogen selectivity of the Pt-Re-C catalyst may discourage the practical considerations. Also, targeting application for the SOFC system does not seem to be a good strategy

for the intended distributed biomass utilization as SOFCs are considered suitable for centralized power production where bottoming technology could be used to enhance the overall energy efficiency.

- The use of precious metals at high loadings is a concern.
- A high residence time is needed in this process.
- No long-term stability is shown.
- The biggest weakness of the project is a lack of defined metrics for success. A simple listing of the parameters that the researchers think they need to achieve regarding criteria such as selectivity and yield would be beneficial.
- A very small number of catalysts were tested. This project looks like catalysis by chemists with little chemical engineering input. The project needs a stronger emphasis on chemical engineering for kinetic analysis of reaction networks to optimize the network.
- This presentation does not address practical commercial issues. For example, there is no consideration of reactor design or heat transfer. Also, under the optimum conditions for desired conversion and selectivity, the space velocity is too low to be practical.
- Not enough detail is provided on economic analysis to judge the validity of assumptions and to assess practical applicability of the findings from this study in a commercial system.

Specific recommendations and additions or deletions to the work scope

- The Project Weaknesses” section above contains many recommendations.
- Selectivity improvement should possibly be prioritized to a higher level.
- Researchers should seek collaborations with potential users of this technology.
- The work needs to address long-term studies (i.e., long-term testing of the catalysts). Also, other basic supports should be considered to decrease the acid character of oxidized rhenium. The project needs to address the role of inorganics present in biomass. If possible, either platinum should be replaced by a cheaper transition metal or the loading should be lowered.
- More work should be done on catalyst synthesis. Researchers need to screen additional catalyst variables including support, total platinum concentration, impregnation method, and reduction temperature and rate.
- A better kinetic analysis is needed.
- Based on the findings as stated, the project seems to have been redirected to develop a process to produce a renewable fuel for SOFCs. The cost and other parameters should then be compared accordingly to see if this is a viable and cost competitive process. The original objective of hydrogen production is clearly not met in the current form.

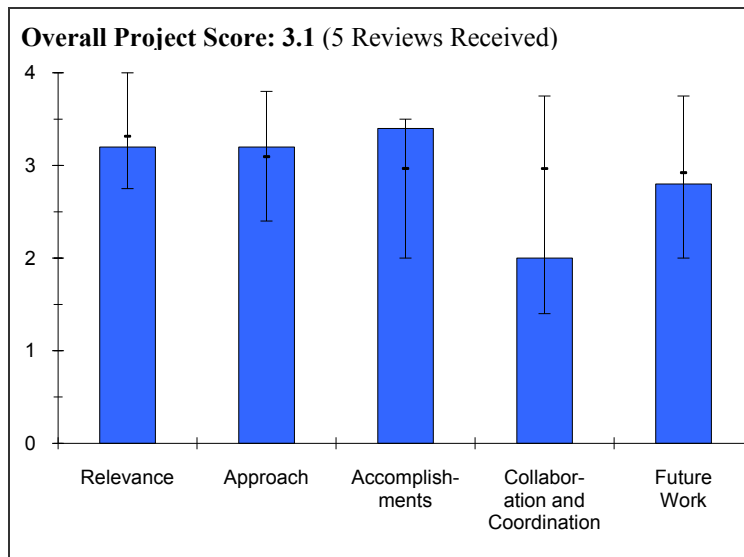
Project # PD-03: Hydrogen from Glycerol: A Feasibility Study

Shabbir Ahmed; Argonne National Laboratory

Brief Summary of Project

The objective of this project is to evaluate the economic feasibility of producing hydrogen from glycerol derived as a byproduct of the biodiesel industry: 1) for the distributed production of hydrogen and 2) based on the steam reforming of glycerol, followed by purification using pressure swing adsorption. This project will review the availability and price of glycerol, evaluate the hydrogen-from-glycerol process at a distributed hydrogen production facility using systems analysis, and estimate the cost of hydrogen and its sensitivities.

Question 1: Relevance to overall DOE objectives



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

- The success of this project would support DOE objectives for the Hydrogen Program by providing an alternative reforming process that utilizes the possibly abundant volumes of glycerol from biodiesel production.
- A realistic and reliable economic evaluation of hydrogen production from biomass (and from any stocks in general) is critically important to guiding R&D efforts for the DOE Hydrogen Program.
- It is important to have independent analysis of the economic feasibility of various processes. Economic analyses performed by individual teams are difficult to compare. Studies such as this will allow a bias-free comparison of different approaches on the same basis.
- Glycerol is a scarce resource. The presenter did a great job in quantifying the resource and he estimated 43 stations that could operate on glycerol throughout the United States. As the volume of production required for low cost is approximately 500 units (according to better assumptions from the Hydrogen Analysis project (H2A) sponsored by DOE), this system would be designed at a significant volume of production disadvantage. There is still potential for it if it leverages ethanol reforming technologies. Glycerol as a feedstock for reforming may be better suited to a fuel-flexible reformer. Typically the fuel feed and treatment system is the biggest difference from one steam methane reformer (SMR) feedstock to another. Thus, the researcher could focus on this type of system aspects.
- This project assumes that the highest value for waste glycerol is to produce hydrogen, which is a false premise. Once the one dollar credit for biodiesel expired, the current transesterification process to make biodiesel from various oils became uneconomical, a number of manufacturing plants closed, and the total amount of biodiesel and glycerol dropped. Currently, the highest value for glycerol, based on life-cycle analysis, is to produce ethylene or propylene glycol, not hydrogen. Since this is more of a niche market, the assumptions appear to be too optimistic. The capital cost and price of crude glycerol are too low and the efficiency of the combined process is too high.

Question 2: Approach to performing the research and development

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

- The research to date has been well planned and focused on the feasibility of using glycerol as a hydrogen source.

- Since the cost of hydrogen is sensitive to the price of glycerol, it is important to look at the impact of the hydrogen product (if hydrogen production from glycerol really happens) on the price of glycerol (based on an appropriate hydrogen production scale).
- The project is in its initial stages. The team has chosen to follow the H2A model pretty closely. While this is appropriate for the beginning stages, they may want to consider other options.
- The analysis determines the range of costs to achieve the production targets for hydrogen; however, the PI did not provide any evaluation on pathways to achieve the potential reductions and meet the program goal. This was more of a survey project and has not provided an approach to overcome the barriers.

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

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

- The results were presented clearly and excellent progress has been made. The conclusions are supported by the research and the numbers appear to be reasonable. It is clear that if the price of glycerol continues to fall, this process becomes economically viable. It would be interesting to include a water-gas shift membrane reactor into the economic evaluation to see if there is a benefit.
- Progress has been very good on this project.
- The process economic analysis was good, but the assumption of \$1 million for a system is inconsistent with volume of production (43 systems in total). At a replacement life of 20 years, this equates to two systems produced per year, not 500 plants per year as in the Nth plant case}. Additionally, the feedstock cost used was for crude glycerol, which did not consider the cost of cleanup.
- Based on the level of funding, good progress was made to assess if the feedstock could produce hydrogen within the goal of the program. However, there were too many assumptions that cannot be validated to use this analysis as an indicator of what could be achieved.

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

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

- This category is not applicable due to the limited scope of the project.
- There is limited collaboration. It would be helpful to collaborate with teams that are working on experimental aspects of the process.
- It would be beneficial to see if this feedstock could be fed into other existing SMR system concepts. Collaboration in the reforming area could facilitate this investigation.
- The PI should have contacted Archer Daniels Midland Company or the National Biodiesel Board to get more facts on glycerol and its value in the products market. DOE has supported a number of analyses and scoping R&D efforts to help the PI provide a more thorough analysis.

Question 5: Approach to and relevance of proposed future research

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

- It is unclear if this project will continue or not. The rough outline of future work was somewhat general.
- Proposed future work is appropriate. The team should consider looking at the aspects of the process that can be improved by ongoing research in other DOE-funded programs and incorporating data and results from those studies into their analysis.
- The work should focus more on the economics, availability, and market barriers than on the reforming challenges.

Strengths and weaknesses

Strengths

- This is a well-defined project with logical conclusions.

HYDROGEN PRODUCTION AND DELIVERY

- Although the project is at a very initial stage, the results show good potential in the economical use of glycerol as a renewable stock for hydrogen production.
- The analysis is based on sound assumptions.
- For a new project with a PI that does not have a great understanding of glycerol, the project was well documented. The approach used some sensible values for categories such as efficiencies and feedstock cost, even though the capacity values were not realistic.

Weaknesses

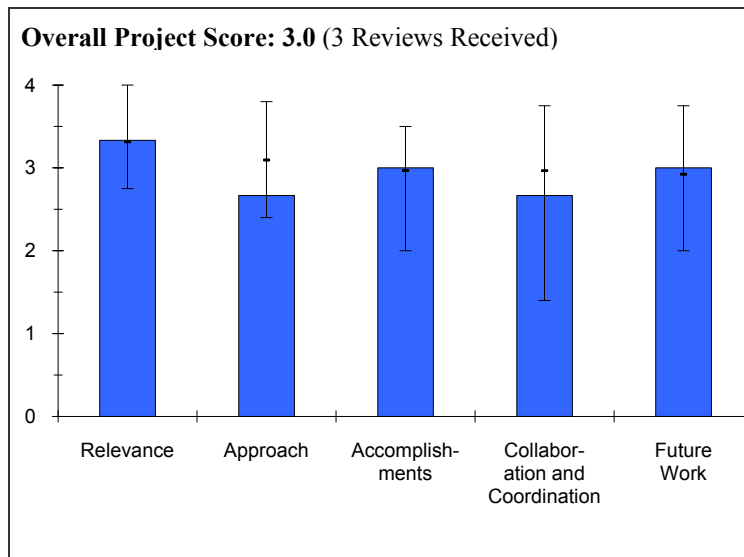
- The project had no significant weaknesses.
- Partners need to be identified to provide realistic operation parameters, system design, and reforming performance data, e.g., kinetics, conversion, and catalyst cost. More efficient, emerging reaction (e.g., aqueous phase reformation, high-temperature reforming, and membrane reaction) and separation (e.g. membrane) activities need to be included as a case study that may provide useful information for the ongoing and future R&D efforts.
- The project should perform sensitivity analyses of the factors that contribute to the cost.
- The PI did not appear to have much understanding of the biodiesel and glycerol market issues.

Specific recommendations and additions or deletions to the work scope

- If this project continues, it would be interesting to include a water-gas shift membrane reactor into the economic evaluation to see if there is a benefit.
- It would be very helpful to the R&D community if the PI could include some important developing or emerging technologies (e.g., membrane reactors, and membrane separations) in the assumed production flow chart to see their economic validity.
- Uncertainty about future funding makes it difficult for the team to plan their future approaches.
- It would be good to see how glycerol could be used as a fuel additive for other processes. The quantity available does not seem to justify development unless other pathways are identified for glycerol production (e.g., biological or bacterial)

Project # PD-04: Distributed Bio-Oil Reforming*Stefan Czernik; National Renewable Energy Laboratory***Brief Summary of Project**

The overall objectives of this project are to 1) 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 and 2) demonstrate the technical feasibility of the process. The objectives for fiscal year (FY) 2010 are to 1) demonstrate catalytic partial oxidation/steam reforming of bio-oil to syngas at bench scale, 2) demonstrate long-term catalyst performance, 3) provide mass balance data for the H2A project, and 4) make a “go/no-go” decision.

**Question 1: Relevance to overall DOE objectives**

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

- Developing an advanced reforming approach to produce hydrogen from "bio-oil" derived from pyrolysis of biomass supports the Hydrogen Program goals. Such an approach, if successful, could have an important impact on renewable, distributed hydrogen production.
- The project is well-aligned with the DOE RD&D objectives.
- It is not clear that hydrogen production is the best use of pyrolysis oil.
- Stability issues may make transportation difficult.
- Environmental and toxicity issues associated with pyrolysis oil at a forecourt location, as described in this work, are significant enough to preclude its use in forecourts.

Question 2: Approach to performing the research and development

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

- A two-step oxidative cracking/catalytic steam reforming process for producing hydrogen from hydrocarbon oils is a sound technology approach.
- The reviewer is unclear on whether the use of precious metal catalysts is a concern and if an investigation of alternatives is planned. The formation of carbon species (lightweight, solid particles) is a concern. The team should look into this and try to get a better understanding of the reaction network and product distribution.
- The approach appears to be essentially Edisonian with little or no guidance from theory or fundamentals. Hence, many more catalysts should have been tested or process variables should have been explored much more extensively.
- No catalyst characterization was included.

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

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

- The project has met many of the reported milestones and has made good progress despite having lost all funding for FY 09.

HYDROGEN PRODUCTION AND DELIVERY

- The team is tackling a challenging process quite well. So far, the progress has been substantial.
- Progress in the last year seems minimal. The main accomplishment seems to have been a 2-1/2 day run, a couple of new catalysts, and minor temperature variation. This is not a lot of progress for \$500,000.

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

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

- The project requires collaboration with multiple entities. Two universities are providing expertise in cracking and catalyst development. A collaboration with an oil company is providing help with feedstock effects.
- The collaboration with the partners may be better defined. For example, what is the role of the University of Minnesota versus BASF Corporation?
- Cooperation seems limited to obtaining three catalysts from outside sources, including one a commercial catalyst.
- Chevron and Colorado School of Mines collaborations were not discussed in any detail and no impact on the work was mentioned.

Question 5: Approach to and relevance of proposed future research

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

- It is a good idea to focus on testing of catalyst life and obtaining mass balance data for use in analysis before proceeding forward with a prototype. A detailed well-to-wheels systems analysis will be required since the technology requires a number of steps.
- It may be overly ambitious to go to a prototype system in 2011. The team has several more questions that need to be addressed at the bench scale.
- The team needs to look for a cheaper catalyst. Just because nickel did not work once does not mean it cannot work. A United Technologies Research Center program had a similar result, but they modified their nickel catalyst to make it work. This type of catalyst modification is simple, allowing catalysts to be easily modified one day and screened the next.
- Long-range testing is a good direction. The PI should calculate the effect of run life on process costs in determining "how long is long" and carry out tests for a relevant length of time.

Strengths and weaknesses

Strengths

- The project used excellent facilities, R&D infrastructure, and a qualified staff to conduct the project to completion.
- The team chose a good research area. Bio-oil from biomass pyrolysis could become an important and prolific energy source.
- The progress on bench scale process is impressive.
- The system is giving reasonable conversions.

Weaknesses

- The use of methanol as a diluent is a weakness. On a large-scale use model, methanol supply and distribution becomes a problem.
- The team should not move to a scale-up stage too fast. The project's future plans may not be realistic.
- There has been a lack of accomplishment. The project has no apparent efforts on catalyst fundamentals, though for the amount of money invested between 10 and 100 catalysts should have been tested instead of only three.

Specific recommendations and additions or deletions to the work scope

- The project should continue to be funded.

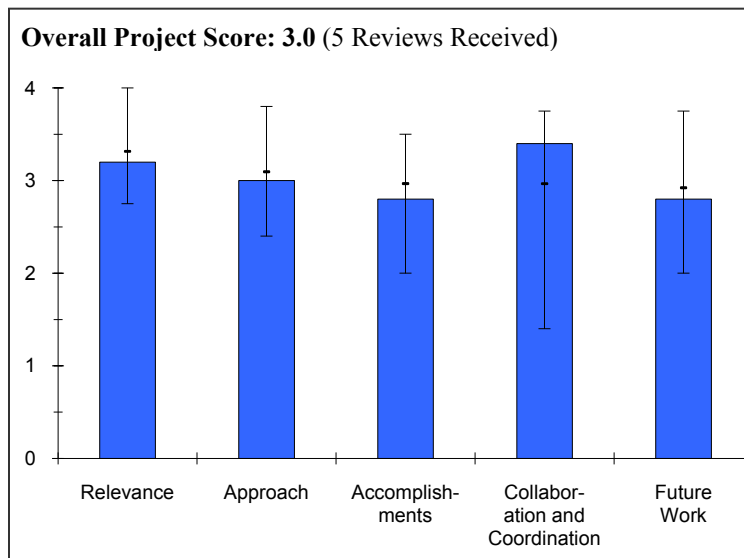
- This project needs to systematically study bio-oils of different qualities and types derived from different feedstocks. A task should be added to investigate alternative means for bio-oil stabilization other than alcohols. For example, hydro pyrolysis front-end processing could be used instead of solvent addition.
- Long-term testing is necessary. Two days is not enough to see poisoning effects.
- The project should include a detailed feed analysis for various feedstocks with attention to contaminants (e.g., sulfur, nitrogen, chlorine, metals). This analysis should identify which feedstocks would pose problems for catalyst poisoning, corrosion, etc.
- The project should detail the costs throughout the value chain and identify the most promising candidates to cut total cost.

Project # PD-05: High-Performance, Durable, Palladium Alloy Membrane for Hydrogen Separation and Purification

Ashok Damle; Pall Corp.

Brief Summary of Project

The overall objective of this project is to develop, demonstrate and perform an economic analysis of a palladium alloy membrane that enables the production of 99.99% pure hydrogen from reformed ethanol at a cost of less than \$3/gallon gasoline equivalent. The objectives for the past year were to 1) continue optimization and characterization of the membrane formation process, 2) conduct extensive testing of palladium alloy membranes in pure gas streams and in syngas/water-gas shift (WGS) reaction environments for parametric evaluation of their performance, 3) demonstrate membrane performance milestones for Phase III “go/no-go” decision, and 4) complete the techno-economic modeling in collaboration with Directed Technologies, Inc. to determine the influence membrane parameters have on the cost of hydrogen production.



Question 1: Relevance to overall DOE objectives

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

- This project is critical to the success of the Hydrogen Program. The development of robust, inexpensive membranes is necessary to meet DOE’s RD&D objectives.
- Production of pure hydrogen is critical for the use of fuel cells.
- Membrane separation is only one approach to purifying hydrogen for fuel cell applications.
- Relevance is fair. There are purity and pressure issues when membranes are used for separation. In most cases membranes do not ensure 99.99% pure hydrogen over lifetime and membranes reduce the pressure of hydrogen product gas.
- DOE seems focused on membranes as the leading separations approach,
- Palladium membrane implementation is under investigation by others and is especially useful for operation in WGS environments. Palladium-gold alloy membranes show improved performance and durability within cost targets.
- Improving the cost effectiveness of ethanol reforming for hydrogen production is in line with DOE goals. It would be helpful to emphasize module reactor development in addition to membrane development while keeping commercial targets in mind.

Question 2: Approach to performing the research and development

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

- The team’s approach for this project is excellent. The approach addresses the technical barriers and, if successful, will result in a significant progress in membrane technology.
- Approach for development, testing and cost analyses are well defined. Work on membrane characterization after impurity testing is needed to better understand how to improve membrane tolerance.
- Investigating the full performance spectrum, including flux, durability, and cost, is a good approach.
- Looking at the impact of impurities is a critical task.

- Consider porous metal substrate as a membrane support.
- Including integrated membrane reactors for system intensification, is critically important to reducing cost.
- Membrane design and fabrication is well-conceived, but the performance testing is not well defined. There seems to be significant variation in the performance level requirements for various tests. Sensitivity of hydrogen recovery or hydrogen purity to pressure differentials and flux rates is not documented. Testing to demonstrate performance targets should also be performed at other target levels. Alternatively, target parameter sensitivity to other performance parameters should be documented.
- Suggest developing a protocol for performance testing.
- The approach is well thought out and is focused on the key barriers, with the exception of addressing the manufacturing cost barrier.

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

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

- Great progress in membrane development and economic analysis. Thinly coated membrane material on a porous substrate is a solid approach. Polarization research and the economic analysis comparing the flux, cost, and percentage of hydrogen recovery is very important.
- Progress has been made evaluating reaction environments, and determining the effect of carbon monoxide, hydrogen sulfide, and steam content in the feed gas on the hydrogen flux. Techno-economic modeling and determining maximum operating conditions was completed.
- 500 hours of stability testing is not sufficient to determine the life of a membrane with a 5,000 hour lifespan.
- Need more information on actual durability results because it appears that the flux is degrading with time. Why do stability test show that hydrogen purity is 99.8% after 500 hours?
- Technical progress seems limited and improvements marginal since the last review.
- Actual cost analysis information is needed including a comparison with pressure swing adsorption (PSA)., PSA, including the pressure loss effect, is the current industry workhorse.
- Results appear unclear at this time. Results seem to be a combination from several different membrane types and test conditions. The PI needs to look at one membrane test setup and one set of test conditions.
- The cost analysis focuses on hydrogen recovery performance in the range of 70%- 90%. The target recovery is greater than 80% in FY 10 and greater than 90% in FY 15. Documented performance in long term tests is only about 67% recovery and one test showed recovery of 82%. The performance table dated FY 09 (but presented as "Accomplishments" for FY 10) showed recovery greater than 60%. There was no clearly documented test at target levels showing recovery levels in accord with the FY 10 target. This deficiency could be a fault of the presentation or it could be because no appropriate testing was done. Nevertheless, the choice of hydrogen recovery as the cost sensitivity parameter demands that hydrogen recovery performance be adequately documented.
- The lack of a well-defined protocol for performance testing inhibits understanding of progress toward resolving issues and overcoming barriers.
- Progress has been slow. Much of the FY 10 presentation was presented in the previous AMR presentation. Significant progress has been made however, the results appear mixed. While durability and resistance to impurity improvements are demonstrated, the flux and hydrogen recovery values are inconsistent. It is not clear what the optimum operating mode (e.g., integrated WGS), operating conditions (e.g., temperature and pressure), and performance should be.
- Results for flux and hydrogen recovery values are confusing and attributed to different experimental conditions. It is unclear if there is a specific value or range under typical operating conditions (e.g., slides 10 and 11). Slide 10 indicates 78% hydrogen recovery is notable but no temperature conditions are noted. Compared to hydrogen recovery rates using PSA, 78% is not impressive.. On slide 11, #4 uses 90% recovery at a lower flux. The recovery and flux values reported on slides 13 and 14 need clarification.
- No details were provided on how the cost estimating was done. Information should be provided on the mode, operating conditions, flux, and recovery values that were used in the techno-economic analysis to arrive at the \$2.99/kg of hydrogen mentioned in slide 11, #7. A comparison between this separation process and PSA as a base case needs to be done.
- The statement on slide 8 that any improvement in the separation has minimal effect on the overall cost of hydrogen is a concern. It suggests that efforts on this approach are not worthwhile. The statement, "Greater

HYDROGEN PRODUCTION AND DELIVERY

membrane recovery however significantly reduces the cost of hydrogen," needs to be quantified and compared to demonstrated value.

- The results of the techno-economic analysis show that ethanol conversion efficiency is critical. More information is needed to show how the membrane separator influences the conversion efficiency.

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

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

- The collaborations with the Colorado School of Mines, ORNL, and others are excellent. The addition of a potential end user is critical.
- The project had very close collaboration to address the different aspects of the development of a commercial membrane. From membrane fabrication to cost analysis, all of the issues are being investigated.
- This project includes a good list of collaborators with right skill sets.
- The project would benefit from collaboration with a PSA manufacturer or industrial gas company as the end-user.
- The work performed by partners was not specifically identified in the presentation. However, material characterization by ORNL was referenced in the oral presentation. Materials science work at Colorado School of Mines was not identified. Additional detail on collaboration will help promote access by other program efforts to specific and unique skills and facilities.
- Collaboration efforts seem appropriate and well-coordinated. The presenter stated that an end user has been identified. End-user participation is critical in developing a meaningful product.

Question 5: Approach to and relevance of proposed future research

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

- The proposed future work is detailed and well thought out.
- Future work is very well defined. The project is only 65% completed and is already in the stage of scaling up and collaborating with end users.
- The cost of hydrogen seems to depend on developing a good strategy for increasing hydrogen recovery
- A lot of work remains to determine commercial viability of this approach.
- More emphasis is needed to ensure consistent experimental design for example, the targets should include the costs measured for 5,000 hours an end-of-life target purity of 99.99% , as well as the additional cost associated with loss in membrane pressure.
- Testing protocols need better definition to assure that material components will meet target performance levels and do not remain a barrier to implementing scale-up design and fabrication. The plan to scale-up to fabrication plan is good assuming appropriate membrane material characteristics have been defined..
- Techno-economic analysis results indicate Phase III work, as described, might not be justified Unless there is clear value demonstrated for the efforts, it would not make sense to proceed to the next phase.
- Without results incorporating the membranes in the reactor (i.e., WGS) or the reformer, this approach does not appear to offer sufficient economic benefit. The plans, as described, do not seem to include any actual testing of a membrane reactor.

Strengths and weaknesses

Strengths

- To date, the researchers have done an excellent economic analysis detailing the strong influence that percent hydrogen recovery has on the cost of hydrogen compared to other factors such as membrane cost and permeance (flux). In addition, the recognition of and the subsequent addressing of the potential boundary layer/polarization effects will be valuable information for membrane development.
- Long-term evaluation of the hydrogen flux in the presence of WGS products has been accomplished.
- A determination on the effect of impurities (hydrogen sulfide, carbon monoxide, water) completed.
- A determination of the cost has been accomplished.
- The membrane is being designed for high pressure changes and high levels of impurities

- This project is comprised of a good technical team with lots of good ideas.
- Good overall progress was made on membrane separations as a generic approach.
- The palladium-gold alloy membrane appears to be effective for separation and purification of hydrogen, especially in WGS environments.
- Membrane development, fabrication and manufacturing capabilities are clear strengths of the project team. Collaboration with appropriate entities has added value.

Weaknesses

- More extensive testing of membranes needs to be conducted in the presence of contaminants, especially hydrogen sulfide.
- A comparison with commercial membranes is needed.
- The team must understand the mechanism of deactivation due to carbon monoxide and hydrogen sulfide. Conduct postmortem analyses of the membrane and determine if there are any issues with embrittlement.
- A focus on hydrogen recovery is needed.
- An end user has yet to be added
- The team needs to establish the right basis for comparison. For this application it is a PSA system.
- Hydrogen sulfide should be taken care of before it reaches the reformer and WGS reactor since catalysts will likely be deactivated.
- The team needs to get the user industry perspective (e.g., industrial gas companies [and fuel providers) on their criteria for deployment.
- Systematic planning and testing has no logical framework that assures efficient progress toward the project goal. No decision points were identified. To be relevant the test conditions need to be more focused on realistic operating conditions. There should be a systematic effort to optimize operating conditions to leverage the advantages of this membrane
- The economic analysis indicates that using ethanol reforming to reduce hydrogen production costs is questionable

Specific recommendations and additions or deletions to the work scope

- None
- Hydrogen purity analysis should be done to ensure the product meets the impurity concentrations standards listed in SAE J2719 & ISO 14687-2.
- This separation approach and PSA need to be compared for pressure loss and economics.
- Essential individual performance targets for each critical path need to be identified and demonstrated. The team should also establish and document a test protocol that assures that simultaneous target performance levels have been achieved.
- There has been a significant body of work to date on palladium alloy membranes for hydrogen separation and the benefits and limitations are well known. It is clear that unless these membranes are incorporated in the reactor to eliminate the number of unit operations, there would be no cost benefit. The project scope should therefore include this type of testing.
- The team should clearly define “go/no-go” decision points. At present, the results reported suggest that the approach will not be able to meet the stated goal of significantly reducing ethanol reforming cost. In the absence of that promise, the project needs to be reexamined.

Project # PD-06: A Novel Slurry Based Biomass Reforming Process

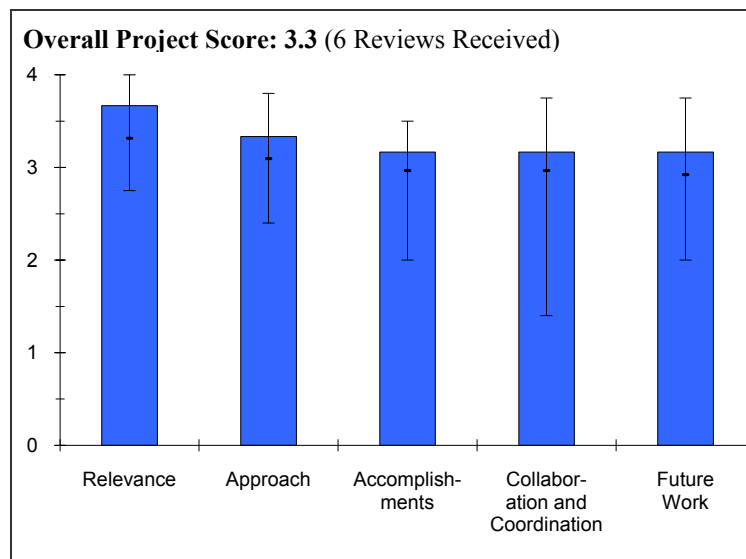
Thomas Vanderspurt; United Technologies' Research Center

Brief Summary of Project

The objectives of this project are the 1) development of an initial reactor and system design, with cost projections, for a biomass slurry hydrolysis and reforming process for hydrogen production; 2) development of cost-effective catalysts for liquid phase reforming of biomass hydrolysis-derived oxygenates; and 3) proof-of-concept demonstration of a micro-scale pilot system based on liquid phase reforming of biomass hydrolysis-derived oxygenates.

Question 1: Relevance to overall DOE objectives

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



- Hydrogen production from biomass, or other renewables, is critical to the Hydrogen Program.
- Reducing the hydrogen production cost is critical to the long-term viability of these technologies.
- Hydrogen production from renewable sources such as biomass is a key component of the DOE Fuel Cell Technologies Program.
- This project addresses renewable hydrogen production with potential application to distributed production of high-purity "fuel-cell"-grade hydrogen. The requirements of a very high pressure reactor with corrosion-resilient steels, need for caustic recycle, build-up of contaminants and solids in the process, and uncertainty of contaminants in downstream palladium separator may be barriers that are difficult to overcome. This may prevent commercial implementation.
- This project clearly supports the DOE Hydrogen Program goal of producing low-cost hydrogen from renewable feedstocks. The project needs to consider focusing on renewable feedstocks that are available in the United States and are sustainable at large scales.
- This process was very well communicated this year and it shows very good progress by the team.
- This project is relevant if hydrogen is to be produced from renewables. An extremely large range of capital and production costs exist due to membrane, catalyst, and high reactor cost. A more detailed analysis should be done to improve the accuracy of the cost estimates.
- Although the reactor design has safety factors that exceed the expected operating temperature and pressure, there is still concern of metal fatigue over extended operation. Accelerated coupon testing should be done to prove there would not be a safety issue.
- Although the Raney catalyst technology is well developed, a concern of loss in performance after repeated cycles of pressure and temperature exists. This should be validated in any follow-up work before scaling up.

Question 2: Approach to performing the research and development

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

- The biomass slurry-to-hydrogen concept seems to be a working technical approach. The costs for the palladium membrane currently seem excessive, however, due to the conditions where the liquid phase reforming take place and the high degree of technical integration required. Due to the cost, the secondary approach for gasification has to be examined.
- The base hydrolysis has been shown to work, but the complexities and high cost associated with this approach are present.

- The project was originally proposed to use acid catalyzed, but now uses base facilitated reforming. The use of a base is established in the literature for processing biomass. The key challenges will be recovering the catalyst and the unreacted base. The project investigator mentions these issues in the future work section, but they are not to be covered until the last year of the project. Base recovery should have begun earlier.
- The team is using an expensive metal membrane for hydrogen recovery and metal membranes are known for failure. They should have provided analysis to indicate that the metal membrane would be less expensive than traditional pressure swing adsorption (PSA) for hydrogen recovery. The team's approach does not include examining the performance of the metal membrane with the very aggressive base (potassium hydroxide [KOH]) and with the expected products from the wood processing. Ethanol is a much cleaner and easier-to-use material.
- Autoclaving cellulosic biomass in caustic media at high pressure is not a new concept. Antal et al. at the University of Hawaii, for example, achieved similar results (high biomass conversion to hydrogen) with a similar approach using a supercritical gasifier. The team should seek some collaboration for this project.
- Much work was done on base-lining autoclave work on alcohol reforming and not much time remains for the biomass solids, which should have been the focus of the project. This is where the most value to the program would have been gained.
- Bench scale testing of individual components (hydrolyzer, reformer, and membrane) of the integrated system might be worthwhile at this early stage. However, the project investigator needs to consider testing the whole system together to prove the concept from an integrated system standpoint. The earlier this can be done, the more credible the cost estimates will become. For example, testing with a furnace to provide heat for the endothermic reaction will not give one the answer on how to integrate a burner into the system. Issues with impurities will not be addressed by testing with ethanol as a reformer feed.
- The project is following in a very good path to designing a complete system. Details were addressed besides design components (e.g., the reliability impact of palladium membranes). The process is in line with practical implementation.
- The project has an excellent scope of work to address an alternative approach to thermochemical conversion processes. Good progress against the catalyst and selectivity issues has been made.

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

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

- This project has demonstrated excellent conversions of synthetic and real feedstocks.
- The use of a base to facilitate wood processing is not a new concept nor is the use of supported Raney nickel. Both can be found in the literature.
- The team is making progress towards the flow reactor.
- Membrane demonstration for less than one hour is nice but not impressive. The membrane represents a large cost for their proposed system and its replacement will have a significant negative impact on the cost analysis. The team needs to demonstrate that they can run the membrane for thousands of hours with a gas mix that represents the expected products from their reactor, including impurities and the potassium hydroxide KOH base
- The team needs to demonstrate KOH recovery, which will be a significant challenge.
- The project investigator has demonstrated the basis of the technology and addressed several issues, such as catalyst type, that would be cost barriers. Many barriers and issues remain, such as corrosion and caustic recycle. The effects of contaminants also need to be addressed.
- Though hydrogen and capital cost projections appear to be close to the DOE targets, this reviewer has serious reservations that these numbers will hold true once all of the issues are identified and resolved. For instance, the caustic corrosion, metallurgy, and contaminations issues often drive the cost prohibitively high.
- The work on the flow reactor with integrated system shows good progress so far. Strong progress has also been made toward hydrogen cost reduction. A palladium membrane cost reduction from 85% of the capital cost to 50% at the current stage shows some promise. However, it still represents a large portion of capital cost that could jeopardize the economic viability of the integrated process.
- Very good progress has been made to date, but more details on the separation process should be shown. The team appears to have addressed most of the issues with the palladium-copper membrane and it would be beneficial to see some of the information behind it.

HYDROGEN PRODUCTION AND DELIVERY

- Strong progress has been made on milestones for selectivity, catalyst selection, and yield as compared to 2009. Too much range of cost and performance still exists to scaling up.

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

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

- Most of the collaboration is being provided with hydrogen separation membranes.
- The project has some collaboration, but the team needs to be more specific in their presentation on what the partners are doing.
- Collaboration with Energy & Environmental Research Center (EERC) to do autoclave optimization testing is a plus. EERC has excellent facilities and support staff. Consulting with the forest products industry or similar industries with experience in alkali pulping, biomass feedstocks, and other areas could be advantageous.
- The project has good collaborations with various entities. The team should work with the H2A project model to refine cost as more information is obtained from testing.
- This project went through a competitive process development and a lot of collaboration was not possible. However, the team does not appear to have been working in vacuum, as they have achieved great technology incorporation into their process.
- The team had some collaboration with the University of North Dakota. However, there is not much detail on scope, communications, coordination, and review of the results.
- Clear identification of roles and responsibilities should be present as applied to the reporting of results and scale-up.

Question 5: Approach to and relevance of proposed future research

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

- Moving the catalyst to nickel seems like a move that will be unsuccessful, unless this approach will also incorporate regeneration schemes. Sulfur poisoning of nickel is well known, as is carbon formation in heterogeneous gas phase catalysis. Thus, this may work for the pure synthetic feedstocks, but poisoning is very likely with real biomass.
- In terms of cost, reductions are more likely in dealing with the palladium membrane and the caustic base hydrolysis.
- The team is beginning to look at caustic recycle, which is good. However, this should have begun earlier.
- Durability testing will be very interesting. This test should include the membrane.
- This project is worth continuing to the end of this phase to complete lab prototype testing to obtain better data for use in process economics assessments. The project investigator is aware and sensitive to cost issues and has structured a future test plan accordingly.
- The project investigator needs to consider addressing issues with scale up, reactor metallurgy at high pressure, temperature, caustic conditions, and feasibility of using Raney nickel at a larger scale. The investigator should also consider focusing on heat integration.
- The proposed work does address information from previous work; however, it still does not identify who is performing the research and development. It also does not explain the strategy if the catalyst does not scale and the prototype fails the durability testing.

Strengths and weaknesses

Strengths

- This project has an interesting approach.
- This project has potential for low-cost hydrogen production.
- It is leveraging information and technology development from other DOE projects such as membrane technology, which was developed under DOE's Fossil Energy program.
- The project uses excellent facilities and staff for conducting this type of research.
- The proposed recycle and durability study is critical to project success.
- Good fundamental research and development is used to understand reaction mechanism.

- The project has a good research and development plan to evaluate the hydrothermal conversion process.

Weaknesses

- The development of base metal catalysts needs to examine the poisoning issues with real feedstocks, not just the pure feeds. The cost of the metal catalysts seems tertiary to the overall cost compared with the palladium membrane and the caustic hydrolysis steps.
- The work is not extremely innovative. For example, the use of bases to facilitate the reaction is known and Raney nickel is a well-known catalyst.
- The team needs to demonstrate caustic solution recovery, which will most likely be more difficult than what they expect.
- The cost advantage of using the palladium membrane over traditional PSA has not been demonstrated.
- It is not clear how carbon balance was achieved. This data needs to be reported.
- There are huge hurdles which could prohibit implementation, including the requirement of a high-pressure reactor with corrosion-resilient steels, the need for caustic recycle, and buildup of contaminants and solids in the process.
- This project has a very aggressive schedule. It is unknown if all of the issues can be satisfactorily resolved in six months or that adequate testing can be completed to address technical feasibility related to all of the concerns.
- It appears that the United Technologies Research Center (UTRC) elected to use palladium membrane for purification. However, this appears to contribute to a large portion of the capital cost and also represents a higher technical risk with this particular application.
- Limited data was presented on the different runs. It is unclear based on what was presented if the experimental design had to be redefined due to problems or poor performance. It is unclear what the risk for completion is based on current progress.
- No clear roles and responsibilities are provided for EERC and UTRC.

Specific recommendations and additions or deletions to the work scope

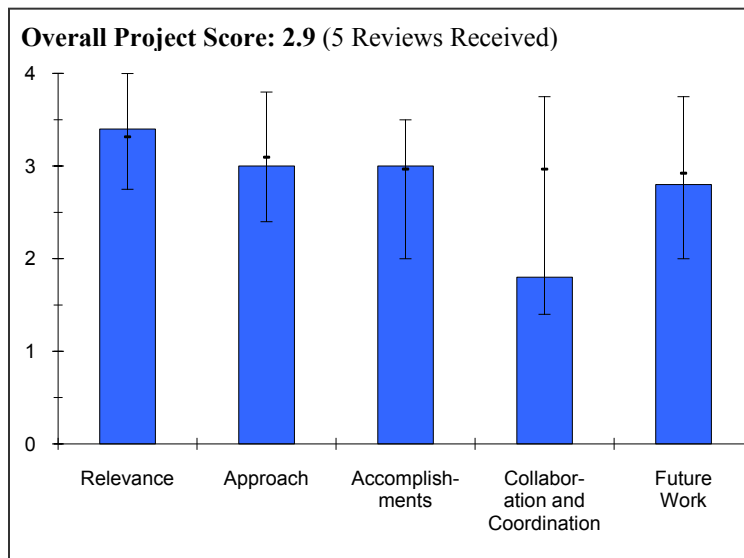
- The team should perform a cost analysis on using the palladium membrane over PSA.
- Continue funding to the end of current project, but future funding should depend on economic evaluation.
- The team needs to look at variations in feedstock composition and impurities and determine their effect on catalyst performance.

Project # PD-07: Composite Pd and Alloy Porous Stainless Steel Membranes for Hydrogen Production and Process Intensification

Yi Hua (Ed) Ma; Worcester Polytechnic Inst.

Brief Summary of Project

The objectives of this project are to 1) synthesize composite palladium and palladium alloy porous Inconel membranes for WGS reactors with long-term thermal, chemical and mechanical stability with special emphasis on the stability of hydrogen flux and selectivity, 2) demonstrate the effectiveness and long-term stability of the WGS membrane shift reactor for the production of fuel-cell quality hydrogen, 3) research and develop advanced gas clean-up technologies for sulfur removal to reduce the sulfur compounds to less than two parts per million (ppm), 4) develop a systematic framework towards process intensification to achieve higher efficiencies and enhanced performance at a lower cost, 5) perform rigorous analysis and characterization of the behavior of the resulting overall process system as well as the design of reliable control and supervision/monitoring systems, and 6) assess the economic viability of the proposed intensification strategy through a comprehensive calculation of the cost of energy output and its determinants (e.g., capital cost, operation cost, fuel cost), followed by comparative studies against other existing and pertinent energy technologies.



Question 1: Relevance to overall DOE objectives

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

- This project addresses barriers related to long-term stability and hydrogen flux targets for hydrogen separation membranes. Therefore, it is relevant to overall DOE objectives.
- This project needs an additional advanced sulfur cleaning unit (see slide #4) for the membrane developed in this project to work.
- High-flux membrane development is very relevant to hydrogen production.
- The work is focused on realistic and required performance specifications. The team should strengthen economic targets and better communicate how the work is aimed at meeting these targets.
- The project is comprehensive for development and testing of palladium and palladium alloy membranes for hydrogen separation. It is relevant to the Hydrogen Program as well as the goals and objectives in the multi-year plan.
- This project is relevant to the DOE Hydrogen from Coal Program's advanced concept/process intensification objectives by eliminating several unit operations and replacing them with the WGS step. The process concept could enable high-purity production of hydrogen from a gasifier gas stream in a single step assuming contaminant removal steps can be done successfully, though this is a big assumption.

Question 2: Approach to performing the research and development

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

- The approach in this project is not clear. It appears this team is fabricating a number of membranes of the same composition and testing them, but it is not clear what is changed between membranes (except probably

thicknesses). This approach sounds Edisonian. No attempt is made in developing sulfur- and carbon monoxide-tolerant membranes. These are the primary weaknesses of this project.

- These tests seemed to be targeted to reproduce the attractive results achieved in previous tests, but they did not seem targeted towards moving the project forward. Cycling tests and the use of larger membranes would add value, as would tests on membranes that were sulfur-tolerant. Also, the membranes tested were largely thicker than the ones targeted to meet the cost objectives of the project.
- This work represents very good technique and is at the leading edge of dense metal membrane development. The reviewer ranks this work in the top 5% of palladium membrane development worldwide. However, a few shortfalls remain that should be addressed.
 - The reported results are from a collection of different, individual membranes. This suggests that one membrane sample (or possibly a reproducible set of membrane samples) is not capable of achieving all the reported technical progress metrics (i.e., flux, selectivity, durability, and economics). The weakness here is that the technology appears to be immature, suggesting that transfer from the lab to industry may be exceedingly difficult or perhaps impossible. The project investigator should be reminded that a low degree of reproducibility represents low manufacturing yields and consequently higher cost.
 - Economics need to be addressed, not only in the abstract (e.g., against DOE targets) but also in the real world (e.g., competing solutions). The project investigator stated that the goal is to achieve a robust membrane in the thickness range of about 7-8 microns, though current results for WGS use membranes that are approximately 18 microns thick. Thus, the project investigator should provide a critical economic comparison with other dense metal membranes, which include three classes: 1) dense drawn tubes, 2) rolled planar foil, and 3) palladium alloys deposited on a porous tube. It is virtually impossible to assess economic viability without this type of comparison.
- For mixed gas membrane tests, a plot of flux versus hydrogen recovery (rather than space velocity) would add value to the project.
- Any results of poisoning experiments (sulfur tolerance) must report the hydrogen recovery as well as flux and inlet sulfur concentration.
- The project approach is good for developing and testing membranes that address the barriers of membrane selectivity and hydrogen flux.
- The technical work plan for the project is well-designed, comprehensive, and considers all of the relevant issues to test the feasibility of the concept at the laboratory scale. The fundamental studies contribute to the state of the art.

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

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

- Higher fluxes are obtained only in ideal gas conditions.
- The membrane is not tolerant to even very low concentrations (less than 2 ppm hydrogen sulfide) of sulfur. Flux is inhibited by the presence of even about 1% carbon monoxide, which is a serious problem for the real-world application of this membrane.
- This group has shown similar, good results with this type of small, palladium-coated membranes for the past decade. The reviewer would like to see more tests with larger membranes or with membrane modules, as well as tests with membrane coats that were more likely to withstand cycling or sulfur. Finally, progress on commercialization is absent. Membranes and results in the 2010 report are virtually identical to those in the 2009 report.
- This project is representative of the best metal membrane work being done at this time. The project investigator has demonstrated steady progress toward the goals and a clear understanding of how to continue this trend.
- The project has successfully achieved hydrogen flux of 359 standard cubic feet per hour per square foot (scfh/ft²), which exceeds DOE's 2015 hydrogen flux targets. It successfully addressed the barrier of developing steady state and unsteady state membrane reactor modeling simulations. The project also developed simulation models that are useful for predicting membrane performance over a range of conditions. The project obtained good long term hydrogen selectivity over a period of 147 days.
- Substantial progress has been made toward completing the testing of the membrane in long-term tests using simulated gas mixture streams.

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

This project was rated **1.8** for technology transfer and collaboration.

- A gasifier partner is not included in this work.
- The membranes are made in house by graduate students and are tested in house only by these graduate students. Based on the present year and 2009 activities, it appears that the only route to commercialization of these results is if the graduate students continue to pursue work in this area.
- The project investigator reports that only one collaborator is involved, Adsorption Research Inc. (ARI). The project lacks a collaborator who can provide module design input and commercialization/industrialization knowledge. This is a significant weakness that should be overcome.
- The project does not demonstrate collaboration or communication with the coal gasification industry. It does not appear to have internal expertise in scale-up, plant equipment, or economic analysis.
- The project has identified a key industrial partner who is making substantial progress in the upfront pressure swing adsorption (PSA) clean-up step (to remove sulfur), which is critical to the technology. No other collaborators are mentioned.

Question 5: Approach to and relevance of proposed future research

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

- No plans are presented to study the mechanical durability of the membranes. Hydrogen embrittlement is an issue for palladium membranes.
- Thin membranes have pinholes and, therefore, the selectivity is decreased. The future plan is to make thinner membranes, but the method for fabricating defect-free thin membranes is not explained.
- The project investigator reports a sound strategy for dealing with sulfur tolerance. However, results need to report hydrogen recovery in the presence of sulfur since sulfur will be concentrated on the feed side of the membrane as hydrogen permeates it. The plan lacks a clear and compelling strategy for reducing the membrane thickness from 18 microns to the target of about 7 microns, which is key to achieving competitive economics. Little information was provided on how this will be done without sacrificing selectivity and durability. The success of the project is pinned to this question.
- No evidence exists of a plan to test with a coal-based feed stream. Future work needs to identify the barriers associated with scale-up and a plan to mitigate them. The project indicated it plans to initiate an economic analysis but did not commit to complete an economic viability analysis for commercialization.
- The project is focused on the barriers and plans to conduct economic evaluation before proceeding through into a follow-on phase.

Strengths and weaknesses

Strengths

- A good number of publications are presented.
- This project trains graduate students and post-doctorates.
- This project performs good fabrication and testing of palladium membranes.
- The project presents great flux, durability, and selectivity for small membranes with pure gases and no cycling.
- The project demonstrates a good track record of steady membrane improvement, which is mostly due to significant advances in porous support structure and development and palladium deposition process.
- Project strengths include good membrane testing procedures. Membranes have been developed that exceed DOE flux targets for 2015 and selective hydrogen permeabilities have been demonstrated for long periods of time.
- The project made a good choice in partners. The team demonstrated comprehensive testing capability and considerable progress toward targets. The project is very well organized and addresses the major issues.

Weaknesses

- The membrane is not tolerant to few ppm levels of sulfur.
- Membrane flux is inhibited by the presence of 1% carbon monoxide in the gas stream.

- No plans are presented to study mechanical durability.
- No techno-economic analysis is provided.
- A gasifier partner is not included in this project.
- It is unclear who the end user of this technology would be.
- The project uses small membranes, and different membranes are used to test flux, lifetime, and selectivity. The project did not show any real progress in membrane size, connections, sulfur tolerance, cycling, collaboration, or commercialization.
- The project has a lack of connection to real-world economics. This could be overcome through proper selection of an industrial/commercial partner to help with module design and economic evaluations, relative to competing technical solutions (not only DOE targets).
- The project investigator should be devoting more effort to demonstrating a reasonable degree of reproducibility. For example, report results for 10 nominally identical membranes that are fabricated according to a method that is expected to yield the best membrane performance. It is currently unclear how many meet the expected performance. A statistical treatment of the results (e.g., flux, selectivity, durability, and sulfur tolerance) will provide enormous insight into further required effort.
- There is no indication that the project has plans to interact and communicate with the industrial coal gasification community. A plan is needed to obtain membrane performance data using a coal gasification-based slipstream. Though the project's future work indicated "initiation" of an economic analysis, no plan is presented to complete an economic viability analysis. The project investigator did not discuss plans for significant scale-up of the membrane reactor module.
- The project needs to collaborate with industry partners beyond ARI to be in position to conduct integrated system testing, obtain reliable process economic data, and potentially be in position for technology transfer.
- The team needs to build an integrated system and run pilot tests using real coal-derived gasifier effluents.

Specific recommendations and additions or deletions to the work scope

- As per slide #2, the work is 100% completed. The future plans are not well defined and the approach is not clear. Therefore, this project can be terminated. DOE should revisit the project once this team finds an end user to work with them.
- This project is completed. For future projects, it would be nice to see a demonstration of cycling stability with these membranes or membranes made with palladium-silver, palladium-copper, or palladium-gold coats. These are materials that might be expected to withstand cycling. Hydrogen sulfide should be added to the gas. The team should test larger membranes in addition to modules made of several membranes or membranes with much larger surface areas. The team should also increase collaboration with other groups.
- The strategy for achieving suitable thin membranes that are economically viable needs to be explicitly communicated. The strategy should be convincing and compelling.
- The team should bring on a partner to assist with commercialization. In addition, a comprehensive economic analysis should be conducted against the best alternative solutions (e.g., membrane, PSA).
- The team should begin to address reproducibility using statistically significant populations of membranes made according to best methods.
- It is recommended that this project complete an economic viability analysis and design of module(s) for scale-up. The project uses expensive membrane materials (e.g., palladium and gold), and the process may not be economically viable.
- This project should continue to be funded. Besides ARI, the team should engage user industry partnerships to assist in process and economic analysis as well as development of integration approaches as the project moves forward. The project should generate sufficient information at the end of the current phase to be able to design and test an engineering prototype to run pilot trials using gas streams generated by a real coal gasifier. The project team should also be ready to begin technology transfer activity.

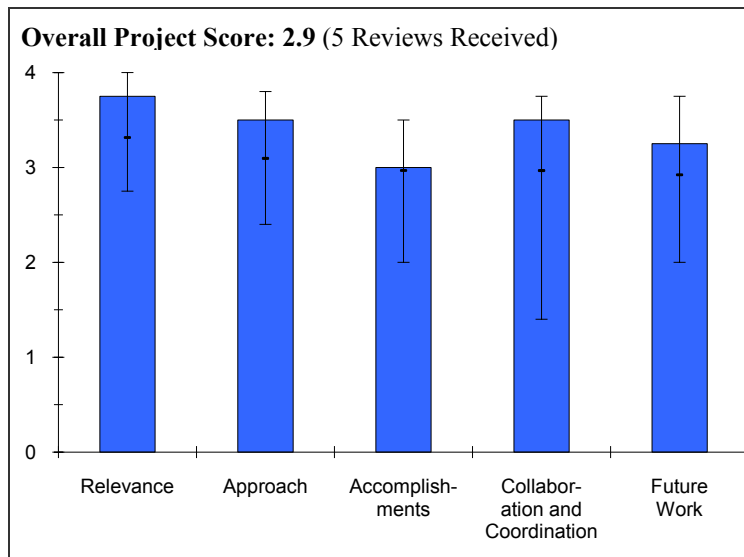
Project # PD-08: Development of Robust Hydrogen Separation Membranes

Bryan Morreale; National Energy Technology Laboratory-Office of Research and Development

Brief Summary of Project

The objective of this project is the development of robust hydrogen separation membranes for integration into coal conversion processes, including integrated WGS membrane reactors. Studies suggest that incorporating separation membranes into coal conversion processes can reduce costs by 8%. Task one is the performance testing of external membranes and the National Energy Technology Laboratory (NETL) hydrogen membrane test protocol. Task two is the development of robust metal membranes.

Question 1: Relevance to overall DOE objectives



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

- This project is relevant given that it is attempting to develop a robust hydrogen separation membrane for integration into coal conversion process. Also, the performance testing of hydrogen separation membranes fabricated by other researchers working in this area are being tested in this project.
- Development and testing of this type of hydrogen permeable membranes is very relevant to the DOE Hydrogen Program goals.
- The work is clearly focused on sulfur poisoning mechanisms and speculates methods to improve sulfur tolerance of palladium alloy membranes. However, little else is being reported that is strategically relevant to program goals.
- Although a fair amount of effort appears to have been directed at defining standardized membrane testing protocols, this is not specifically on task with program targets.
- The overall goal of this project is to develop robust dense metal hydrogen separation membranes for integration into coal conversion processes. This project is highly relevant to DOE Hydrogen Program objectives as well as the goals and objectives of the multi-year plan.
- Hydrogen separation is critical to the Hydrogen Program. This project has established a joint laboratory and university collaboration. Through this collaboration, it has established a hydrogen membrane testing protocol to allow competing developing technologies to undergo unbiased performance verification on a common basis.

Question 2: Approach to performing the research and development

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

- The pure palladium and 60 weight percent Pd-40 weight percent Cu (60Pd-40Cu) membranes are tested under different temperature conditions, the former at 450°C and the latter at 350°C. Based on this test result, two types of decay mechanisms, namely, corrosive decay and catalytic poisoning, were presented. It would be valuable to show the effects of the two membranes tested at the same temperature (350°C or 450°C). It would be interesting to see if these two decay mechanisms occur in both cases, or if the "corrosive decay" mechanism is valid only in the case of pure palladium. The experiments conducted to date are unclear. This shows a well-thought-out approach was not followed.
- It is stated in one of the slides that the approach is to develop a multi-layered membrane system that utilizes the catalytic activity seen with palladium sulfide. However, the results show that the flux decreases drastically (from about 12 to less than 4) in 150 hours of testing and the flux continues to decrease beyond 150 hours (slide

#13). The rationale in developing a multi-layered membrane system that utilizes the catalytic activity of Pd₄S is unclear.

- The topic is broad, including the development of robust membranes, but the materials tested come from a rather narrow range of options of binary Pd-Cu alloys. The reviewer would like to see results with a broader range of membrane materials tested over a broad range of temperatures, both with and without sulfur.
- The technical approach proposed to improve sulfur tolerance of palladium-alloy membranes is weak, primarily because the probability for the approach to yield success is low. The team should become intimately familiar with the large body of data addressing coatings on metal membranes. This work has been underway for decades and yet little awareness was communicated in the briefing. In particular, metal coatings are well known to be fraught with problems (e.g., pinholes, cracks, and intermetallic diffusion). Oxide and other inorganic coatings are also known to be problematic. For example, coatings can be dense, pinhole-free coverage is difficult to obtain, and hydrogen permeability is often low.
- The project applies engineering principles, membrane technology, and coal conversion processes to define a sequential protocol for study and testing. This approach provides a better understanding of membrane surface fouling by unwanted contaminants, such as hydrogen sulfide.
- The project has comprehensive experimental test rigs combined with materials and a computational support capability. The research endeavors are focused, specifically on poisons and structural integrity testing.

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

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

- A test protocol has been developed and test systems have been modified to allow testing of various membrane geometries.
- Several multi-layered membranes have been fabricated.
- Flux is very low (see slide #19) and dropped to zero in two hours.
- This project included some interesting results on palladium-copper, but the reviewer has seen some of these results before. A broader range of materials tested would have been beneficial.
- Too much of the briefing time was spent describing the development of standardized membrane test methods. While this is necessary (as is, for example, instrument calibration), it does not specifically address program goals.
- The relevant reported progress was related to understanding sulfur poisoning. However, this was earlier work, which leads the reviewer to wonder what the team has been doing on this program.
- A test protocol was developed and test systems were modified to allow testing of various new membrane geometries at various performance levels. It was found that the loss of flux was due to hydrogen sulfide, which caused the corrosive decay of palladium membranes. The corrosive decay was associated with the reaction of palladium and hydrogen sulfide to form palladium sulfide.
- The project demonstrated excellent progress and results in just nine months with research focus initially on sulfur contamination, which is the major barrier.

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

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

- Several partners are listed on the slide, but the role of each partner is not explained with the exception of the important roles played by collaborators from Carnegie Mellon University (CMU) and the University of Pittsburgh (Pitt).
- Collaboration is limited to researchers from Pitt and CMU, but there are no industrial collaborators. Therefore, there is likely no route to commercialization on the horizon.
- The list of collaborators is impressive on first examination. Then, one sees that most or all of the collaborators are related to NETL. The reviewer did not see mention of industrial/commercial partners, which suggests that the connection to commercialization could be strengthened.
- The project partners include two universities, a national laboratory, and a research organization Gas Technology Institute (GTI).
- There is no evidence the project includes, or has plans to include, a partner from the coal gasification industry.

HYDROGEN PRODUCTION AND DELIVERY

- Partners are well integrated and each contributes their area of expertise to the testing protocol. GTI is part of the project, but no mention is given to its role.

Question 5: Approach to and relevance of proposed future research

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

- Information of future plans are absent in the slides and no discussion about these plans were included in the oral presentation.
- Future work is not very well defined. The plan seems to be to do everything and the reality is certain to fall short. The reviewer would have liked more information of a specific plan, such as testing these membranes at these conditions.
- The proposed approach is based on establishing protective coatings to yield sulfur tolerance. Decades of effort to develop protective coatings have not yielded any practical solutions. However, the project investigator is proposing repetition of the same techniques that have been examined previously (e.g., metal coatings and inorganic coatings).
- The suggestion to use a coating formulation that is similar to an hydrodesulfurization (HDS) catalyst is intriguing. However, the rationale for this is unclear. The coating layer must be resistant to poisoning by sulfur species, active for dissociation of hydrogen, and permeable to hydrogen atoms. It is unclear what properties of HDS catalysts lead the investigators to believe these functional requirements will be met. HDS catalysts lose catalytic activity in the absence of sulfur. The side of the coating facing the inside of the membrane will be devoid of sulfur and rich in hydrogen, which is not good for an HDS catalyst. It is unclear why the team thinks they can deposit a dense, pinhole and crack-free layer of these materials (or any inorganic coating).
- Previous work conducted by the reviewer for DOE in the mid-1990s demonstrated the short-term effectiveness of glasses in retarding hydrogen sulfide corrosion of stainless steel. However, the glasses were not an impermeable barrier to hydrogen sulfide. The reasoning behind suggesting that glasses can meet the required functionality is unclear to the reviewer.
- Proposed future work includes testing with contaminants other than hydrogen sulfide, such as chlorine and nitrogen-based compounds. Future work also includes integration of the WGS reactor and membrane separator.
- The future work plan is based upon sound and important technical criteria.

Strengths and weaknesses

Strengths

- The team has a good understanding of engineering principles, membrane technology, and conversion processes.
- The facility to test membranes operates under NETL-established test protocol.
- The project investigator provided unbiased performance verification testing of membranes made by other researchers.
- The project demonstrated very good computational capability.
- The team used a nice setup. They conducted nice work with palladium-copper alloys and sulfur.
- The team developed a solid understanding of sulfur poisoning of palladium and palladium-copper alloys. The work also shows that palladium sulfide coatings are tenacious and yet they grow to remarkable thickness. This should provide important clues into potentially fruitful future directions aimed at increasing sulfur tolerance. Typically, protective oxide coatings on metals are effective because the oxidation stops once a thin surface coating forms. It is unclear to the reviewer why the tenacious sulfide coating does not stop further sulfidation.
- The project includes a good combination of in-house technical expertise and willingness to address the effects of a range of contaminants on membrane materials and performance. Progress is being made in understanding how loss of membrane flux occurs due to unwanted contaminants.
- This is an excellent project that combines computational and experimental protocols that have already demonstrated capabilities for standardization and controlled testing of various types of membranes. The laboratories and the various teams of project investigators that are participating in this project are outstanding.

Weaknesses

- Flux is very low.
- No future plans are included.

- The approach followed in this project is not good.
- The project seems to be going “everywhere and nowhere” in terms of materials and collaboration.
- The project has a lack of compelling arguments as to why the proposed future work in coatings will yield success.
- The project shows no evidence that it is making progress on understanding the challenges associated with implementing a hydrogen membrane into a coal gasification plant.
- It is probably worthwhile to work with a “user industry” team to obtain direct commercial guidance and to gain consensus on process and process economic considerations. It is also probably worthwhile to advertise the capability to ensure that all DOE membrane projects are subjected to the standard testing protocols developed under this project.

Specific recommendations and additions or deletions to the work scope

- Continuation of the computational study is recommended.
- It is recommended to maintain the test facility to test the performances of membranes fabricated by outside researchers.
- The project should pick a few more membranes to test, perhaps palladium-gold alloys. Also consider a lower-cost, higher-flux option.
- The project should pursue collaboration in a direction towards commercialization.
- The team should review the body of prior work on metal membrane coatings, including both metal layers and inorganic layers. The team should also develop a strategy for either stabilizing layers that provide all the requisite functionality or come up with an alternative program plan.
- The project should take a closer look at the mechanism for palladium sulfide formation and layer growth.
- It is recommended that the project add an industrial partner from the coal gasification community.
- DOE should continue to fund this project.

Project # PD-09: Scale-Up of Hydrogen Transport Membranes for IGCC and FutureGen Plants

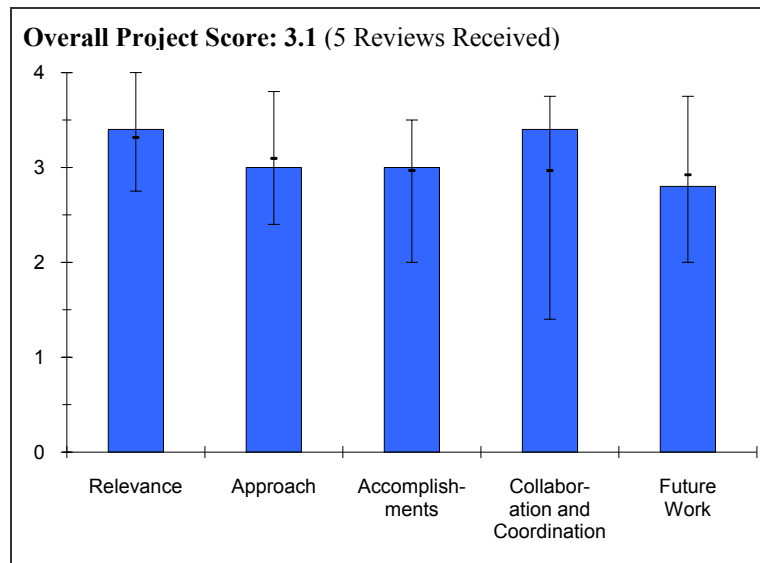
Carl Evenson; Eltron Research Inc.

Brief Summary of Project

The overall objective of this project is to create hydrogen transport membranes that: 1) are a cost-effective hydrogen/carbon dioxide separation system, 2) retain carbon dioxide at gasifier pressures, 3) operate near WGS conditions, and 4) tolerate reasonably achievable levels of coal impurities. Objectives for June 2009 to May 2010 include 1) scale-up of membrane manufacturing, 2) lifetime testing, 3) impurity testing, and 4) design of a 12 lb/day membrane reactor.

Question 1: Relevance to overall DOE objectives

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



- The objective of this project is to develop a cost-effective hydrogen/carbon dioxide separation system that retains carbon dioxide at gasifier pressures, operates near WGS conditions, and tolerates reasonably achievable levels of coal impurities. These objectives are relevant to the DOE Hydrogen from Coal Program.
- Metal membranes are very relevant to hydrogen generation and delivery.
- This project is definitely aimed at the technical goals, but no communication of accomplishments toward economic goals is presented. Economics cannot be ignored. More importantly, the technology under development must be assessed in comparison to other available technical solutions, not only DOE economic targets, which can become obsolete as other solutions are developed.
- Mixed gas testing should be reported with a plot of flux versus hydrogen recovery since comparison to pure hydrogen flux under equivalent hydrogen partial pressure provides the necessary reference point. Sulfur poisoning results must also be reported with the hydrogen recovery since impurities are concentrated on the feed side of the membrane as hydrogen is removed.
- The project clearly supports DOE's Hydrogen Program. The overall goal is to develop a cost-effective hydrogen/carbon dioxide separation system. The objective is to develop a hydrogen recovery system that retains carbon dioxide at coal gasifier pressures, operates near WGS conditions, and tolerates impurities.
- The Eltron membrane project is yet another technology that can recover hydrogen at high purity from integrated gasification combined cycle (IGCC) syngas streams, which is critical to the economic production of hydrogen from coal and which forms the basis of the DOE Hydrogen from Coal Program element.

Question 2: Approach to performing the research and development

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

- Approaches for the past year were to procure membrane materials prepared by different manufacturers and processes for testing and evaluation, select the preferred manufacturing process and catalyst deposition technique for scale-up in process development unit, collect lifetime data on a 6-inch tubular membrane with electrodeposited catalysts, and deposit catalyst on a 5-ft tubular membrane.
- Without knowing the composition of the membrane, these approaches seem to be fine. The reviewers have to take the presenter's word that this membrane is good.
- More information on seals to the membrane tubes would be useful (e.g., hot-seal or cold seal). Additionally, more information on membrane designs and materials and on cycling or sulfur content would be useful.

- The technical results communicated in this briefing are primarily scale-up of the membrane fabrication (and module), some durability data, and some mixed gas data, including sulfur tolerance.
- The module design is fairly standard (tube in shell) and yet the team has been slow to recognize mass transfer challenges associated with this design. Furthermore, no guidance is provided to the reviewers with respect to the composition of the permselective layer of the Eltron membrane. This is unfortunate, since even some general information would be extremely helpful in reviewing this work. Therefore, the reviewer can only conclude that the very thick (500 micron) permselective layer, which is reported to not contain palladium or copper, must be comprised mostly of Group 3, 4, or 5 metals. These are extremely reactive metals and three concerns arise immediately. First, alloying with the catalytic coating (intermetallic diffusion) is a concern. Second, oxidation from carbon dioxide, carbon monoxide, and water in the feed stream is a concern if the coating is scratched or otherwise damaged. The third concern is hydrogen embrittlement. This is not a good approach. Furthermore, it has been previously investigated and found to be deficient.
- The project seeks to demonstrate performance and economics of metal membranes using coal-based feed streams. The project has developed a high level of expertise in bench-scale testing of membranes.
- The technical approach cannot be assessed due to the “proprietary” nature relative to other hydrogen membranes. It is excellent to focus on lifetime and durability testing, making technical decisions based upon cost considerations (e.g., moving from planar to tubular platform), and partnering with a company that can provide a host test site for prototype testing using actual coal gasifier streams.

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

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

- Tubular membrane manufacturing was scaled-up.
- Membrane flux decreased drastically upon exposure to gasified coal syngas that was passed through a zinc oxide sorbent bed. It is not clear what is going to be done to prevent this serious problem. Without knowing the composition of the membrane, it is impossible for the reviewers to offer suggestions or recommendations.
- The team found a good collaborator. Some tests on real gases were conducted and the team has switched geometry of membranes to tubes.
- The team’s plans are to work with larger membranes. Cycling tests and tests with sulfur would have added value in addition to some arm’s length sales. Still, the project seems quite good and attractive.
- The key successes reported are scaling up to practical membrane modules and forming the partnership with Eastman. If not for these two facts, the reviewer would rate this as fair.
- Unfortunately, the negatives include lack of demonstrated reproducibility; flux decay, which the reviewer believes is inherent in the membrane structure; apparent restriction to low operating temperature, which is expected if the aforementioned alloying/intermetallic diffusion results in membrane structural degradation; and complete lack of economic benchmarking.
- The project reported that “the two key advantages of its dense metal membrane are that it is ten times cheaper than palladium membranes and has ten times better performance.” Tubular membrane manufacturing was successfully scaled up. Membrane lifetime and impurity tests were conducted.
- The project has completed all objectives on track for installing a prototype system in the last quarter of FY 10.

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

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

- It is good to see a gasifier partner, Eastman Chemical Company (Eastman), is participating in this project.
- Eastman is a great collaborator.
- Bringing Eastman on board is a big plus as this represents a pathway to commercialization.
- A critical new partnership with Eastman has been developed. Eastman will provide a coal gasification facility in Kingsport, TN, for membrane testing.
- The team did a commendable job obtaining a key partner such as Eastman, as a host site to provide actual gasifier effluents is critical to the success of any membrane development project.

Question 5: Approach to and relevance of proposed future research

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

- The plan to design, build, and operate a 12 lb/day hydrogen unit seems good. Eltron should test this unit in a real gasifier slip stream before proceeding further with the design of the 250 lb/day unit. The stability of the membrane-to-coal gas impurity is a very serious issue and this must be solved before proceeding with the 250 lb/day unit.
- Technically, the future work is perfect. The reviewer would like to see some aim for arm's length sales or publishing of technical information. It seems that the alloys would be sufficiently covered by patents by now, if they ever will be.
- The briefing did not explain how the following deficiencies would be overcome: 1) feed side mass transfer resistance, 2) achieving adequate sulfur tolerance, 3) achieving reproducible membrane performance, 4) resolving the problem of gradual flux decline, and 5) achieving competitive economics. All of these challenges need to be addressed.
- The bright side is that Eastman should be able to either assist with a compelling economic assessment or validate that done by Eltron. The field tests scheduled to be done at Eastman's plant will provide valuable and useful information.
- The project appears to be effectively planning its future work in a logical manner by incorporating appropriate decision points. Future work includes scale-up testing on a coal gasification feed stream, based on construction of a 1.5 lb/day unit to a 12 lb/day hydrogen unit (followed by a "go/no-go" decision to build a bigger one), preliminary design of 250 lb/day unit (followed by another "go/no-go" decision), and later development of a 250 lb/day hydrogen membrane unit.
- The aggressive future work plan assumes success. No alternative research and development plan is presented should performance and cost targets not meet the DOE targets.

Strengths and weaknesses

Strengths

- The team finally managed to get an end user (Eastman) onboard.
- Eastman as a collaborator is a strength. Some work with hydrogen sulfide also contributes to the success of the project.
- The scale-up of membrane modules to practical size is a strength, as is planned field tests on slipstreams.
- The project has developed a high level of expertise in bench-scale testing of membranes. It was reported that "the two key advantages of its dense metal membrane are that it is 10 times cheaper than palladium membranes and has 10 times better performance." A systematic plan has been developed involving "go/no-go" decisions for the scale-up from 1.5 lb/day to 250 lb/day of hydrogen, based on a shell and tube module design.
- The choice of an industrial partner (Eastman) as site for prototype coal gas testing is a strength. Eltron has excellent research staff and research and development facilities.

Weaknesses

- The membrane composition is unknown.
- Flux degrades rapidly upon exposure to the coal gas stream.
- Precious metal catalysts are used. The Palladium catalyst layer will be poisoned by carbon monoxide and hydrogen sulfide in the gas stream, which will limit the dissociation of hydrogen molecules and hence flux will be reduced with time.
- The project is secretive. No cycling work or work with hydrogen sulfide is included. Also, when asked technical questions, the presenter said "Eltron believes...", not "I've found...", or "the experiments support."
- The membrane composition is questionable. The reviewer speculates that this approach has been previously tested and rejected. It is uncertain how the team will overcome the challenge of limited operating temperature and flux decline. It is also uncertain how the team will protect the membrane against oxidation from feed stream components (e.g., carbon oxides, water, hydrogen sulfide). Hydrogen embrittlement and the implication for process control is a concern since it cannot be at low temperature in the presence of hydrogen.
- Information on the projected cost is lacking and it should be expressed as a range since it is probable that all variables are not resolved. In particular, the membrane is extremely thick and most likely a reactive metal that is

relatively expensive to produce in high-purity, fabricated shapes. It is a fundamental mistake to ignore cost analysis throughout the project. In other words, this should not be deferred until the end of the project.

- The lack of relevant information regarding composition of the membrane for this project makes it difficult to evaluate. Though the project is very close to scale-up and testing in the Eastman coal gasification plant, no economic results were reported.
- The loss of membrane performance is cause to be concerned about the commercial viability of the technology under gasifier conditions. This needs to be confirmed and the impact process analyzed before decisions are made to scale up to the larger unit proposed. The project appears to be on the fast track to scale up and it is not clear what targets define the “go/no-go” decision.
- The presentation was silent on the process design and economics task and there is no mention of that in future work. Understanding the cost is critical to success.

Specific recommendations and additions or deletions to the work scope

- The project should address the membrane stability before proceeding further.
- Oxidation of refractory materials is a serious issue.
- A technical publication of alloy composition is recommended. Information on arm's length sales would be helpful.
- Further funding should be significantly reduced until the membrane stability issues are resolved. Three concerns related to membrane stability (and durability) have been raised: 1) flux decline, 2) oxidative stability if there is a defect in the catalytic coating, and 3) hydrogen embrittlement under off-design conditions.
- The team should present a complete and realistic economic assessment of the membrane module cost that includes real prices for materials and fabrication. It is not adequate to say metal “X” costs \$“Y”/lb, as actual cost may often be many times more for fabricated articles. The analysis should include a comparison to other membrane solutions, not only the DOE targets.
- It is recommended that the project add at least one membrane manufacturer as a partner. Economic viability should be determined for the commercial plant, using data obtained from bench-scale testing.
- Continue to fund this project.
- Though performance tests have been done in simulated gas streams as well in a simulated coal syngas, which contains sulfur, the reviewer thinks the results show an unfavorable response. Thus, the project should give expanded attention in laboratory studies to better understand the performance loss and seek a material or engineering solution before a lot of time and effort is spent running membrane tests at larger scale at Eastman.

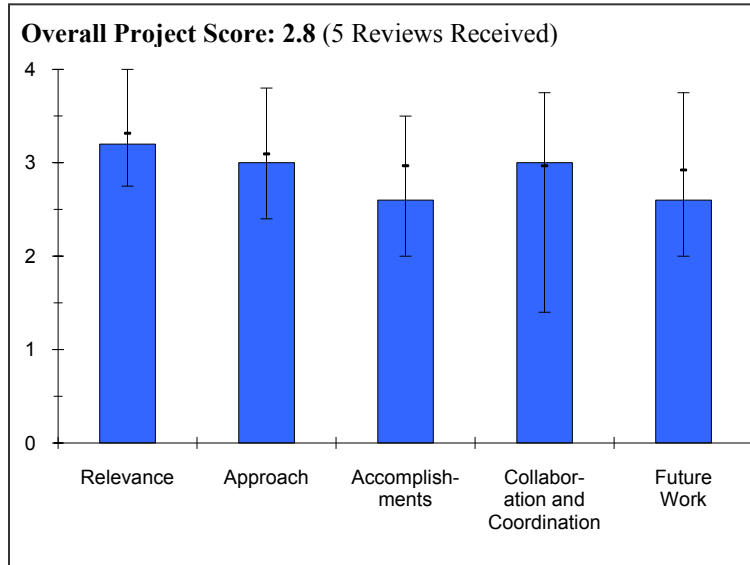
Project # PD-10: Amorphous Alloy Membranes for High Temperature Hydrogen Separations

Kent Coulter; Southwest Research Institute®

Brief Summary of Project

The overall objective of this project is to develop advanced and novel energy technologies that will facilitate the use of our nation's abundant coal resources to produce, deliver, store, and utilize affordable hydrogen in an environmentally clean manner. The program will model, fabricate, and test thin film amorphous alloy membranes that separate hydrogen from a coal-based system. The program's objective is to have performance meeting the DOE 2015 targets of flux, selectivity, cost, and chemical and mechanical robustness, without the use of platinum group metals.

Question 1: Relevance to overall DOE objectives



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

- The scope of this project is to model, fabricate, and test thin film amorphous alloy membranes that separate hydrogen from a coal-based system with performance meeting the DOE 2015 targets of flux, selectivity, cost, and chemical and mechanical robustness, without the use of platinum metal groups. This scope is relevant to the DOE Hydrogen from Coal Program.
- Good alloy membranes are very important for DOE's hydrogen generation goals. Nickel is much cheaper than palladium.
- The program is aimed at meeting the technical goals stated by DOE and the economic goals. The approach is rather novel as well, both in materials selection and analysis/fabrication techniques.
- The project objective is to model, fabricate, and test thin-film amorphous alloy membranes that separate hydrogen from a coal-based system and meet DOE 2015 targets for flux, selectivity, cost, and chemical and mechanical robustness (without the use of platinum group metals). It is relevant to the DOE objectives and supports the Hydrogen Program in addition to the goals and objectives of the multi-year plan.
- This project is yet another membrane separation approach aimed at lower cost materials to achieve economical hydrogen separation and production from coal gasifier syngas. Developing a viable method for separating hydrogen from gasifier gas is critical to the DOE Hydrogen from Coal Program. It would be a great benefit to find a replacement for palladium at comparable performance and much lower cost.

Question 2: Approach to performing the research and development

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

- The results show that the amorphous alloy membrane is not thermally stable. Crystallization of amorphous alloys is well known and should not be a surprise to the project investigator.
- The refractory alloys will oxidize easily.
- It is a good approach to use computer modeling coupled with experiment.
- The computational tasks performed by Georgia Institute of Technology (GIT) represent a very useful contribution to the science of metallurgy. However, one has to question the time value of this approach as the project investigator stated that three weeks of supercomputer time is required to complete the evaluation of one hypothetical alloy composition. This greatly limits the utility of the approach.
- Fabrication of ultra-thin alloy foils by vapor deposition is also a very interesting and useful technique since the size of foils that can be made is large.

- No evidence supports that the project approach will achieve results needed to move forward on a timely basis.
- The project approach is based upon sound fundamental scientific principles and is managed by experts in different institutions who bring together a full complement of technical know-how. The technical approach is sharply focused on the technical barrier of replacing palladium with amorphous metal alloys and it is difficult to improve significantly.

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

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

- So far, only a few samples are fabricated and none of them are tested.
- It is early in the project. An investigation of a higher nickel content alloy would be beneficial so the team could go to higher pressures and lower temperatures, which would add value. Still, the team is learning.
- The project investigator admitted that little effort has been expended due to a slow start on the computational tasks. As a result, the reviewer is taking this into consideration and is expecting to see much more progress over the next year.
- The vapor deposition process seems to result in carbon incorporation in the resulting foil films (see composition reported for nickel zirconium binary alloy fabrication). It is uncertain why this occurs. If this is inherent in the process, it must be fixed. The fabrication process must be capable of producing alloys of the desired composition and purity. Otherwise, the technique is of limited value.
- As a relatively new project (start date is October 1, 2009), no significant technical accomplishments were noted. It appears the most of past eight months have been spent planning the project and budget.
- Although the project is early, preliminary work completed shows a promising methodology.

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

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

- Georgia Institute of Technology (GIT) and Western Research Institute (WRI) are collaborators.
- The collaborators' roles are defined.
- Good collaborators are included in this project. More materials expertise would be beneficial since they would have known to expect metal rearrangements at the high temperatures of the study. They would also be familiar with the high hydrogen contents.
- During the next year, a commercialization partner should be brought on board. The other partners represent a sound basis in the fundamentals.
- The project appears to collaborate and work well with academic and research entities. GIT will select alloy compositions using first principle calculations for membrane permeability. Southwest Research Institute (SwRI) will perform fabrication of the alloy membranes, and WRI will test the membranes. However, there is no evidence that they plan to collaborate or partner with someone in the industrial coal conversion community.
- The project has close, appropriate collaboration with other institutions and partners are full participants and well-coordinated.

Question 5: Approach to and relevance of proposed future research

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

- The focus of the second year effort will be to evaluate the performance and fabrication options to produce membranes.
- It is not clear who will perform the preliminary evaluation of membrane performance before the membrane system is tested in the gasifier stream.
- The team needs to get the membrane durability up before moving to sulfur, which means the membranes will probably have to operate at lower temperatures.
- The reviewer faults the program plan for placing much effort (at the expense of both manpower and money) on theoretical calculations of amorphous metal alloys that do not address a key requirement of stability in hydrogen at operating temperatures. This is an easy experiment to conduct. The project investigator stated (in questions

HYDROGEN PRODUCTION AND DELIVERY

after the briefing) that a few known glassy alloys with high reported transition temperature will be tested for stability. This should have been done as the first task, rather than being delayed until this point in time.

- It appears the proposed future work will move slowly. The first year of the project will be used to demonstrate an amorphous alloy, based on six membrane samples to test and establish thermal stability.
- The project has just begun and the proposed work plan is solid.

Strengths and weaknesses

Strengths

- The project did well at modeling to predict alloy compositions. It was also a good move to add WRI as a partner in the team.
- The project is innovative and exploratory.
- Alloy structural and property calculations have been validated with published results and ultra-thin film fabrication methods.
- The project is a good example of how different research groups can work together to achieve a common goal. It appears their goal is more about providing information to others who are interested in commercializing membrane separation for hydrogen recovery than commercializing the unit themselves.
- This is an excellent collaborative study. Though the project is in the early stage and has started late due to staffing reasons, much progress has been made to lay the foundation for the remainder of the project.
- The systematic approach with the use of combinational screening techniques and computational modeling is a plus and should lead to some very useful results.
- The project will be using actual gasifier feeds to test their membranes, thus being able to identify contaminant performance issues early before designing and scaling larger units.

Weaknesses

- The project lacks a research plan to stabilize amorphous phase.
- The project lacks collaboration with researchers involved in industrial operation.
- The reviewer did not see a plan to prevent oxidation of the refractory alloys.
- This project is innovative and exploratory.
- It is unclear whether the fabricated ultra-thin foils are free of pinholes. A statistical treatment of this question is required. In other words, if “X” m² of foil is fabricated, the occurrence of pinholes (or other defects) should be provided. In addition, conclusions should be drawn on whether the fabricated foils can be handled and at what thickness. The reviewer has some experience testing the foils made at SwRI and believes they can be difficult to handle.
- A fundamental question must be answered immediately about whether it is possible to have a stable (with respect to crystallization) glassy metal alloy of a composition likely to be permeable to hydrogen that is stable at operating temperature and in the presence of hydrogen. If the answer is no, this program should be stopped or redefined. Assuming the answer is positive, the project should determine how a catalytically active protective coating will be applied to the glassy membrane and how the coating will be stabilized. A large body of experience exists that shows simple metal coatings are not stable with respect to intermetallic diffusion in the presence of hydrogen at operating temperatures.
- No evidence is provided that shows the project team is working to understand specific challenges involved in implementing and operating a membrane process in an industrial coal gasification plant.
- Though this is an academic collaborative study, the reviewer recommends that the team try to include someone from the user industry to provide process and economic guidance. Sometimes, the best catalyst or the best material can be developed, but in the end it has no major impact on the final cost of using the technology. When at the proper stage of the project, the team should try to collaborate with NETL and have their membrane concept tested using the NETL testing protocol.
- There are no permeability tests or contaminant tests scheduled until the third year. It is suggested that some earlier testing be included in the research plan.

Specific recommendations and additions or deletions to the work scope

- The team should get stability under control, and then move to testing with sulfur, etc.

- Demonstrate that developing a stable glassy metal alloy is possible, and then offer a compelling plan to achieve success with respect to applying a catalytically active protective coating.
- The team should address the alloy foil composition with respect to carbon inclusion (Ni-Zr binary alloy results). If this is a problem, a solution must be found soon.
- It is recommended that the project develop a broader vision that includes an understanding of the challenges involved in operating a hydrogen membrane separator in a coal gasification plant.
- Continue to fund this project.
- Add a task to do some early process and economic evaluation to develop a sense of the elements important to the eventual cost of the membrane system.

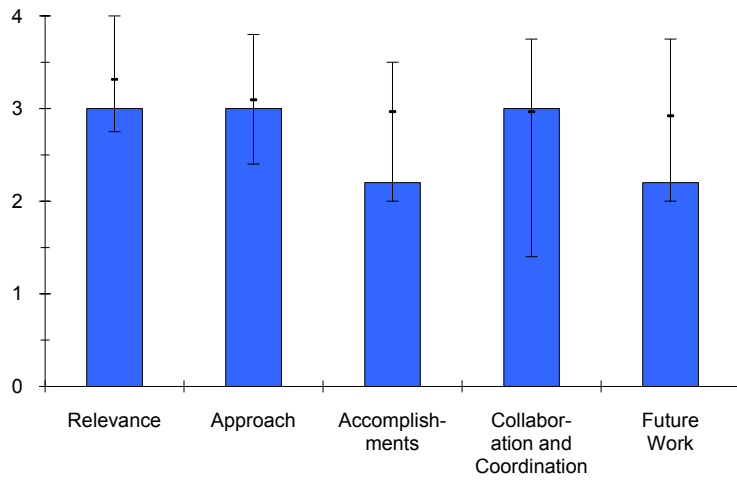
Project # PD-11: Experimental Demonstration of Advanced Palladium Membrane Separators for Central High-Purity Hydrogen Production

Sean Emerson; United Technologies' Research Center

Brief Summary of Project

The objectives of this project are to 1) confirm the high stability and resistance of a palladium-copper tri-metallic 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 $25 \text{ m}^3/(\text{m}^2 \cdot \text{h} \cdot \text{atm}^{0.5})$ at 400°C and capable of operating at pressures of 12.1 MPa (~120 atm, 1,750 psia); and 3) construct and experimentally validate the performance of 0.1 kg/day hydrogen palladium-copper tri-metallic alloy membrane separators at feed pressures of 2 MPa (290 psia) in the presence of hydrogen sulfide, ammonia, and hydrogen chloride.

Overall Project Score: 2.6 (5 Reviews Received)



Question 1: Relevance to overall DOE objectives

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

- The objective of this project is to develop an advanced palladium-based alloy membrane to separate hydrogen from a coal gas stream. There is not a gasifier partner in this team.
- Better membranes are very relevant to meeting hydrogen production targets, which are the aims of the project.
- A project objective is to confirm the high stability and resistance of a palladium-copper tri-metallic alloy to carbon and carbide formation. In addition, resistance to sulfur, halides, and ammonia is also very important.
- Most of the technical goals appear to have been addressed, although sulfur tolerance was weakly addressed and the reviewer is not convinced that any new advancements were made. For example, sulfur tolerance of palladium-copper and palladium-gold alloys has been public knowledge for decades.
- This program mostly fails to meet the economic requirements necessary to be commercially feasible. The developed membrane and module is prohibitively expensive for all but a small handful of applications that are limited in market size. This work has done very little to advance the state-of-the-art of palladium membrane technology.
- Most project aspects, such as testing for membrane flux and durability, are relevant to the Hydrogen Program. The objectives of the project include testing of palladium-copper and tri-metallic membranes for hydrogen purification that are resistant to poisoning by syngas contaminants.
- Development of advanced palladium membrane separators for central high-purity hydrogen production is critical to the Hydrogen Program and fully supports DOE research and development objectives.

Question 2: Approach to performing the research and development

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

- The approach is to use atomistic and thermodynamic modeling calculations to predict palladium-based ternary alloy compositions, fabricate the membranes, and evaluate membrane performance.
- Modified palladium-copper membranes seem like a reasonable approach. The tests seem reasonable. Unfortunately, no work was done on the majority of the goals. Instead, only stability and resistance to sulfur were covered.

- It appears to the reviewer that two different branches exist in this program. One involves module development and testing based on existing Power+Energy (P+E) commercial module designs. The other branch is the UTRC effort to develop a ternary alloy that has better performance (e.g., flux, cost, sulfur tolerance) than can be found with known palladium-copper alloys.
- The briefing did not convey any new learning from the modularization of palladium-copper membranes in P+E's module design.
- UTRC has an interesting approach of developing a ternary alloy of palladium-copper-X (X denotes a third metal) that retains the body-centered cubic (BCC) phase under operating conditions and has sulfur tolerance. However, it is not a totally novel approach. Regardless, the reviewer thinks this approach has merit.
- The project approach is to use membrane property simulations by atomistic modeling and experimentally verifying performance of hydrogen separation membranes. Unfortunately, chronic membrane failures have made many of the results inconclusive.
- The approach identifies the key barriers, and the research plan is focused on key performance verification including stability, sulfur, and other contaminants found in gasifier streams. Lab testing protocol clearly addresses the addition of contaminant at levels appropriate for gasifiers.

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

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

- The diffusivity of membrane is low due to segregation of metal oxide.
- The team successfully developed an atomistic modeling screening approach for sulfur tolerance.
- Too many defects exist in the tube. Tube performance is not satisfactory.
- The project has reasonable results. No progress was made on anything but sulfur; and nothing was presented on ammonia or halides. The price is still prohibitively high. It is not clear that the ternary is any better than plain palladium-copper. Perhaps the team should have tried more than one ternary.
- The reviewer is hard pressed to point to any key results of this work. The modularization effort is not new work. The briefing reported that P+E used its existing module design and existing membranes as a reference point for new membranes developed by UTRC. The UTRC ternary alloy membrane does not offer improvement in performance or cost over the existing palladium-copper membranes. Indeed, the project investigator reported that the cost of a commercial-scale membrane module assembly would be hundreds of millions of dollars (as expected for a relatively thick-walled tubular membrane). There is no reason to believe this work will result in any commercial value for the stated goal of DOE.
- Mixed-gas test results should be plotted as hydrogen flux versus hydrogen recovery, with a reference line showing the flux obtained with pure hydrogen at a similar hydrogen partial pressure. Poisoning experimental results must state the hydrogen recovery since impurities are concentrated at the feed side of the membrane as hydrogen is removed.
- Though the project has quantified the effects of hydrogen sulfide, carbon monoxide, carbon dioxide, nitrogen, and water on hydrogen permeability and demonstrated sulfur resistance of the palladium-copper alloy, significant membrane failures tend to occur. The hydrogen permeability needs to be substantially improved. When a single-tube separator with the ternary alloy composition was tested, it was found that a compositional barrier formed on the membrane surface. A polishing process was identified to remove the barrier, which allowed performance improvement of the membrane by a factor of two compared to 2009 results. There are unresolved problems that still exist at the bench scale, including issues with membrane flux, durability, and performance.
- Considerable progress has been made to understand sulfur tolerance and test the performance of the membrane under a wide range of conditions. Too much detail was presented in slides to ascertain key results and accomplishments, and what is yet to be achieved. However, the summary slide lists key accomplishments thus far.

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

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

- The team is collaborating with P+E to fabricate membrane tubes.

HYDROGEN PRODUCTION AND DELIVERY

- Informal collaboration with two universities is occurring.
- A gasifier partner is not included in this project.
- The team has a good partner and seems well-coordinated. Given the poor results with the ternary, it would have been nice to know the identity of the third element.
- P+E is a good addition, as their experience in modularizing small-diameter, thick-walled tubular membranes is very good. UTRC itself brings a lot of commercialization experience, but perhaps not so much in the areas of chemical processes.
- The project collaborates with P+E to manufacture the separators and fabricate alloys.
- Thermodynamic phase modeling has been done in collaboration with Metal Hydride Technologies. The Colorado School of Mines is also a valid collaborator. However, there is no evidence the project has actually approached a coal gasification plant operator to test their scaled-up membrane process with a coal gasification-based feed.
- The team has close and appropriate collaboration with membrane fabricators and institutions. Partners are full participants, and the team is well-coordinated.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.2** for proposed future work.

- The project includes future plans to construct ternary alloy separator for testing, conduct DOE testing protocol tests to validate performance and durability, and move to larger scale demonstration (e.g., 100 lb/day of hydrogen) with real gasifier exhaust in a follow-on effort. Before the team embarks on this plan, they must develop a technique to fabricate defect-free membranes. Also the transition metal (TM) oxide segregation problem must be avoided.
- It is unclear how the team plans to address the problems with sulfur tolerance and price that have appeared. There is no indication that plans exist to study 1% ammonia, for example, or halides.
- The project investigator stated that the project is essentially completed, so this question is probably not relevant. However, the reviewer strongly urges the DOE to require compelling arguments for achieving economic feasibility before funding further projects that are similar to this one. Thick-walled (on the order of 50 micron) small-diameter tubes simply do not show any chance of economic feasibility if palladium is a major constituent. Tubes made of Group 3, 4, and 5 metals also have significant costs of fabrication, and proposed programs aimed at using these metals to avoid the cost of palladium must be scrutinized for convincing arguments for achieving success.
- Proposed future research includes constructing ternary alloy separators for testing. Tests are planned to validate that performance and durability can meet DOE targets. The project also proposes to move to a larger-scale demonstration unit (e.g., 100 lb/day of hydrogen) with real gasifier exhaust. This project has encountered significant problems in conducting membrane tests due to failures of the membranes themselves and low flux rates. These problems need to be resolved well in advance of any consideration to move to a larger scale demonstration with a real gasifier exhaust.
- Plans clearly build on past progress and are sharply focused on barriers. It appears that this project ends with lab verification of performance. Then, based upon preliminary economics, the team may elect to move to a larger size unit to test feasibility with actual gasifier exhaust.

Strengths and weaknesses

Strengths

- The team is conducting modeling to predict alloy compositions.
- The team has demonstrated the ability to test membranes.
- This team uses a good approach, and they are likely to produce some valuable and practical products. The project team has good collaboration.
- The technical approach of developing a ternary alloy of palladium-copper- X to achieve a BCC structure that is resistance to sulfur poisoning bears further investigation.
- This project tested membranes that had been exposed to a number of impurities that closely approximate industrial plant conditions. The results were valuable in understanding factors affecting performance of hydrogen membrane separation processes.

- Key performance issues are identified and are an integral part of the project.
- Membrane fabrication testing is an “art in itself,” and the project includes team members who are industry experts.
- All operating performance targets, especially sulfur and ammonia tolerance, appear to be attainable.
- This project has an excellent team of companies and institutions and adequate research facilities or expertise that will be beneficial to completion of the project.
- The team uses NETL testing protocol.

Weaknesses

- A gasifier partner has not been identified.
- The team was unable to fabricate defect-free membrane tubes.
- The team was unable to prevent segregation of TM oxides.
- Flux is not high enough.
- The method is too expensive, and sulfur tolerance and flux are still below desired levels. No publication of the third element is provided, and no results with halides or realistic ammonia contents are included.
- Adding oxophilic elements (metal X) to the palladium-copper alloy must be approached cautiously. One commercial supplier in Asia offers a ternary of palladium-copper-X where X is an oxophilic transition metal, and this alloy is susceptible to oxidation in air as well as in the presence of reformat when at operating temperatures. The project investigator stated that the third alloying element X in the UTRC alloy does oxidize in air. This represents a potential weakness in the composition that could make it unsuitable for commercial applications.
- Long-term durability testing of any new alloy needs to be done under realistic operating conditions.
- The economic analysis should have signaled a problem much earlier in the program. Effort should have been redirected long ago to a pathway that offered promise of meeting acceptable economics.
- Chronic failures of the membranes resulted in pinholes and leaks, and it appears that membranes manufactured and tested in this project have not performed as desired. Significant improvements are needed in the hydrogen membrane flux to achieve DOE flux targets of 200 scfh/ft² in 2010.
- Nothing is reported about how the project will attempt to improve the hydrogen flux, which is about four times short of the target.

Specific recommendations and additions or deletions to the work scope

- The team should focus effort on fabrication methodology to minimize defects in the membranes.
- The team should select a ternary composition to avoid oxide segregation.
- The project is nearly done. The team should test high ammonia and hydrogen chloride and publish the third element.
- Any further work on this program (or similar programs) should be deferred until the cost objection is overcome.
- It is recommended that the project focus on improving flux and manufacturability of membranes that will achieve DOE targets.
- Continue to fund this project.

Project # PD-12: Supported Molten-Metal Membrane (SMMM) for Hydrogen Separation

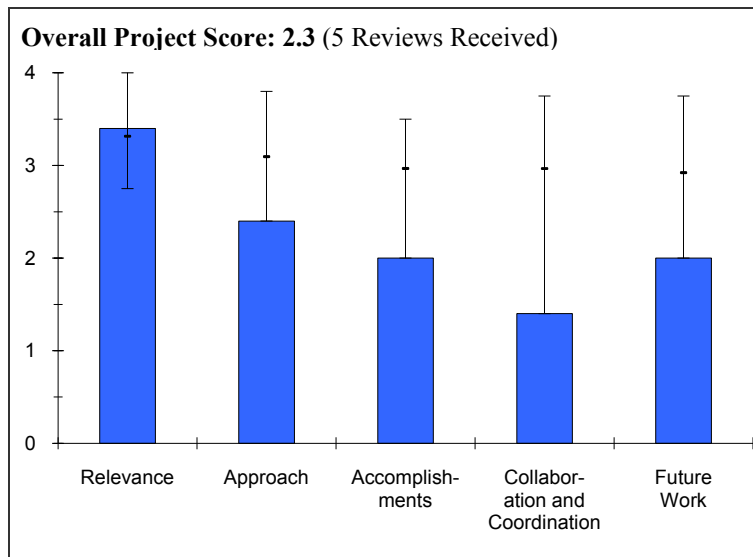
Ravindra Datta; Worcester Polytechnic Institute

Brief Summary of Project

The objectives of this project are to 1) enhance hydrogen diffusion via more open lattice, 2) enhance hydrogen dissolution via a more open lattice, and 3) enhance density of surface dissociation sites. The goals of Phase 1 are to 1) select a molten metal and catalyst, 2) select suitable porous supports (porous metal, with or without a diffusion barrier, or ceramic), 3) develop membrane fabrication protocols, and 4) establish basic feasibility of the SMMM.

Question 1: Relevance to overall DOE objectives

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



- The objective of this project is to develop a SMMM for hydrogen separation. There are serious issues regarding the stability and structural integrity of the molten membrane.
- This project is certainly in line with DOE goals.
- The stated objectives and program plan are clearly aimed at the DOE goals. This is a novel approach, and the reviewer is unaware of any direct precedent.
- The goal is to develop hydrogen separation membranes to recover hydrogen produced by coal gasification.
- The project appears to support the Hydrogen Program.
- The objective of this project is to validate the technical and economic feasibility of a SMMM for hydrogen separation, which clearly supports the Hydrogen Program objectives.

Question 2: Approach to performing the research and development

This project was rated **2.4** on its approach.

- The approach lacks several important points. For example, the identity of the porous substrate to be used in this work is unknown. The structural integrity of SMMM on porous support tubes is also unknown.
- This is an innovative approach. The team should have looked at membrane materials that are more likely to wet but not alloy with the substrate.
- The technical approach seems to lack direction and priority. The project investigator could make more efficient use of time and money by prioritizing the technical challenges and then addressing them in a thoughtful and systematic fashion, which was not evident in the briefing. Indeed, a lack of recognition of fundamentals (e.g., wetting, surface tension and capillarity, and alloy) seems to pervade the effort to date.
- It appears that the approach of the project is to develop a molten metal alloy membrane that will enhance hydrogen diffusion and dissolution via a more open lattice. There is no evidence that the project has a plan to address the challenge of achieving immobility and stability requirements for the molten metal alloy membranes.
- This is an interesting and innovative membrane approach worth studying to lower cost and possibly improve performance regarding operating issues. However, many issues in membrane fabrication and contaminant tolerance could and should be integral to the fabrication and materials choice decisions. Economic considerations need to guide even the early research, as many technical hurdles exist here.

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

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

- The project investigator has attempted to fabricate membranes but was not successful. Poor selectivity was reported.
- Practically speaking, the results were poor. Still, the project is innovative and the team is still at an early stage of the work. The team has not even developed good membrane development methods.
- The briefing did not communicate any significant positive results toward the objectives. This is a high-risk project, and unless the project investigator can refocus on the immediate technical challenges and demonstrate progress, the program should be either halted or redirected.
- Early work in the project has to do with the construction of a porous Inconel support. Progress was made on identifying candidates for molten metals and supports. Electroless/electroplating methodologies for SMMM fabrication were developed.
- The project is early (only nine months old), but good progress on screening methodologies, identifying materials, and conducting some preliminary tests has been made. It is too early to judge this project relative to meeting targets.

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

This project was rated **1.4** for technology transfer and collaboration.

- No outside collaborators participated in this project.
- The team should collaborate with a metals and materials expert. They need a better method to test wettability and undesirable alloy formation. Still, this may be an area where some ignorance helps.
- No other collaborators were communicated in the briefing materials. This may be sufficient at this early stage, but if the program is to continue it is vital to involve collaborators with modularization and commercialization experience.
- No evidence is presented that the project has established any outside collaboration or technology transfer. The team appears to have no plans to do so.
- All work is done at the sponsoring organization with no identified outside collaboration. There needs to be partnering at some point with actual membrane fabricators and a team member that can provide process economic guidance.

Question 5: Approach to and relevance of proposed future research

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

- The project investigator is going to look for alternate support and metal compositions to fabricate membranes.
- If metal alloying and inorganic wetting are both unsolved problems, it is not clear that a combination will not suffer from the combination of the problems.
- The project investigator presented no compelling plan for the future in the slide presentation. Only during questioning did he hint at plans to test zirconia substrates because he has reason to believe they may wet better with the molten metal phase. When questioned about the catalytic metal phase, the project investigator offered ideas that dissolving (alloying) a catalytically- active metal in the molten metal might offer good results.
- Overall, the briefing did not offer a convincing plan to overcome the two most important technical challenges, which are finding a substrate that is wetted strongly by the liquid metal phase and finding a way to catalyze hydrogen dissociation at the surface of the liquid metal phase.
- Proposed future work of the project includes an investigation of alternate supports and molten metals as well as feasibility and permeability studies on SMMMs.
- Future plans build on early results and generally address overcoming barriers. The plan includes investigating alternate molten materials and supports, but needs to include continued work in fabrication methods, which is integral to the choice of and behavior of the materials and the support.

Strengths and weaknesses

Strengths

- The project investigator has extensive experience in fuel cells and hydrogen catalysis. He has developed the technique of supported molten-metal catalysis.
- The co-project investigator is a leading researcher in palladium and palladium alloy membranes.
- This is an novel, innovative project, but risky.
- The project's theoretical basis may justify the research associated with SMMMs for hydrogen separation.
- This project offers a different membrane approach with distinct operating advantages, if successful.

Weaknesses

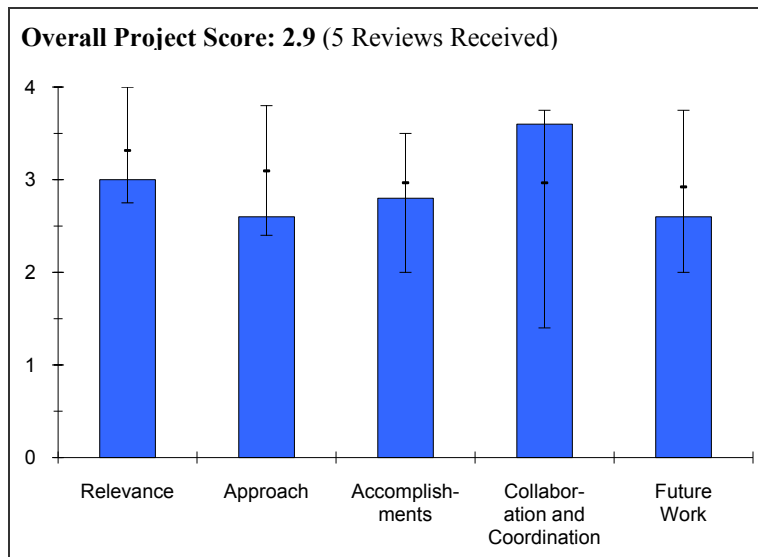
- No good plans to fabricate a durable SMMM were presented.
- The team needs an expert on metals and materials. The project may never work, but the lack of expertise makes it hard to tell if the problem is fundamental.
- This project is very high risk.
- An inert porous structure/material must be found that is wetted strongly by the molten metal. This is a requirement to the liquid metal being held in the pores (capillarity) at reasonable trans-membrane pressures. No evidence currently exists that a solution is possible.
- A molten metal that is permeable to hydrogen and chemically stable in the presence of reformat must be identified. The project is risky, and feasibility has not been established yet.
- A catalyst for dissociating hydrogen may be needed depending on properties of the molten metal phase. This catalyst needs to remain active when in the presence of the liquid metal phase and reformat. Again, no evidence has been presented that this is possible.
- The project does not demonstrate an approach of how to address the requirements of immobility and stability of the liquid molten metal membranes in the environment of a coal gasification plant. The team does not appear to have secured the expertise to address the challenges associated with operating a membrane unit in the industrial coal gasification plant.
- There are numerous technical and cost issues associated with this approach. Therefore, there is a low probability of success. It is worth pursuing at least to the point of showing that the idea is technically feasible, but that must include a demonstration of contaminant (e.g., sulfur) tolerance as well as flux and selectivity. This was not included in the plan.

Specific recommendations and additions or deletions to the work scope

- This project should be discontinued.
- The team needs an expert on metals and materials.
- This project must be significantly reorganized. The above technical challenges need to be addressed individually to establish a reason to believe the overall approach has technical merit.
- The question of a liquid (molten) metal wetting the porous support can be addressed easily and quickly by measuring the contact angle of a drop on the material in question. From the contact angle, one can calculate the capillary force within the support material's pore structure. If the bubble pressure is not at least 200 psi, success is unlikely.
- Hydrogen permeability of the molten metal phase can be experimentally probed, but the project investigator has some literature data and this should have been communicated. Specifically, the reported hydrogen permeability, if known, for tin should be communicated. The diffusivity/solubility is not reported.
- It is even easier to evaluate the chemical reactivity of candidate molten metal phases in reformat at the intended operating temperature.
- The probability of identifying suitable catalytic materials should not be overlooked. The feasibility to have discrete metal particles (probably not due to alloying with the molten metal phase) is unclear. Inorganic compounds might be considered rather than metals.
- It is recommended that the project add a partner from the industrial coal gasification community to understand the challenges associated with operating an industrial membrane unit.
- Develop a preliminary economic model and use it to conduct preliminary economics to guide the research.
- Continue to fund this project.

Project # PD-13: R&D Status for the Cu-Cl Thermochemical Cycle-2010*Michelle Lewis; Argonne National Laboratory***Brief Summary of Project**

The overall objective of this project is to develop a commercially viable process for producing hydrogen that meets DOE cost and efficiency targets using the copper-chloride thermochemical cycle. The features of copper-chloride thermochemical cycle that promote meeting targets and overcoming barriers are that: 1) the 550°C maximum temperature allows coupling with the solar power tower, which is near commercialization; 2) the conceptual design uses commercially practiced processes; 3) the high yields in thermal reactions mean that no catalysts are required; 4) preliminary Aspen flowsheet indicates it is possible to meet the efficiency and cost targets. Key challenges are to 1) inhibit copper crossover and achieve stable cell performance in the electrolyzer, 2) identify and cost materials of construction, and 3) reduce steam demand for hydrolyzer.

**Question 1: Relevance to overall DOE objectives**

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

- The copper-chloride thermochemical cycle remains one of the most promising approaches for large-scale water splitting that meets the DOE targets for hydrogen cost and efficiency.
- This project has a well-designed process for generation of hydrogen. Good attention has been paid to the impact of cost as well as design and material selection.
- The production of hydrogen fits in the DOE portfolio.
- This is a program to desirably supply "green" hydrogen via water splitting using a combination of thermal and electrical energy, with the latter preferably from renewable resources.
- The program proposes to utilize thermal energy to synthesize hydrogen.

Question 2: Approach to performing the research and development

This project was rated **2.6** on its approach.

- The primary focus should remain on potential showstoppers such as copper crossover in the electrolysis step.
- Copper crossover is a critical path. It is unclear whether anyone on the team calculated what level can be accepted and turned this level into a membrane specification.
- The project uses a good approach in systematically identifying weak sections of the technology and pursuing solutions for these issues.
- The electrolyzer is very inefficient. Even if the team hits their target voltage and current, the performance may not be substantially better than that of water electrolysis.
- The critical path is the electrolyzer development, which is where the majority of the team's effort should be focused.
- The voltage reduction targets (a decrease of 0.07 V in ten years) do not seem very aggressive.
- The chemicals being used are very aggressive, but minimal effort is discussed in the approach on to how the team will handle these materials.

HYDROGEN PRODUCTION AND DELIVERY

- The team is building a large-scale demonstration reactor before having identified proper materials. This does not seem logical.
- They are using the H2A project to identify operating conditions that are needed to meet their cost targets, which is good.
- The team uses two lab-demonstrated chemical transformations that are coupled with an electrochemical step and further processing to, in effect, split water. At the present 0.7 V for the electrolysis, the latter would consume at least one half of the overall needed energy. An apparently ongoing study of the inherent thermodynamics should allow an estimate of the minimum voltage for this electrolysis.
- The proposed chemistry, which uses a combination of hydrolysis and electrolysis, involves difficult processing conditions. Clearly, some excellent engineering design is required to make this successful. The approach did not address a solution to some very key issues. No mention of anticipated yields is provided. The concept of using a "solar power tower" obviously means that the process cannot operate at night and, thus, will be subject to periodic "on" and "off" cycles. The technical and financial implications of this operational mode were not addressed.

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

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

- The progress has been very good on improving the electrolysis performance, although there is still a substantial gap to reach the DOE target with a cell that exhibits a long operating lifetime.
- Very good progress has been made in moving towards integrating the individual systems.
- It is unclear why or how the team expects to find a membrane. The desired qualities of a membrane that could work are not stated. It appears that if a good membrane cannot be found, the process as described will not work.
- When asked about the current membrane status, the project investigator responded that Pennsylvania State University used a proprietary membrane that has worked 100 hours to date. While this is very encouraging, a minimum of 1,000 hours of durability is expected.
- The team shows modest improvement on the electrolysis. They need to demonstrate longer life at lower voltages, and they need to immediately test at the higher temperatures.
- The team is scaling up the chemical reactor now. This appears premature since they have not finished the benchtop reactor development.
- The team constantly refers to their H2A analysis, but it is not in the material. They are using the H2A to direct their work, which is very good. More projects should do this. They should have included the H2A analysis, perhaps in the supplemental section. In particular, inclusion of the electricity cost would be valuable. If they use grid electricity, many of the benefits of this project disappear, whereas if they use solar power, then it is unlikely they will meet the cost targets. Therefore, it would be interesting to see how they did this.
- The chemicals to be used are extremely aggressive, especially at the operation temperatures. They did not discuss any materials compatibility testing, though this is a very important area. It seems that the team should have done materials compatibility testing before constructing a large-scale demonstration.
- Excellent progress was made in the copper-chloride hydrolysis to Cu_2OCl_2 reaction and in the selective decomposition of the latter to oxygen and copper-chloride. However, many issues remain with the electrolysis step, and details were not well conveyed. Thus, it is not clear exactly what the actual membranes were. They should be chloride instead of chlorine carriers, and they should be anion- (i.e., Cl^-) instead of cation-exchange membranes as is written in the slides. Also, the catholyte and anolyte concentration steps are clearly a remaining challenge.
- The project seemed to be in early stages, and most of the results appear to be planning activities and organizational tasks.

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

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

- A great international team with highly relevant partners is identified.
- In the past, this project had poor collaboration with some of the partners. It seems they have remedied the situation.

- Excellent collaboration has been shown with the other cited laboratories. More input from Pennsylvania State University in detailing progress on the electrolysis would have been welcome.
- Argonne National Laboratory plans to outsource most of the work, much of which is to Canadian interests. The competency and qualifications of these organizations were not discussed.

Question 5: Approach to and relevance of proposed future research

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

- The membrane may be a key component to success. It would be useful to include a membrane development plan and how this piece of the system is expected to be improved to meet the critical challenge of reducing crossover.
- The future work listed by the team seems appropriate. More effort needs to be directed to the electrolyzer development.
- On slide 15, the team discussed the large-scale demonstration, but this is not mentioned on slide 16, which discusses future work. It seems premature for them to proceed with the large-scale demonstration when they have so many other critical issues to address.
- The proposed future work addresses most of the remaining issues.
- Some of the technical challenges were mentioned (e.g., copper crossover in the electrolysis step and management of hot, strongly acidic media), but the technical steps proposed to address them were not.

Strengths and weaknesses

Strengths

- The project involves good collaborations with competent partners such as Commissariat à l'Énergie Atomique (CEA) and universities. The focus should be on solving the problems that are potential showstoppers.
- The international team members bring a wealth of experience in the specialties relevant to making this program a success.
- This is an innovative process that appears to have a good probability of success.
- Good progress has been made at this point.
- A large team has been assembled.
- The remarkably selective chemical steps of the process, which are conducted without need of catalysis, is a strength.
- The strengths clearly must involve the people working on this activity. Unfortunately, the Canadian technical and intellectual resources were not discussed.

Weaknesses

- The use of unusual process conditions and equipment (e.g., the ultrasonic nozzle and sub-atmospheric pressure for the hydrolysis reaction) could limit the ultimate practicality of the cycle.
- Since little was presented on the membrane, by default, this is the weakest link. It is not known which properties of a membrane are critical. For example, it is unclear whether only a custom membrane will work. In addition, the level of difficulty of making this custom membrane for a commercial process is unknown.
- The approach does not seem logical. For example, the team reports having large-scale reactors to perform the testing, but they say that in their future work they will identify compatible materials. It would make more sense to identify compatible materials and then build large-scale demonstrations.
- The copper-chloride electrolysis is very inefficient. It is not clear how this system would be superior to high-temperature electrolysis.
- The team has made some limited progress on electrolyzer life testing, but they need to be testing for thousands of hours as opposed to a couple of hours.
- The team correctly identified corrosion as a significant problem, yet they did not report any work in that area. They need to do some corrosion testing since this is a large gap in the project.
- The team needs to get thermodynamic data for all three steps of the cycle. Specifically, this data is needed for the optimization of each and for estimating the true potential maximum energy efficiency of the process.
- More transparency is needed on the electrochemical step, including details and discussion.

HYDROGEN PRODUCTION AND DELIVERY

- Although the program seemed new and just becoming focused, the plan for making necessary progress was inadequate.

Specific recommendations and additions or deletions to the work scope

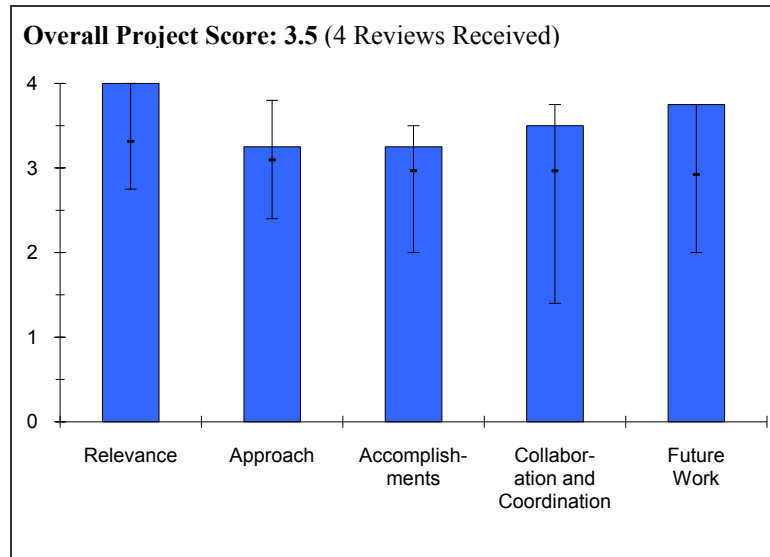
- The project needs more membrane work on lifetime, characterization under high acid concentrations, development of membrane cost models, and a back-up plan if the membrane does not work as expected.
- The team needs to identify a critical path to success and follow it. Critical areas include electrolyzer development, reactor optimization, and materials. Once these are addressed, then they should consider scaling up.
- The team needs to address the corrosion issue. If they cannot find any materials that have a reasonable life under the operating conditions, then there is no point in continuing this research. However, they did not report any work in that area. It should not be the main focus of their work, but they should be looking at it in parallel. Perhaps instead of scaling up the reactor, they could do some materials testing.
- These "thermochemical" processes have been around for decades. This project needs to address the key technical issues, which are copper crossover and material design, and work those tasks before a "system" is built. A "go/no-go" milestone written around the electrolyzer would be a good addition.

Project # PD-14: Hydrogen Delivery Infrastructure Analysis*Marianne Mintz; Argonne National Laboratory***Brief Summary of Project**

The objectives of this project are to 1) provide a platform for comparing alternative component, subsystem and system options to reduce the cost of hydrogen delivery; 2) analyze delivery options (e.g., wind-to-liquid hydrogen); and 3) develop new tools that build off existing DOE-sponsored tools (e.g., the H2A project, with a focus on production; Fuel Cell Power Model; and the Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation Model [GREET]).

Question 1: Relevance to overall DOE objectives

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



- Although DOE focuses on future large-scale stations, it is important to not forget that in the near to intermediate term, the implemented stations will be much smaller. This must be dealt with first. The cost of dispensed hydrogen if multiple stations use the same design should be investigated instead of funding and building multiple "unique" station designs.
- The topic is very relevant to research and development objectives because it helps define future funding priorities within DOE. As far as immediate relevance for near-term costs, it is less so.
- This project is necessary to explore the costs of options for hydrogen delivery. This allows the Delivery Team to focus on high-cost items to target research.
- This project is very important to assessing the hydrogen delivery infrastructure, and it supports the DOE research, development, and deployment objectives.

Question 2: Approach to performing the research and development

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

- More actual data from industry and current projects can always improve models like this, especially when it relates to the verification of underlying assumptions.
- This project provides a good framework from which to analyze tradeoffs, but more description of uncertainty is needed. More information on the uncertain processes or technologies that make a large difference in final cost and why this occurs would be helpful. For example, the level of confidence in the team's cost estimations would be helpful if construction of infrastructure began today. Expert opinions on which aspects are most subject to change would be useful. Information on the ramifications on the future direction of research is requested, though perhaps this in the main report and not contained in the presentation.
- A stronger tie-in with current technology costs for comparison could be provided. Information on how to bridge the gap from now until a final state and how to phase this in may be helpful. Also, a little more comparison to costs for onsite SMR should be included. Again, this information may be contained in the full report, and the presentation was simply too time-constrained to go into detail. Overall, the approach seems sound.
- A great approach and interaction with stakeholders to get accurate input is presented.
- The approach of developing a flexible, user-friendly spreadsheet-based tool will be beneficial for the industry to utilize and analyze various strategies. It would be useful to have further information regarding the validation of

HYDROGEN PRODUCTION AND DELIVERY

the assumptions in the tool. The approach for the fuel station footprint needs to be further explained regarding the actual constraints and options.

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

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

- Input from gasoline station owners is urgently needed on station footprint feasibility since future hydrogen stations and equipment will most likely be added to or replace existing gasoline stations.
- The team presented very interesting work on the tradeoffs for cold gas pathway. The team demonstrated a more realistic station footprint. Version 2.2 of the H2A Delivery Scenario Analysis Model (HDSAM) was posted.
- The team provided good accomplishments and sharing of the technology and model.
- The HDSAM updates and the cold gas pathway are useful progress items. The fuel station footprint and wind-to-liquid hydrogen are only at the beginning stages and need further development.

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

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

- A good referral to other organizations with whom the project participants work was provided.
- Other national laboratories and DOE are involved with the project, which shows good collaboration.
- Good collaboration is demonstrated with other partners, but perhaps a bit more emphasis on their individual contributions should be given in the presentation. The project provided great acknowledgement on industry input toward station design.
- The collaboration with the other national laboratories is appropriate. It may be useful to have some collaboration with an energy company.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.8** for proposed future work.

- The team should not get wrapped up in exploring all potential options, especially when current pathways can be strengthened.
- The renewable hydrogen pathway analysis mentioned is very important. The costs for renewable hydrogen are not well understood and they show great variability. Determining these costs may be very important in influencing policy and decision making.
- Great plans for future work are presented.
- The future work with corresponding projected dates appears to be focused and builds on the past progress.

Strengths and weaknesses

Strengths

- This project includes many of the variables that are involved with getting hydrogen to the vehicle users.
- This project provides overarching direction and good framework for future research and development. Having easily changeable values that accommodate different input assumptions is also a strength of the model.
- The model provides the best assessment to focus research.

Weaknesses

- The project looks far into the future, and the further out, the more uncertain the reality of the specific pathway becomes.
- The project should include realistic footprints. Distances can generally be minimized by adding specific solutions and measures to the station (e.g., fire walls).
- Relevance to near-term costs could be a little more explicit. For example, information on how the model results guide next steps would be useful.
- The project needs industry input to calibrate models.

Specific recommendations and additions or deletions to the work scope

- Information is requested on how much additional use of unused capacity of hydrogen stations can bring the cost down.
- A slightly more explicit comparison (although some is already given) to onsite SMR costs would help frame the results. This would be especially useful going forward with regard to the renewable option. One of the discussed pathways for renewables is distributed natural gas production from renewable sources and renewable credits being given for SMR hydrogen production at the other end. The reviewer is unsure if this is beyond the scope of the project since this would really be natural gas production and delivery rather than hydrogen. A good understanding of these costs would still be helpful in order to compare to other scenarios such as wind or solar to hydrogen.
- The reviewer recommends including sensitivity analysis results as well as some explanation and/or validation assessment of assumptions.

Project # PD-15: H2A Delivery Analysis and H2A Delivery Components Model

Olga Sozinova; National Renewable Energy Laboratory

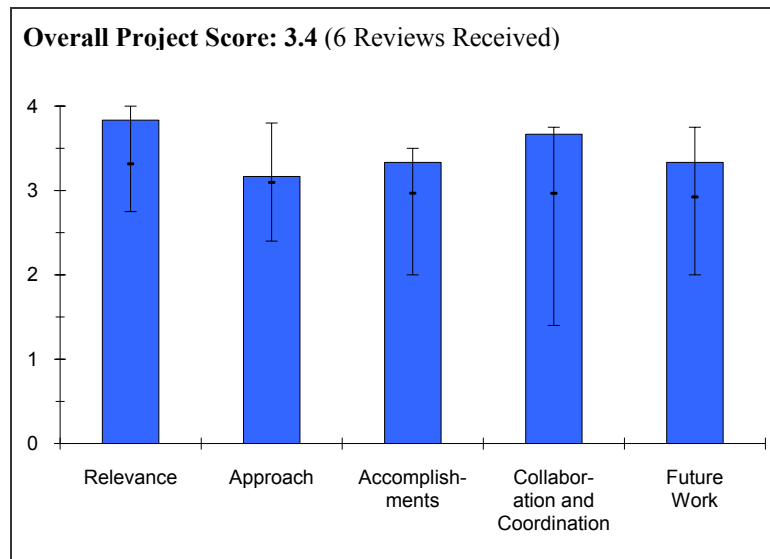
Brief Summary of Project

The objectives of this project are to 1) update and maintain the H2A Delivery Components Model, 2) provide a cost analysis on hydrogen delivery infrastructure, 3) support other models and analysis that include delivery costs, and 4) expand the H2A Components Model by designing new components.

Question 1: Relevance to overall DOE objectives

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

- The team should make sure to continue the verification process with industry as it will be an enormous undertaking for a company to implement a wind-to-hydrogen project and transport it by rail over a distance greater than 1,500 km.
- This project is relevant and provides valuable information on pathways for hydrogen delivery. The addition of a railcar and renewable pathway is extremely important for future infrastructure growth analysis.
- The approach, as outlined in the "Approach" slide in the presentation, outlines the main relevance of the work. It is necessary to maintain commonality to provide a basis for all models using hydrogen costs.
- The modeling work for components allows the delivery team and others to focus on the greatest cost issues.
- The project is highly relevant to the overall delivery objectives as it concerns analysis of delivery costs. This project's outcomes are also coupled to the other cost analysis tools, in particular production and scenario-based models.
- The H2A model aligns with the DOE research, development, and deployment objectives and is an important tool for assessing the hydrogen delivery infrastructure.



Question 2: Approach to performing the research and development

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

- It appears that most aspects/variables are evaluated and included based on industry input.
- The project has good potential to feed information to the H2A model but should also develop simple-to-read, detailed summaries for industry to expand information on preferred pathways to economical delivery.
- Again, the approach seems sound. However, a disconnect appears to exist between the objectives and the approach. Maybe the approach is simply a guideline for the project and all the objectives are guided by that approach. Also, the title of the presentation is "H2A Delivery Analysis and H2A Delivery Components Model," but, in slide 9, no explicit indication of where "Delivery Analysis" fits in is shown. The reviewer is unsure if the delivery analysis was conducted using the Scenario Evaluation, Regionalization and Analysis (SERA) model.
- This project uses a very good approach that allows flexibility in configuration and evaluation.
- Details relating to the unique aspects of this project were lacking in the presentation. However, it was clear that the general objectives and intended outcomes of the modeling effort were well-established. This model also appeared to be highly flexible and capable of interacting with other related H2A (production) and HDSAM models, and the results from this H2A delivery model feed into more detailed analyses which can, for example, provide spatially and temporally variant information.
- The approach of the project of collaborating with the industry to develop the cost input is very good.

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

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

- Make sure to report transportation distances in miles, not kilometers. Even though it may make more sense to use kilometers, industry uses miles.
- Excellent progress was made on updating the H2A delivery components.
- Significant progress has been made, but some questions remain about the SERA model. When looking at the map of pipelines, several seem to go straight through mountain ranges. Therefore, adding some realism based on natural gas pipeline locations and distances would be valuable. It appears this information is available based on slide 29. If the simplified map as shown is used, then perhaps a case study would aid in determining the uncertainty of costs.
- Very good accomplishments have been made to date. The reviewer is not certain if that much emphasis should be spent on rail analysis.
- The upgrades to the refueling stations in terms of dispensing pressure (to 700 bar), as well as inclusion of multiple dispensing options, clearly broaden the scope and relevance of the resulting cost data. While research aimed at understanding the impact of station footprint on cost was useful and appeared to be significant, this information seems like it could have been garnered via more cursory sensitivity analyses rather than the more detailed perspective that was taken.
- The studies related to rail as a delivery method, particularly for long distance transport, appear to be very interesting. The only criticism of the model is its static nature, which does not currently handle economies of scale with respect to component cost. One would imagine that low- versus high-volume component cost should be very different and should impact this analysis.

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

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

- The team is collaborating with an impressive group of companies on this project. Railcar vehicle builders should be included as well, due to potential challenges with developing and building code-compliant railcars with compressed composite hydrogen storage.
- Excellent partners are listed, but the team should try to incorporate more current hydrogen suppliers and state governments working with industry.
- This project is highly integrated and requires tight collaboration with other institutions.
- Good collaboration with others and industry is presented. The team should consider input on rail viability and costs from ethanol producers and their industry associations.
- This project relies heavily on interacting with multiple developers and specialists to obtain reliable input information. The investigators appear to be very proactive in seeking out the correct institutions for this information (e.g., talking with railroad entities for the rail analysis). Additionally, the highly interactive nature of this H2A delivery cost model with other related cost models (e.g., production and HDSAM) was made evident and appears to be in place.
- The collaboration effort appears to be highly coordinated with this project.

Question 5: Approach to and relevance of proposed future research

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

- Make sure to consider fueling and defueling times of hydrogen transported by rail and potential related challenges for compressed hydrogen.
- A “go/no-go” decision on natural gas pipeline delivery is excellent since there is no need to waste resources if the pathway leads to a dead end. It is important to include buildup of hydrogen from wind scenarios.. Additional information on emissions is critical. Perhaps some help from Argonne National Laboratory could be incorporated.
- Future work seems appropriate and in line with the approach and objectives.
- Good plans are presented for the future.

HYDROGEN PRODUCTION AND DELIVERY

- The future work clearly builds on progress and is appropriately tasked toward refining previous "mature" delivery components as well as expanding into new directions in terms of delivery options (i.e., hydrogen from wind).

Strengths and weaknesses

Strengths

- The project is very inclusive.
- Railcar delivery is very important, and the reviewer is glad to see it included. The project provides good industry values on delivery that assist with analysis.
- This project is important because it maintains commonality with other models.
- The model allows the costs that are first addressed to be those that most greatly affect the overall costs of hydrogen delivery.
- This project is comprised of a very competent team capable of analyzing diverse delivery pathways. The team is able to quickly modify the model to efficiently make delivery cost comparisons.

Weaknesses

- It is not clear what the current baseline is for hydrogen delivered cost.
- The project has some low volume delivery pathways that should be dropped since these are short term. The 100 kg station information is not currently relevant and should be wrapped up so the focus can be on the larger stations.
- The project seems to be a bit disjointed from the way it was presented. It is unclear whether the main purpose of this work is to maintain the components and delivery costs or to develop new models such as SERA. Some background information would be helpful.
- The model needs accurate and representative data for calibration and good predictions.

Specific recommendations and additions or deletions to the work scope

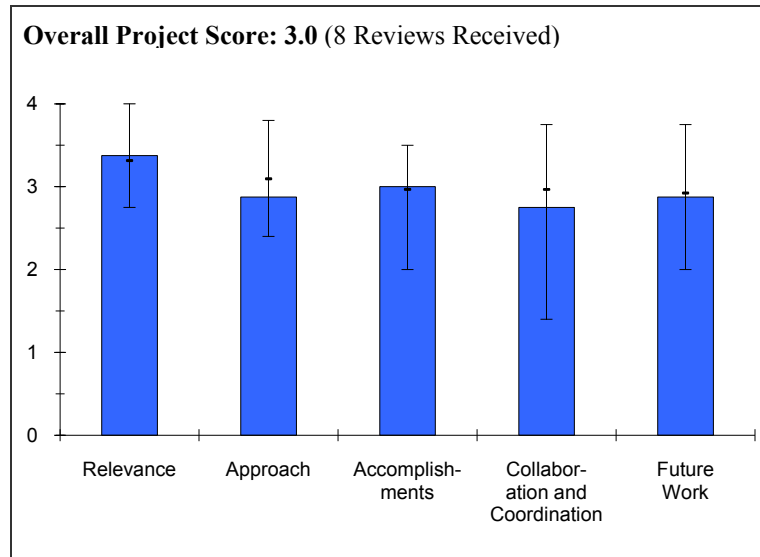
- The current baseline of hydrogen cost and improvement over last five years should be added.
- Continue with the detailed analysis of the railcar delivery. Renewable delivery is critical for California and should be examined in detail for specific station pathways in the Los Angeles and San Francisco Bay areas.
- The team should run the model at multiple assumed component volumes to get some sensitivity of the extent of delivery infrastructure versus component cost.

Project # PD-16: Oil-Free Centrifugal Hydrogen Compression Technology Demonstration*Hooshang Heshmat; Mohawk Innovative Technologies***Brief Summary of Project**

The objective of this project is to demonstrate key technologies needed to develop reliable and cost-effective centrifugal compressors for hydrogen transport and delivery, including 1) flow of 500,000 to 1,000,000 kg/day; 2) pressure rise to 300-500 psig up to 1,200-1,500 psig; and 3) contaminant-free and oil-free hydrogen.

Question 1: Relevance to overall DOE objectives

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



- The reduction of hydrogen cost per kilogram at the production plant is best for current technology improvement, since the production plant is where the majority of hydrogen production will occur for the foreseeable future.
- Pipeline delivery would be the long-term low-cost supply option and will require compressors for pipeline transportation.
- This is an excellent engineering project. The reviewer is not sure it supports mid-term goals, but believes it is very relevant in long-term goals. The project may be at too early of a stage for a decision on mid-term delivery methods.
- This project is very relevant to the hydrogen delivery arena. Compressor costs at the terminal/plant can have a significant impact on hydrogen delivery cost.
- This project supports DOE Hydrogen Program's effort to advance hydrogen compression from central production for pipeline transportation, as long as research and development is being supported in other areas of central production and delivery of the hydrogen to the pump (e.g., central production, pipeline, and storage and dispensing).
- Centrifugal compressors are a vital enabling technology for hydrogen pipelines and would lower forecourt costs as well.
- Oil-free compression leading to contaminant-free and oil-free hydrogen is a major step in the direction necessary for fuels from hydrogen to work.
- This project could be more relevant if it also developed compression for dispensing at 6,250 psi and/or 12,500 psi.
- The project target was clearly explained, but additional linkage of targets to the overall DOE research, development, and deployment objectives would be useful.

Question 2: Approach to performing the research and development

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

- It is unclear whether input was obtained from hydrogen plant operators. If not, communication with engineers at a plant that operates with current hydrogen compression equipment would be helpful. Often compressors are cause of plant shutdowns if they break down, resulting in several millions of dollars in revenue lost per day of non-operation.
- The team incorporated an excellent use of computational fluid dynamics (CFD) and finite element analysis in design prior to constructing test rig.

HYDROGEN PRODUCTION AND DELIVERY

- The project does not appear to be integrated with other efforts. Technical barriers are being addressed and have yielded some results, but work needs to continue to address further barriers.
- A focus on technology development and new concepts is the right approach for development of ultra-high capacity hydrogen compressors under these conditions since existing capabilities are limited.
- The approach is fairly comprehensive and very representative of how typical development happens in the large compressor industry.
- Testing of a single compressor stage is key to validate the success of theory.
- Design development tied to manufacturability is key to successful manufacturing of the technology.
- The approach addresses materials, design, modeling and simulation, and fabrication/manufacturing. The project team should consider looking at Design for Manufacturing and Assembly early in the design.
- The design work has proceeded well.
- Mohawk Innovative Technology, Inc. (MITI) is carrying out all aspects of design, including CFD and mechanical stability.
- Flexibility in drive (electric or turbine) is a plus.
- Foil bearings and seals are the key to this project. It is unclear whether work has been for hydrogen compression or other scenarios. The presenter mentioned that the work is from NASA's Space Shuttle Main Engine work with liquids, which raises questions on how well they are working with gas and what issues have arisen.
- Materials are believed to be the critical initial design component. More work and discussion of the materials issues would be helpful. There was much discussion of stresses but little information about embrittlement and hydrogen loss due to leaks.
- Compressors may not be run at a constant rate as the design requires. Further work to deal with turn-up and turn-down is necessary.
- The approach should be expanded to the complete compressor including the gearbox assessment.

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

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

- It is unclear why within a 15-year durability target this equipment would be rated for 30,000 start and stops, as stated during the presentation project. This would translate in close to 5.5 starts and stops daily, though none of the pipeline-connected hydrogen production plants shut down this many times.
- Model projections look promising to meet or exceed DOE targets with an opportunity to demonstrate in a test rig this year.
- Good progress has been made on overall design of the compressor, including stage selection and other compressor parameters.
- Good progress has been made on numerical and CFD design of impellers and stress criteria.
- A very solid approach is used to design and manufacturing, with progress on track.
- The project seems to progress down the front-end design work. However, the project needs to proceed to on-stream testing of the design concept to determine strengths and weaknesses in the design and to show how this design differentiates from other competing DOE-funded projects in this area. This will help DOE downselect the "winning" design.
- The design and CFD work in 2010 clears the way for prototype construction.
- Good progress was made in materials selection.
- Only preliminary testing has taken place to date. The reviewer is concerned about the long life requirements of pipeline delivery and the testing necessary for such. The design incorporates these issues but not enough information was provided to warrant sufficient durability.
- More work should be done on hydrogen embrittlement and the potential related issues.

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

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

- It is unclear whether or not input was obtained from hydrogen plant operators. If not, communication with engineers at a plant that operates with current hydrogen compression equipment would be helpful. Often

compressors are the cause of plant shutdowns if they break down, resulting in several millions of dollars in revenue lost per day of non-operation.

- The presentation did not reflect input from entities besides DOE, MITI, and two consultants. It was unclear if any input was received from national laboratory material scientists on potential challenges.
- A small list of partners was provided, but they appear to have the experience necessary to execute design and testing.
- There appears to be very little collaboration or coordination among organizations.
- Mitsubishi Heavy Industries (MHI) and MITI are the right partners for this approach given that– they are the technology leaders in this industry.
- Good work was achieved with MHI. The team should consider consulting with a metallurgist with expertise in the hydrogen embrittlement area to review the design and selection of wetted parts.
- Collaboration with MHI (or equivalent) is essential to move this technology toward commercialization.
- The companies necessary to produce and sell these compressors are involved and coordinated.

Question 5: Approach to and relevance of proposed future research

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

- Data from single-stage device tests will demonstrate whether or not all of the efforts and calculations were correct.
- Reducing the design to practice with single-stage performance testing will be a large step in this year's plan.
- Single-stage testing is critical to validation of the approach.
- Economic estimate updates will help the program determine feasibility of this approach.
- The team needs to get to proof-of-concept testing on a full compressor system.
- Construction and operation of a prototype and completion of an economic analysis will be critical.
- The team is at the point where testing is appropriate and is the major priority for future work. More information on the testing plans would have been useful. Most concern lies with the durability of the compressor as a system.

Strengths and weaknesses

Strengths

- This project appears to cover all variables.
- The novel design used in this project is promising.
- No oil is used in this project.
- The project's projected low cost and small footprint are strengths.
- This project provides good engineering analysis of a compressor design.
- An excellent technical team and approach are used in this project.
- Solid design and analysis is combined with MITI and MHI's expertise in compressor and bearing technology.
- Near-term applications in chemical and refining industries provide a "market pull" independent of hydrogen-powered transportation.
- It is important to the program's objectives to develop efficient, contaminant-free compressors.

Weaknesses

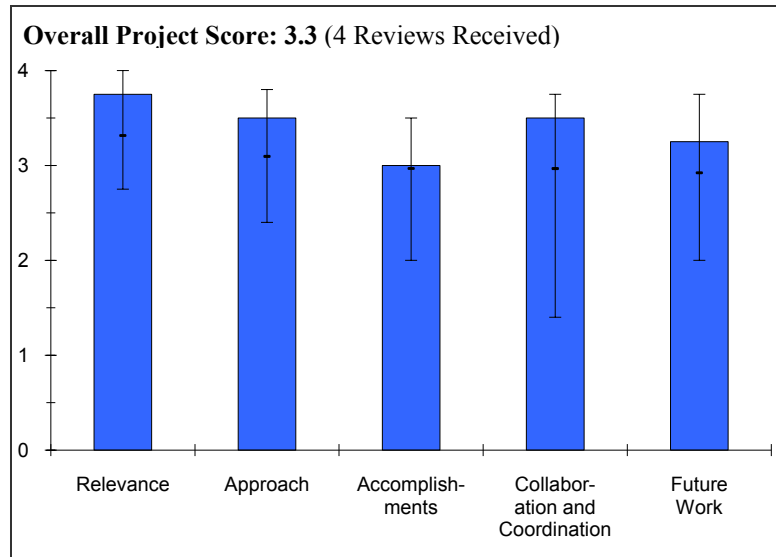
- No (single-stage) system testing data is provided.
- The presentation gave very optimistic numbers compared to DOE targets.
- The project funding is high for results provided so far. The project should be further along, and a single-stage compressor should be in the manufacturing stage. The team needs to account for two years and \$1.5 million.
- No significant weaknesses were determined.
- The design is for constant use with little turndown. The reviewer is doubtful that this service will be available within the next 20 years, so further work on turndown is necessary.
- Further testing on materials is necessary. The reviewer has low confidence that the foil bearings and seals will be as leak-free as the project investigator indicates.

Specific recommendations and additions or deletions to the work scope

- The project should add a benchmark compressor (rated for same throughput) set up to compare cost, durability, reliability, maintenance, and efficiency numbers, even if the new compressor design has not been tested.
- A production rate of 200,000 kg/ day is a long-term need. The team should consider feedback from the analysis group for pipeline compression requirements in the transition phase. They may be able to coordinate scale-up of the equipment with transition requirements.
- The scope is appropriate, but more testing and an expedited move to actual building of a single-stage compressor would be preferred.
- The team should work on compressor technologies that do not need consistent service.
- Further testing on materials is needed.
- The team needs to include the reliability and robustness assessment of the design versus existing technologies.

Project # PD-17: Development of a Centrifugal Hydrogen Pipeline Gas Compressor*Frank Di Bella; Concepts NREC***Brief Summary of Project**

The overall objective of this project is to demonstrate an advanced centrifugal compressor system for high-pressure hydrogen pipeline transport to support DOE's Strategic Hydrogen Economy Infrastructure Plan. Objectives are to 1) deliver 1,200+ psig and 100,000 to 1,000,000 kg/day of pure hydrogen to a forecourt station at less than \$1/gge; 2) reduce initial installed system equipment cost to less than \$5.4 million uninstalled based on DOE's HDSAM 2.0 Economics Model, which is a component of the H2A project; 3) reduce operating and maintenance costs via improved reliability; and 4) reduce the system footprint.

**Question 1: Relevance to overall DOE objectives**

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

- Pipeline compressors will be required for the projected low-cost long term-pipeline delivery option.
- The pipeline compressor can provide a critical component to the long-term success of the hydrogen infrastructure, and this project provides a key piece of development to the process.
- Compression cost is one of the key barriers preventing cost-effective delivery of compressed hydrogen for fuel cell vehicles. This project, along with the project conducted by MHI, are critical to reduce the high cost of compression.

Question 2: Approach to performing the research and development

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

- A phased program approach and use of state-of-the-art and acceptable engineering practices reduces risk during development.
- The team established a sound approach to project barriers, and it appears the project will address all issues associated with pipeline compressors.
- The project has a good approach, using various outside experts to provide the key component technology. The reviewer has concerns about the assumption of hydrogen contamination by the outside seal vendor. The team should consider a demonstration of this contamination level.

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

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

- Passing the “go/no-go” decision on December 9, 2010, is an accomplishment for the team.
- Accomplishments to date show good results towards DOE goals. The material selection method is good; however, more analysis is needed on the embrittlement and stress factors at tip speed.
- Good progress has been made on reaching project objectives.

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

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

- An excellent mix of industry, academic, and national laboratory partners is established for this project.
- Collaborations are solid and appear to be appropriate.
- Good collaboration is demonstrated with outside compressor vendors. Detailed input from university partners would have been appreciated to see how they contribute.

Question 5: Approach to and relevance of proposed future research

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

- A complete detailed cost analysis is included to confirm the low \$4.5 million compressor package cost.
- The amount of future project work and the timeline appear to be a challenge. It will be a difficult task to complete design, component procurement, and testing within a year. DOE should ensure they are on target.
- Good plans are provided for the next step of assembly and testing of detailed designs.

Strengths and weaknesses

Strengths

- Identification of commercially available components and multiple suppliers has been done.
- The project appears to have reliable results and should achieve most DOE targets.
- The project will prepare an effective centrifugal design and demonstration for large-scale hydrogen compression.

Weaknesses

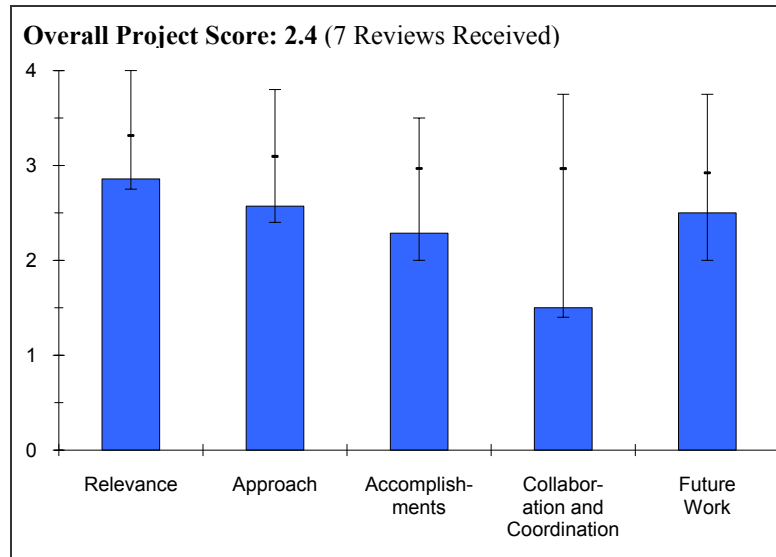
- The overall vision for the industry is not presented well. The goal of achieving 1,000,000 kg/day is not clearly defined.
- This project relies on assumptions of performance by collaborators in this project.

Specific recommendations and additions or deletions to the work scope

- The team should consider increasing the number of stages and lower the tip speed if the cost is determined within reason.

Project # PD-18: Advanced Hydrogen Liquefaction Process*Joe Schwartz; Praxair***Brief Summary of Project**

The overall objective of this project is to develop a low-cost hydrogen liquefaction system for 30 and 300 tons/day that meets or exceeds DOE targets for 2012. Objectives are to 1) improve liquefaction energy efficiency, 2) reduce liquefier capital cost, 3) integrate improved process equipment, 4) continue ortho-para conversion process development, 5) integrate improved ortho-para conversion process, and 6) develop an optimized new liquefaction process based on new equipment and new ortho-para conversion process. Goals for Phase II include 1) process development to establish performance targets for process equipment and ortho-para conversion and 2) development of a preliminary capital cost estimate.

**Question 1: Relevance to overall DOE objectives**

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

- This is a very relevant project since liquid hydrogen is especially important to keep early hydrogen infrastructure equipment design as simple as possible and to capital cost down.
- Any improvement in the efficiency and cost of liquid hydrogen production will benefit dispensed hydrogen cost per kilogram in early stages. This is especially true because, at lower delivery quantities, liquid hydrogen is very expensive due to the limited number of liquid hydrogen production facilities. The distance the customer is from a liquid hydrogen production point significantly influences the cost of 1,000 scf delivered.
- Liquefaction supports the transition cost goals, but not long-term hydrogen cost goals.
- Improved efficiencies are an important part of developing hydrogen pathways; however, this only partially supports the goals and objectives of the Hydrogen Program. These challenges may be addressed by individual companies and not necessarily DOE.
- Liquefaction is very relevant to mid-term hydrogen infrastructure deployment, and the cost of liquefaction is key to the success of this approach.
- Praxair, Inc. already employs hydrogen liquefaction as part of its commercial business. Thus, it has a vested interest, for its own business purposes, to improve the efficiency of hydrogen liquefaction. This project could then be seen as government support of hydrogen liquefaction business development. The project investigator stated that this approach will find "limited application in a potential hydrogen economy..." The reviewer would add "...as it pertains to the specific DOE Hydrogen Program objectives," because it may be a different story elsewhere.
- The project's goal to reduce energy and the cost of liquefaction has a direct impact on delivered hydrogen cost reduction.
- Given that hydrogen liquefaction is becoming increasingly important and relevant as a potential delivery option, this project's scope supports the overall DOE effort. In particular, efforts to achieve the delivery cost and efficiency are core to this project's principle objective of developing a new liquefaction system.

Question 2: Approach to performing the research and development

This project was rated **2.6** on its approach.

- Software modeling may be very valuable for future efforts, development theories, and knowledge pertaining to ortho-para conversion.
- The team has a good approach to build on previous success with Edison Material Technology Center (EMTEC) funding.
- No details are provided on ortho-para conversion experimental work.
- The approach is not clearly defined and the results to date are not clearly stated. The project does not appear to be on track to overcome specific barriers of high energy use for liquefaction. Instead, only incremental improvement has been made.
- This project's approach is fair and is comprised of a combination of modeling and prototype concept testing.
- Praxair's expertise in liquid hydrogen should help in a successful development and delivery of this concept. They are among the experts in the gas liquefaction field; hence, it is assumed they know what they are doing.
- The project has a good approach to use an idea to reduce the energy requirement for ortho-para conversion. The team should review and cite any new literature and research on ortho-para conversion technology developments.
- It is clear that this project builds on work and results from a previous short-term study (EMTEC-funded). At the broadest level, this project focuses on expansion of that program to investigate similar liquefaction processes that involve minimization of the effects of ortho-para conversion during liquefaction. Beyond that, it is unclear what the specific technical approach is since it appears to be proprietary. The programmatic approach, which includes process design and optimization, equipment evaluation, and demonstration, is appropriate.

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

This project was rated **2.3** based on accomplishments.

- The “go/no-go” indicators for efforts on this topic are not clear. From a cost perspective, it may not be worthwhile to continue efforts in this area at some point in the future because, for example, pipeline implementation may outdo this technology when passing 100,000 kg/day production.
- DOE has performance indicators for large-scale liquefaction (300,000 kg/day of hydrogen), but there are no installations in the United States of that scale for liquid hydrogen production. According to the presenter, 30,000 kg/day of liquid hydrogen is the largest existing production volume in the nation. A pipeline as an alternative option may be a better alternative from a cost, efficiency, and environmental perspective.
- The model ortho-para conversion was delivered to DOE but was not included in the presentation.
- The addition of ortho-para to the simulation program is an improvement in the state-of-the-art of modeling.
- Currently could achieve 75% efficiency (11 kW/kg 2012 target), but the reviewer does not expect to be able to get to 85% efficiency (6 kW/kg 2017 target).
- The technical progress is difficult to determine. Model development has shown modest progress with the ortho-para additions to the model.
- The team needs to show the current projections and status of this approach against the DOE targets. None of those was mentioned in the slide package.
- Good progress on ortho-para conversion reduction was documented. The team needs to mention exact numbers on efficiency with the new conversion approach.
- Fair progress on thermodynamic model was made, but it is still hard to determine the exact technology status.
- The project investigator was unable to provide cost figures for current or projected hydrogen liquefaction production, though they must know how much it costs to do the hydrogen gas-to-liquid conversion. Also, DOE targets for 2010 should be given in dollar units.
- The cost of liquefaction may not be important for the Praxair liquid hydrogen business, but it is critical for this DOE Hydrogen Program mission.
- Good accomplishments have been made since the 2009 review.
- The results of modeling efforts were vague (because of proprietary nature), but certain processes appeared to show promise for meeting the efficiency targets. No information on the cost of this process was currently given, but this was listed as future work. Progress on constructing and demonstrating large and small test fixtures were evident, but data from the testing of these prototypes was absent.

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

This project was rated **1.5** for technology transfer and collaboration.

- The team should collaborate with a national laboratory to establish, verify, or evaluate current theories related to liquid hydrogen production and ortho-para conversion, even if this data is not shared with the public. If DOE funds this effort, the numbers should be verified as opposed to Praxair stating that they have the knowledge in house to complete all facets of this program. Alternatively, the process that they use in house can be shown to verify their efficiency and cost numbers. This would provide some sort of process that resembles an independent review. This also follows on the responses given to one of the 2009 reviewer comments.
- No collaboration is demonstrated.
- No collaboration or coordination with other organizations was shown.
- The team needs to have collaboration for verification of existing developments as well as to create more ideas and progress on future developments.
- Collaboration was only with the thermodynamics software provider who was not cited.
- No collaborations were evident. The response to this reoccurring issue, which was given in a supplemental document, was that they are "qualified to complete all facets of the proposed program." While this may be true in some respects, at a minimum, the outcomes of this project should be shared and information exchanged with other relevant projects. External validation of data is also an important part of research and development.
- Part of the spirit of DOE-funded research opportunities is to collaborate with the scientific and engineering community.

Question 5: Approach to and relevance of proposed future research

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

- From the presentation and indications from the presenter, it appears that many unknowns exist about current technology numbers, in particular efficiencies numbers. Benchmarks for or to clarification of these numbers would be helpful for both Praxair and DOE.
- Optimizing the ortho-para conversion process will lead to improved efficiency.
- Future work may provide some insight into future process development. However, it will not address critical barriers or provide large efficiency improvements.
- Many achievements must be made for this project to be successful. The current status is not clear.
- Good plans are provided for future work, including the process design of improved liquefaction.
- The future work seems consistent with the objectives and are logical next steps of the current work.

Strengths and weaknesses**Strengths**

- Liquid hydrogen is currently the highest density delivery option.
- Modeling numbers suggest good potential for this process.
- A knowledgeable industry leader is working on a project, and they likely know best. The project does have potential to reduce energy use in liquefaction by optimizing process.
- No significant strengths were identified apart from Praxair's extensive experience in hydrogen liquefaction.
- Praxair is the leading expert in the business of providing commercial quantities of liquid hydrogen.
- The project team hopes to deliver a more energy-efficient process for liquid hydrogen.
- This competent team is focused on a very relevant topic.

Weaknesses

- Verification process of efficiency numbers is lacking.
- No clear comparison of benefits was provided for alternative production and delivery methods for hydrogen.
- The project leader has not shown potential for large efficiency gains, which are necessary for future hydrogen pathways. The information provided was limited since it was presented at a very high level and lacking detail.
- The project showed a very poor execution and reporting on DOE targets.

HYDROGEN PRODUCTION AND DELIVERY

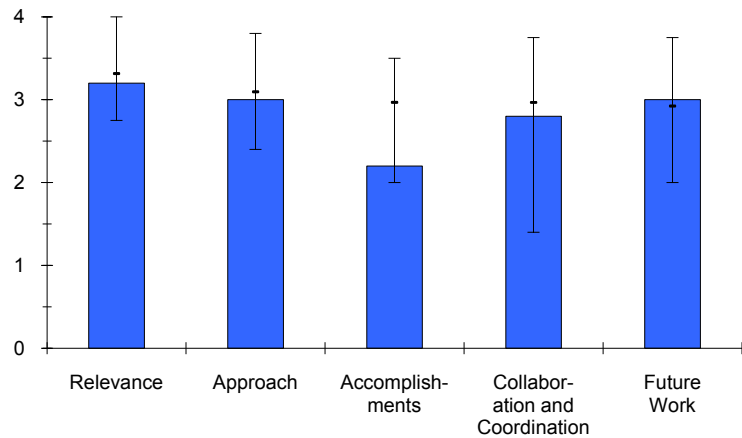
- Due to cost considerations, this project cannot meet the objectives of this DOE EERE mission.
- Technical details of process design improvements are not disclosed to reviewers.
- This project is difficult to review given the very vague descriptions that lack detail. The team is not collaborating.

Specific recommendations and additions or deletions to the work scope

- Clarification of the verification process is needed.
- If possible, add benchmarks with current technology used for liquid hydrogen production.
- Report future work on estimated capital cost as it compares to the DOE target and expected efficiency improvements.
- Clearly outline how the project will improve the liquefaction efficiency. State the status of the industry, and demonstrate how this project will improve industry. For example, if the industry average for liquefaction energy use is 12 kWh/kg, explain that this project has the potential to reduce energy use to 9 kWh/kg. If the project has little ability to reduce energy efficiency, then the project should focus on cost reductions of equipment, which is part of Phase III.
- DOE needs to pursue execution of this project and ensure delivery. Also, the team should adhere to the format of the presentation, such as reporting on current status versus targets.
- Analysis of this approach using H2A/HDSAM is recommended to establish the total costs.
- The team should provide costs of liquefaction in dollars per kilogram of hydrogen. Both current and future targets should be included.

Project # PD-19: Active Magnetic Regenerative Liquefier*John Barclay; Prometheus Energy***Brief Summary of Project**

The main focus of the DOE active magnetic regenerative liquefier (AMRL) project is to analyze, design, fabricate, and test liquefier prototypes to develop advanced liquefier technology that meets DOE's targets for capital cost and energy efficiency for delivery of liquid hydrogen. DOE's efficiency target is 75% at 30,000kg H₂/day with \$40 MM for a 'turn key facility' (~\$353/gpd). In the last year, the objectives have been to 1) design, fabricate, and test the first reciprocating AMRL prototype to successfully span from approximately 290 to 120 K; 2) experimentally answer four key questions that have been identified regarding fabrication of magnetic regenerators with bypass flow of the heat transfer fluid; 3) use measured performance data to validate the sophisticated process simulation model for the design of optimal AMRLs; and 4) incorporate lessons learned from first prototype into the design basis of the second AMRL prototype to span from approximately 290 to 20 K and produce liquid hydrogen with a figure of merit of approximately 0.5.

Overall Project Score: 2.7 (5 Reviews Received)**Question 1: Relevance to overall DOE objectives**

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

- This project is more valuable for liquid natural gas production and distribution than liquid hydrogen production at this point, because liquid hydrogen may be too large of a step beyond current work, especially considering the current delays and complexity of the system.
- Lowering the cost of hydrogen liquefaction is an important goal for improving the economics of hydrogen distribution to the forecourt.
- Relevance to the DOE Hydrogen Program is high due to the ability to potentially provide a step change in the cost, efficiency, and supply of liquid hydrogen.
- Low-cost liquefaction is key to achieving DOE hydrogen delivery cost and performance goals. No cost projections were presented, so it is unclear whether this system would be less expensive than conventional liquefaction processes. Key cost drivers should be presented.
- It would be helpful if the researchers presented their projected efficiency using the same methodology as the DOE program.
- This project appears to be very relevant to identifying new liquefaction technology not based on compression. Since liquefaction is receiving much more attention as a promising method for delivery (and of potential use for cryo-based storage methods), this project is increasingly useful for achieving enhanced efficiency at a reduced cost.

Question 2: Approach to performing the research and development

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

- Many different issues have been considered to design and produce a working device/prototype.
- The project currently appears too complicated to be able to successfully address the development of all the new components of the system and conclude the project.

HYDROGEN PRODUCTION AND DELIVERY

- The technical approach to testing the AMRL prototype is sound.
- The project approach provides good metrics to create a foundation for subsequent steps.
- The project technical approach will allow researchers to test their complex concept in stages. It is not clear how the lessons learned from the reciprocating design will be translated to the rotary design.
- The approach of magnetic regeneration liquefiers is very unique and novel. It is also applicable to this area. The technical approach appears to strike an appropriate balance between materials/components research and selection as well as fabrication and testing, which seems necessary in this project given its relative technical immaturity.

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

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

- It is difficult to see how this project can be accomplished on time if it is already eight months behind schedule. The eight month delay cannot be ignored, even though progress was made.
- No clear comparison of improvement is provided since testing data is not available yet.
- The project has not delivered any data to support the thesis that the AMRL technology can accomplish hydrogen liquefaction with higher efficiency than the current practice. The project is behind schedule on these key objectives.
- Technical accomplishments have been delayed and appear to be not due to technology but instead project ownership and materials. More project accomplishments should be shown, however, to determine future needs.
- The project is behind schedule by over six months. The prototype unit is not complete, so overall progress toward answering the relevant performance questions cannot be determined at this point.
- The assumption that the temperature range can be sufficiently expanded seems optimistic.
- Despite timing setbacks related to transitions in company ownership, a great deal of progress was made with respect to component/subsystem selection and fabrication, creation of a prototype design, modeling, and assembly of hardware.
- This project seems highly efficient and focused on making progress towards demonstration of this technology.

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

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

- Collaboration appears to be sufficient.
- The project should include better comparison with existing technologies and their efficiencies.
- The team has good collaborations with leading academic researchers.
- More collaboration would be preferred, perhaps with Florida State University (e.g., National High Magnetic Field Laboratory) and national laboratories.
- The existing collaborations are appropriate for the project.
- While some collaborations exist, the level of participation in the project for each organization is unclear. However, this team appears to be working very sufficiently despite the lack of collaborators. The only suggested collaborations might be with other liquefier developers for eventual corroboration/validation of results.

Question 5: Approach to and relevance of proposed future research

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

- The “go/no-go” milestones are unclear.
- One of the current manufacturers, users, or experts of liquid hydrogen production units should be included for industry feedback.
- It is important that the future work is directed towards obtaining data with the prototype.
- The next three months of work are critical to the “go/no-go” decision.
- Given progress to date, the researchers' planned progress for the remainder of FY 10 seems optimistic.

- Future work seems well-planned and reasonable to achieve milestones. It is great to see a “lessons learned” activity based on the first prototype. The organization and project management aspects of this project are very impressive.

Strengths and weaknesses

Strengths

- This project has potential, based on the method used.
- Good theoretical background is used to support the development of the AMRL technology. A sound plan is provided for accomplishing the objectives of proving the technology.
- The project has a nice upside potential to dramatically reduce energy use for liquefaction.
- Low-cost high-efficiency liquefaction is critical to achieving hydrogen delivery cost goals.
- The project is comprised of a highly organized, focused, and efficient team. Progress on the project has been great.

Weaknesses

- This project employs a new method.
- No test data of a complete system is available.
- When presented, too much information was given on calculations.
- The presentation of the project needs to show clearer steps.
- The presentation does not clearly show the different components that must be developed or the status and targeted goals for each component.
- The project lacked progress towards meeting the project objectives, although it is unclear how funding limitations may have contributed.
- This project lacks collaboration and cost projections.
- Changing from a reciprocating regenerator to a rotating regenerator appears to require redesign and recalculation of the force balancing mechanisms, heat shields, etc.

Specific recommendations and additions or deletions to the work scope

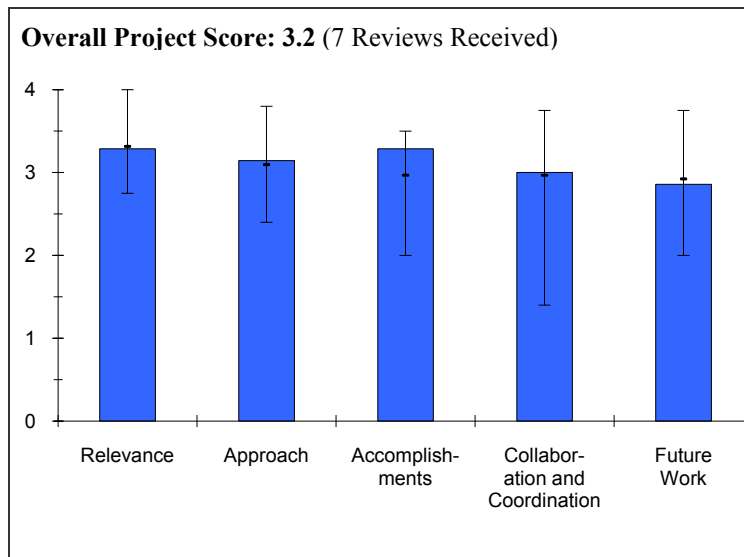
- DOE should better define for what components the efficiency numbers are calculated so that better comparisons can then be made.
- The team should include a comparison with existing liquid hydrogen equipment under strict definition that is set by DOE. This way, an “apples to apples” comparison can be made.
- It is worth questioning at an early stage whether this technology could be utilized at large, commercial scales to produce "tonnage" quantities of liquid hydrogen. A better analysis of the potential to scale up this technology is needed.
- DOE cost goals are mentioned, but no estimates on how this system would help achieve these goals are provided.
- An experimental demonstration of full temperature range cooling with no gaps is recommended before detailed design and efficiency optimization are completed. It was unclear from the presentation whether this has already been done.

Project # PD-20: Inexpensive Delivery of Cold Hydrogen in Glass Fiber Composite Pressure Vessels

Andrew Weisberg; Lawrence Livermore National Laboratory

Brief Summary of Project

The objective of this project is to produce glass fiber composite pressure vessels for the delivery of cold hydrogen. Glass fiber vessels reduce hydrogen delivery cost through synergy between low-temperature (140 K) hydrogen densification and glass fiber strengthening. Benefits of glass fiber vessels include 1) colder temperatures (~140 K) increase density by approximately 70% with small increases in theoretical storage energy requirements and can be achieved at gas-terminal scale with liquefied natural gas refrigerators; 2) low temperatures are synergistic with glass fiber composites; 3) glass fiber minimizes high composite materials cost (approximately \$6/kg for glass versus approximately \$23/kg for carbon fiber); 4) increased pressure (7,000 psi) minimizes delivered hydrogen costs and the same design can deliver up to 12,000 psi or build cascade; and 5) dispensing of cold hydrogen reduces vehicle vessel cost by approximately 25% by avoiding over-pressurization during fast fill.



Question 1: Relevance to overall DOE objectives

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

- This project is very beneficial for developing new tanks for transportation of hydrogen and eventually reduction of cost compared to currently used technologies (e.g., tube and liquid hydrogen trailers).
- Compressed gaseous storage for delivery may or may not be the future delivery method. The project will address the near-term issues if it is a success.
- Reduction of cost for hydrogen delivery via new and different approaches helps to overcome one of the critical barriers for hydrogen infrastructure.
- Project objectives appear to be critical for the Hydrogen Program to meet their long-term goals and objectives. The cold glass process improves strength effect.
- This project is not critical to program success but would make a significant contribution to making hydrogen delivery affordable.
- The team made a good discovery of the effects of cold temperatures on increased strength of glass fibers. National laboratories may not be the ideal entity to be designing cryogenic pressure vessels rather than a vendor who does fiber-reinforced polymer vessels as a business.
- The focus on low-cost pressure vessels is aligned with the Hydrogen Program objectives.

Question 2: Approach to performing the research and development

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

- Great planning and slow scale-up testing was performed in this project, as the team learned the scale presented some unknown issues.
- Glass fibers are a good approach relative to carbon fibers from a cost perspective. The team needs to establish that glass fibers are as good as carbon fibers in terms of reliability and durability since multiple failures have already been seen.

- The team needs to add the infrastructure for low-temperature cooling at the central hydrogen production plant. Therefore, they will need new and totally different infrastructure. First, the team needs to establish the requirements of temperature from full process (e.g., from manufacturing to refueling to vehicle tank). Then, they can go about developing this material.
- The team made good use of advanced materials to incorporate a composite systems configuration. The project contributes to overcoming of economic barriers. The project has a weakness in evaluating pressure cycling and observing the long-term effects to the integrity of the system.
- The program has progressed from fundamental materials to large-scale tanks. Optimization of polymers and fibers has progressed well.
- Short term applications for transport of other cryogenics provide a "market pull" independent of the Hydrogen Program.
- This project has a good approach, but quicker results could be obtained with closer collaboration with a vessel manufacturer.
- The approach for the thermoset liner could be better explained. The previous issues with glass fibers (i.e., chemical exposure) need to be addressed and discussed regarding the validation of the protective coatings. Further validation testing is needed to confirm the cylinder design will pass the certification testing.

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

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

- The prototype is in process of being built.
- Technical accomplishments to date are excellent. The development so far will be critical to future work.
- Much progress on fiber development has been made, but many material failures have occurred. The team needs to establish the right conditions (e.g., temperature) for this operation.
- The team needs to do full value chain modeling for hydrogen, including refrigeration infrastructure at the central plant with more resolution.
- The team needs to describe and optimize the full value chain process for this concept starting from hydrogen production to distribution and refueling into the car tank.
- The team is focused on meeting the program delivery cost projections, which relate to the cost to transfer to storage systems while increasing lifespan.
- Significant progress has been made in moving from laboratory to commercial tanks.
- Good technology accomplishments have been made, but the pace of development may be increased with a vendor performing more of the vessel development based on the laboratory's innovations.

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

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

- The team should consider verifying data with Sandia National Laboratories and codes and standards organizations to determine if this work can be covered under current codes and standards when integrated in trailer and/or railcars. If a gap exists, there should be an effort to address it, because it may cause a hold up for the commercialization of this technology.
- The project has excellent partners and collaborators with alternative goals, which helps move the project along.
- The team urgently needs to collaborate with IGC (and other energy companies) and original equipment manufacturers on the refrigeration and refueling approach.
- Collaboration with industry appears to be good, and partners are fairly well-coordinated.
- Lawrence Livermore National Laboratory has done an excellent job of engaging industry to move this project forward.
- Collaboration could be stronger with a vessel manufacturer rather than working at the laboratory.

Question 5: Approach to and relevance of proposed future research

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

HYDROGEN PRODUCTION AND DELIVERY

- Regulatory initiatives are extremely important and should be incorporated with the container field demonstration. Industrial partnerships will also be critical to the regulatory initiatives and should be involved.
- Much proposed future work is presented, but the team first needs to determine the sweet spot (e.g., temperature and pressure) for this approach.
- Plans for future work need to include full-scale testing of pressure cycling of the storage tank to a projected industry life. Then, the team should conduct a full-scale burst test.
- The team presented a good set of objectives for this near-commercial technology.
- Vessel development should be moved to a competent vendor.
- Future work should include additional analysis of potential failure modes to ensure the project addresses them.

Strengths and weaknesses

Strengths

- The caliber of organizations involved is strong.
- The resulting product and use of cheaper materials are both advantageous.
- A potential end user (Spencer Composites) has shown interest in using the product for integration in existing aerospace, maritime, and energy terminal equipment.
- The team's technical knowledge of testing is strong. The project plan and processes are sound. A cost breakdown of advantages over other methods (e.g., steel at \$485/kg capacity versus glass/epoxy at \$130/kg) is provided.
- Technical execution of development of glass fiber concept has been performed.
- The project has good coordination with the hydrogen industry.
- The project has good involvement of industrial partners.
- The team has demonstrated continual improvement of technology and evolution from concept to real devices.
- The team has demonstrated a novel and insightful knowledge of materials and composites from a fundamental view.

Weaknesses

- This is a new product.
- The safety and standards will be critical to the adoption of this technology. More work should be done concerning this area. This project has great potential to reduce cost for hydrogen delivery; however, the reviewer is concerned with the safety aspects of the final project. Stakeholders may think "this is great but is it still safe?" Great emphasis should be placed on the safety aspects of this technology. Also, it is unclear how volume production of these vessels can be consistent and provide a confidence in the vessel uniformity. The expected cycle life of the full-scale vessels needs to be addressed.
- The team has demonstrated poor coordination on requirements and on determining feasibility of the overall solution.
- The project investigator should talk with other storage tank industries to learn what they are developing as far as new materials.
- The project has no significant weaknesses.
- National laboratories are not manufacturers of vessels.

Specific recommendations and additions or deletions to the work scope

- The team should verify codes and standards. If a gap exists, then it should be addressed.
- The targeted lifetime and number of expected usage cycles should be defined.
- For the production method, the team should find out how the textile industry can contribute to this project, due to the used production methods for weaving fabrics at a fast pace. This may be of use when developing a reliable and fast production method for these storage tanks, which will bring the cost down and possibly improve quality. This last point does not appear to be addressed in the project yet. The team should work with the H2A group to determine when and what would be necessary to add to the model when full-scale tests prove positive (assuming that occurs). The team should also collaborate with hydrogen providers to see which steps they would suggest adding to Phase III (if this has not already been done).

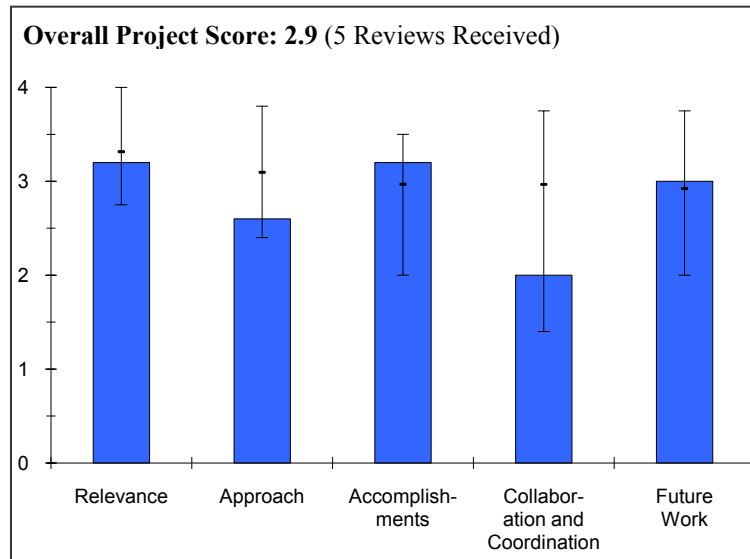
- The project should add the full process design and optimization (from cost perspective) to the scope over the lifecycle of the solution (from manufacturing to storage in the car tank).
- The team needs to pressure cycle the storage tank to projected life and then conduct a burst test. The barrier requirements for water and oxygen should be reviewed.
- The team should move vessel manufacturing from the laboratory to a vendor location.

Project # PD-21: Development of High Pressure Hydrogen Storage Tank for Storage and Gaseous Truck Delivery

Don Baldwin; Lincoln Composites

Brief Summary of Project

The overall objective of this project is to design and develop the most effective bulk hauling and storage solution for hydrogen in terms of cost, safety, weight, and volumetric efficiency. This will be done by developing and manufacturing a tank and corresponding ISO frame that can be used for the storage of hydrogen in a stationary or hauling application. The objective for the first year of this program (2009) was to design and qualify a 3,600 psi tank and ISO frame that will hold 510,000 in³ (approximately 8,500 L) water volume. The objectives for the second year of this program (2010) will be to perform trade studies for a 5,000 psi vessel and, based on the results of the trade studies, move forward on the design, manufacture, and the qualification of a 5,000 psi vessel/system.



Question 1: Relevance to overall DOE objectives

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

- The ability to reduce the cost of delivered gaseous hydrogen is critical to the Hydrogen Program.
- Good progress has been made to date toward alignment with program objectives.
- This project includes the development of a workable truck delivery system which is likely to be necessary for initial hydrogen fuel cell vehicle delivery.
- The presentation indicates that this technology will never achieve DOE volumetric capacity target. The target probably needs to be adjusted.
- The design, development, and construction of a bulk hauling and storage solution is the general objective for this project. While the eventual utility of a bulk hauling/storage container is understood, it is not clear that this topic really requires in-depth research or is really a technological hurdle. Additionally, the benefit of demonstrating this technology (i.e., through a prototype) as opposed to a simple stop at the analysis step is unclear.

Question 2: Approach to performing the research and development

This project was rated **2.6** on its approach.

- This project has established a good approach with task steps and identification of the most cost-effective increase of pressure (5,000 psi).
- This approach is effective towards meeting the barriers defined in the project objective.
- The approach seems sound for developing a tank trailer and appears to include all necessary tests; however, the "Approach" slide discusses a trade study where it really meets an additional DOE target. The "Approach" slide also mentions that "other methods to increase capacity will be researched," although no other methods were discussed. Cooling research does not seem appropriate because of the nature of the composite.
- Under task 6 (on the "Approach" slide), the project investigator states "other methods to increase capacity will be researched." It is unclear to me what other methods might be applicable. The composites will not be able to

hold cooled or liquid hydrogen. A sorption or metal hydride system may not be appropriate for the scope of this project.

- As the approach was presented, some inefficiencies surfaced in the approach. In particular, the cost reduction studies seem like they should come prior to the development and qualification of various pressure tanks. That is, the anticipated performance and cost tradeoffs should be understood at the outset of the project, enabling one pressure technology to be up-selected. A great deal of progress was made for demonstrating hardware (i.e., container and tanks), establishing manufacturing capabilities, and completing qualification (e.g., various mandated tests).
- The approach should include additional modeling and failure mode assessment tools to provide the appropriate level of reliability.

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

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

- The project achieved a tube trailer capacity of 600 kg, which is approximately double that of existing technology.
- Technical targets are being met. The safety factor does not appear to be correct for people.
- All necessary qualification tests were completed for the 3,600 psi vessels this past year. Likewise, ISO container tests were completed.
- The planned trade study appears to have only been completed in a trivial manner, and it is unclear whether 5,000 psi is the correct pressure for the next vessel.
- Based on the current project objectives, a great deal of progress was made on demonstrating hardware (e.g., container and tanks), establishing manufacturing capabilities, and completing qualification (e.g., various mandated tests). It is unclear that such demonstrations are truly needed for all of these various pressures. In other words, the reviewer is not sure why both 3,600 and 5,000 psi were targeted instead of simply trying to demonstrate the more challenging technology.

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

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

- No collaboration occurred in this project.
- No partners for the project were identified.
- There appears to be private collaborations regarding fittings and other equipment; however, the presentation did not make that clear.
- No collaborations were evident in this project.
- There was no collaboration on this project.

Question 5: Approach to and relevance of proposed future research

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

- The team proposes an increase to 5,000 and 8,300 psi that will meet future DOE targets.
- The project is focused on the pressure cycling of liquid natural gas, not hydrogen.
- The criteria for the trade study are unclear and should have been discussed more clearly. It could be on tank capital or a full delivery cost; it is unclear which one will lead to the best selection.
- The completion of tradeoff studies (i.e., between cost and performance) are good, but they should have been done much earlier. It is not clear what the technological hurdle is in demonstrating a 5,000 psi tank after the 3,600 psi tank has been accomplished.
- This project seems like a waste of resources.
- The qualification of higher pressure tanks will be useful

Strengths and weaknesses

Strengths

- The investigator has an excellent background conducting research in this area.
- The team is developing tank-trucks that can be used in the near future, which is needed for the initial delivery and dispensing system.
- The team is competent at designing, manufacturing, and qualifying hydrogen vessel (and container) technology for passenger vehicular and hauling applications.

Weaknesses

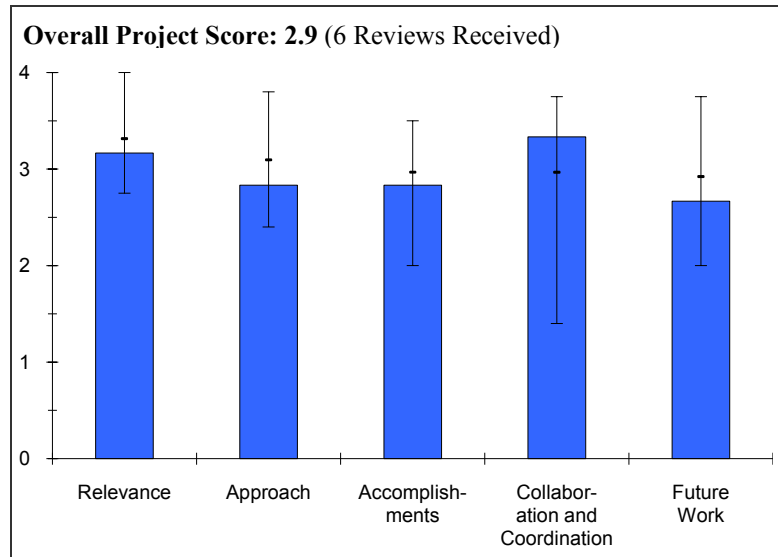
- The project had a big jump in pressure from current conditions of 3,600 psi to end conditions at 8,300 psi.
- The trade study to select the next tank pressure needs to be better defined.
- Inefficiencies exist in the approach. Cost-performance tradeoffs should be done prior to a demonstration. The project is not very technically deep and no collaborations have occurred.

Specific recommendations and additions or deletions to the work scope

- The team should consider comparing projected cost with that of stationary storage steel tanks used in the forecourt.
- Consider approval from the U.S. Department of Transportation for use as a hydrogen shipping container. A trade study at higher pressure should be completed, and a burst testing should be conducted after higher pressure cycling.
- The trade study to select the next tank pressure needs to be better defined.
- The assessment of vibration and mechanical loading on the cylinder neck should be included.
- Failure modes and effects analysis, and other robustness tools should be in the scope and their outcome provided as part of the project.

Project # PD-22: Fiber Reinforced Composite Pipelines*Thad Adams; Savannah River National Laboratory***Brief Summary of Project**

The overall project scope is focused on the evaluation of fiber-reinforced composite piping (FRP) for hydrogen service applications, assessment of the structural integrity of the FRP piping, and development of a life management methodology. Challenges include 1) reduced installation costs for FRP that offer the potential to meet the long-range (2017) cost targets for installed hydrogen delivery pipeline, 2) development of a suite of standardized tests for assessment of hydrogen compatibility of FRP, and 3) development of a structural integrity/life management methodology similar to ASME code B31.8S. The project scope for the past year has been to complete leak testing of commercial FRP joining technologies and initiate life management methodology development.

**Question 1: Relevance to overall DOE objectives**

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

- This project can potentially impact several aspects of the program by developing performance-based standards for FRPs and other similar pressure vessels.
- Pipelines are projected to be the low-cost option for hydrogen delivery, and non-metallic materials could offer the lowest installation cost.
- The success of this project would support the DOE objectives for the Hydrogen Program by assisting in the development of hydrogen delivery technologies.
- Fiber-reinforced pipeline can be a low-cost pathway to hydrogen distribution, so it is an essential element in the portfolio of approaches for hydrogen delivery.
- Reliability issues relating to leakage barriers are not realistic due to the cost of lost revenue.
- Piping costs for hydrogen delivery are very high and are a significant factor in delivery. An evaluation and consideration of FRP may offer lower cost piping.

Question 2: Approach to performing the research and development

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

- A generally good technical approach is used for this project, though it could become even more effective if the experimental approach is consolidated. Specifically, it is unclear whether the accelerated environmental tests are more effective than using actual samples. Optimally, both are needed to calibrate the work.
- A good approach is used for preparing the design and life management for FRPs for hydrogen service.
- The research approach for this project is logical and well thought out. The approach addresses the technical barriers. However, the actual progress did not meet what was proposed.
- The team uses a good approach to develop a life management plan to identify operations and maintenance issues and costs in addition to initial costs.
- Working directly with the American Society of Mechanical Engineers (ASME) is the right approach to establish codes and standards for FRP.
- The team incorporates a good background review of codes process, existing standards, and approaches.

HYDROGEN PRODUCTION AND DELIVERY

- Using performance-based standards is the right objective.
- It appears that FRP will meet program objectives. Once long-term tests are completed, the team may need to perform a burst test to determine safety margins.
- The approach is good for evaluating vendors offerings, but the joints of FRP have not been addressed in this talk.

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

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

- Considering the resources available, the project has shown good progress. The data presentation can be further improved in the supporting documents by providing more details on the methodology and why the technique is used.
- The reviewer questions whether future work on the joints will be conducted.
- The FRP pipe management plan has been completed.
- The fundamental work done for this project is a good basis. However, not enough progress appears to have been made in many areas. Some of these deficiencies include no testing for leakage via permeability, little or no consideration given to different piping materials, and a lack of applied testing.
- Solid progress has been made on establishing pH bounds and stress/strain characterization of glass fibers. Progress has also been made on other environmental factors, but a time factor is needed to assess durability for 25 years.
- Good characterization was completed of flaw impacts on different reinforcement designs. Again, a life of 25 years needs to be put into perspective.
- The project appears to have achieved progress towards meeting the program objectives in its flaw tolerance work with 40% flaw through fiber reinforcement layer.
- Technical analyses of FRP for hydrogen service are good, but it would be beneficial to show the effects of joints and couplings included in the program.

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

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

- The project has a good mix of participation by national laboratories, industry, and ASME.
- Adding AGY to the project team brings fiber experience.
- The collaborations with manufacturers and ASME are excellent. The close work done with ASME is especially well-coordinated and beneficial.
- Collaboration with ASME is important.
- The key to switching to performance-based standards is integration into codes and standards.
- Collaboration with commercial partners and industry standards groups appears to be keeping this work on course. The team needs to combine environmental effects with flaw work. The development of modeling appears to be for FRP materials.
- The project demonstrated good collaboration with piping vendors and other national laboratory and university resources.

Question 5: Approach to and relevance of proposed future research

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

- Future plans are not clear, with exception to the ASME review.
- There does not appear to be any future work proposed because the project is not proceeding.
- A good list is provided for implementing work into standards as an objective.
- Service degradation of material needs to be investigated.
- Future work was indicated, but effects of cyclic pressure were not included.

Strengths and weaknesses**Strengths**

- This project has developed strong collaborations with manufacturers and ASME.
- The team uses a practical approach to solving the problem with current codes and standards with respect to FRP.
- Work completed to date supports the current findings.
- The fundamental approach for evaluating FRP as hydrogen piping should yield new insight for use of FRP substitute for hydrogen service.

Weaknesses

- Many unanswered questions remain for a project that has been in process for over four years .
- The team needs to include the cost of FRP as an estimate for determining commercial potential as compared to steel.
- The team needs to work closer with the construction industry to study the effects of trenchless installation. The team should also study the effects of temperature changes due to reduction of pressure in addition to the overall life of FRP.
- The team did not include cyclic pressure effects and joints.

Specific recommendations and additions or deletions to the work scope

- If not considered previously, it may be worthwhile to expand the project scope to include stationary storage vessels.
- It is unclear whether permeability of the FRP will be measured and if it is part of the less than 0.5% leak rate. The reviewer is unsure whether different composite pipe materials are being considered instead of just one type. Information on how/if the material properties change when exposed to hydrogen for long periods would be useful.
- The team should include the element of cost tracking/targets into the standards development process as a way to compare with the technology with steel pipelines.
- The team should define the comprehensive test metrics for future standards development and modification for FRPs with 25 years of durability timeframe in mind.
- The team should do modeling of failure mode at higher operating pressures and emergency venting of hydrogen.

Project # PD-23: A Combined Materials Science/Mechanics Approach to the Study of Hydrogen Embrittlement of Pipeline Steels

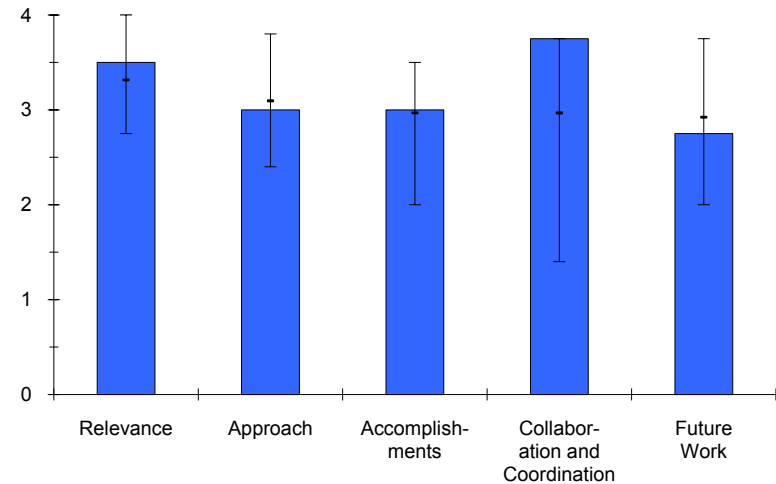
Petros Sofronis; University of Illinois

Brief Summary of Project

The overall project objective is to 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. Specific project objectives are to 1) study existing natural-gas network of pipeline steels or hydrogen pipelines, and 2) work with Oregon Steel Mills to propose steel microstructures with superior tolerance to hydrogen.

Question 1: Relevance to overall DOE objectives

Overall Project Score: 3.2 (4 Reviews Received)



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

- Understanding of hydrogen embrittlement is critical for safe use of hydrogen piping and is aligned with DOE objectives.
- Hydrogen embrittlement is one of the fears of failure mode for hydrogen pipelines and storage.
- The team still needs to define why this work is so important, given the miles of hydrogen pipelines currently in place.
- This topic may be more relevant to DOE's Office of Basic Energy Sciences.
- The project is 75% complete. The following barriers have been identified: high capital cost, understanding of mechanical hydrogen embrittlement, and how embrittlement relates as a function of time and microstructure.
- Steel pipelines are likely to be a key component of a hydrogen distribution network at high penetration. Safety will also be critical.

Question 2: Approach to performing the research and development

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

- Developing an understanding of hydrogen embrittlement in pipelines will allow for safe operation with the cyclic pressures expected in future pipes.
- The team needs to establish a good connection between model and experimentation for validation of the theoretical approach. Carefully constructed experiments are good for validation, but they may not represent the real world situation and makes the model irrelevant for practical situations.
- The team needs to first define the problem in terms of exact range for cyclic pressure, frequency, and type of application for failure modes in actual pipelines due to hydrogen embrittlement.
- The presentation was a little too technical without actually bounding the problem and relating to actual failures in the field.
- Use of scanning electron microscope (SEM) to analyze the particles in the microstructure and characterize them is an excellent method to understand the issues.
- The approach appears to have a good mix of experimental and theoretical approaches.

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

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

- Quasi-cleavage mechanism identification will allow improvement in the model.
- Development of theory is a good idea. The team needs to fully validate the theory with the field application and failures.
- Not much progress has been made in determining actual failure rates and recommending modifications to existing materials.
- To set the bounds on testing, the team needs to establish the magnitude of the problem of hydrogen embrittlement in existing or projected pipelines. This data on this issue was not shared.
- Excellent progress has been made toward understanding suitable steels for construction of pipelines to transport hydrogen. The work to determine if existing natural gas pipelines could, in fact, transport hydrogen is off track. The investigator is only looking at the base pipe materials and not the welds or other higher strength regions within the pipeline system.
- The project's efforts on quasi-cleavage appear to be a significant advance on technology.

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

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

- The team has an excellent mix of industry, university, national laboratories, and international cooperation.
- A good list of collaborators is provided, including the Pipeline Working Group.
- Participation in ASME is a must to get the improvements included in codes and standards.
- Seven industry partners, two national laboratories, and two codes and standards developing organizations are collaborating in this project.
- A good mix of industrial and national laboratory partners appear to be actively involved and engaged in this project.

Question 5: Approach to and relevance of proposed future research

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

- Experiments under cyclic pressure will provide needed knowledge regarding fatigue.
- The list of proposed future work is adequate to achieve the goals of the project.
- A focus on fracture testing is needed along with modeling of the fracture process.
- The team sets a good direction in its extension of modeling efforts to non-steady state and incorporation of new experimentally-observed effects.
- The proposed fatigue studies is a reasonable extension of the current work.

Strengths and weaknesses**Strengths**

- This project provides the basic knowledge needed to understand the effect of embrittlement on future hydrogen infrastructure.
- The team's technical capabilities and theoretical competence are strong.
- The "go/no-go" decision approach for subcritical crack growth experiments is using sound engineering practices. This should assist with the development of a thermodynamic theory of de-cohesion with the use of ab-initio calculations.

Weaknesses

- Slow progress has been made on the actual determination of failure modes, failure rates, and the dependence on various operating conditions.
- Too much theory is presented without defining the real world problem and magnitude of the issues.

HYDROGEN PRODUCTION AND DELIVERY

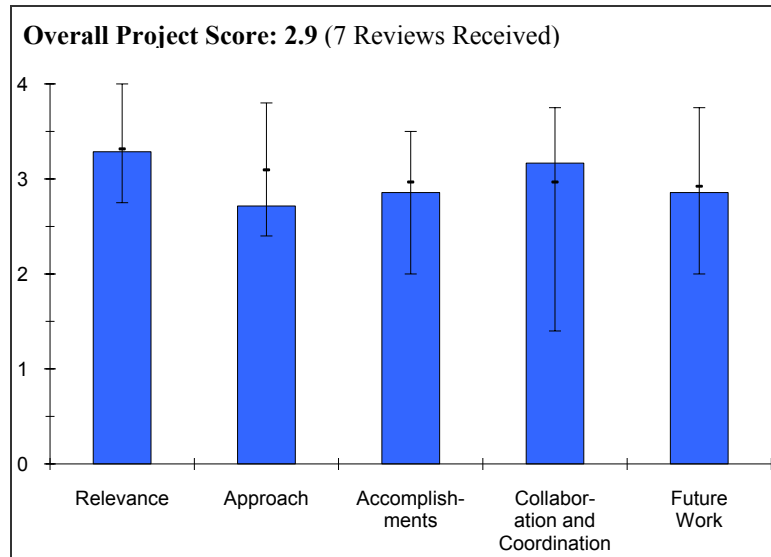
- Sawtooth marking at the top of SEM view is important on how the fracture and crack tip develop. However, this was not well expressed in the presentations or slides, and the reviewer is not sure why.

Specific recommendations and additions or deletions to the work scope

- The team should define an objective in terms of modification of codes and standards.
- The goal of the project should not be to find hydrogen embrittlement. Instead, it should be to define the relevance of embrittlement in the real world situation.
- The team should demonstrate intense dislocation activity for quasi-cleavage fracture. A single-edge notch tension test can be used as a comparison. The team needs to look at fatigue specimens and the characterization of the specimens to show the same mechanics as hydrogen embrittlement.

Project # PD-24: Composite Technology for Hydrogen Pipelines*Barton Smith; Oak Ridge National Laboratory***Brief Summary of Project**

The objectives of this project are to 1) assess, primarily from a materials performance perspective, the compatibility of FRP and engineered plastics in high-pressure hydrogen environments, 2) to define research and development issues for adapting the technology for hydrogen use, and 3) to develop a path to commercialization for the technology. Milestones for 2010 are to 1) conduct hydrogen compatibility evaluations of the next group of composite pipeline materials and construction, 2) perform cyclic testing, and 3) complete the next round of polymer diffusivity and permeability measurements.

**Question 1: Relevance to overall DOE objectives**

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

- The main question confronting this project is whether any one of the composite technologies is appropriate for use in hydrogen pipeline and vessels.
- Non-ferrous piping may provide the lowest cost installation for hydrogen pipelines.
- The presentation material demonstrated that the project is responsive and clearly attuned to DOE objectives.
- Delivery costs dominate the current hydrogen fuel costs.
- Pipeline is the leading future commercial approach to delivery of hydrogen. Current pipeline costs are still too expensive, so this project is very relevant.
- Composite pipelines for hydrogen have the potential to reduce the cost of transporting hydrogen over long distances. The capital cost of composite pipelines is expected to be significantly lower than steel pipelines.
- This project is using existing technology solutions from other industries (e.g., oil and gas) for potential transportation of hydrogen. This project is looking to address long-term gaps that relate to the economics of hydrogen distribution. Over the past couple of years, the project made significant progress; however, it appears to have slowed or stopped over the past 6-9 months.
- Finding low-cost transmission and distribution piping for hydrogen is a necessary requirement for long-term hydrogen infrastructure.

Question 2: Approach to performing the research and development

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

- The authors do not specifically address the approach, but it is evident that they are engaged in a series of empirical tests of various available composite technologies. However, it is unclear if the tests are actually addressing the “go/no-go” decision. For example, the reviewer is interested to know how the team plans to test or address the 25-30 year lifelong reliability of the material.
- The project approach is not covered in the presentation.
- The project is considerably outside of the reviewer’s area of technical expertise, so the reviewer is deferring this question to more qualified reviewers. The approach appeared to be reasonable for addressing a core problem in hydrogen distribution, but this remains a difficult problem that will require substantial effort to resolve.
- A good approach was used to leverage existing oil and gas industry experience in composite pipelines.

HYDROGEN PRODUCTION AND DELIVERY

- The project used a good list of composite pipeline manufacturers.
- The team used a good screening approach to identify issues and leading candidates.
- The overarching approach to the project was not communicated in the poster. No deficiencies in the testing approach were identified. A discussion of “go/no-go” decision points and project milestones would be helpful to better evaluate the approach.
- The original approach was to identify major barriers, which includes the material composition of the pipe. However, the team now needs to refocus and look at secondary issues with using these composite designs. The research team needs to consider the connector materials and other devices needed within the pipeline system and the effects of long-term exposure to hydrogen.
- Generally, the team presented a good approach and good collaboration with FRP pipe vendors. However, some testing should be done early on to examine the viability of pipe connections. This is almost always the weak point in piping systems.

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

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

- The limited resources provided in 2010 may have affected technical accomplishments and progress toward the project and DOE goals.
- The loss of tensile strength is an important issue that is not adequately addressed. The authors attribute this to shipping issues, but this is an inadequate analysis and it raises issues regarding the vulnerability of the fibers to defects and other external damages. The team should consider that this may not be a robust technology to be used in an uncontrolled environment.
- Delamination during the blow-down test highlights a potential weakness for lined pipe in cyclic pressure service.
- The project is considerably outside of the reviewer’s area of technical expertise, so more qualified reviewers should be deferred to in assessing the technical accomplishments of this project.
- Overall, good progress has been made on the screening of leading composite pipeline concepts.
- The projected cost status is quite favorable in terms of costs.
- DOE needs to set proper metrics for hydrogen leak because less than 0.5% is not specific enough.
- The project has demonstrated that the composite pipelines perform better than predicted.
- The projected cost of the composite pipe materials appears to meet the estimates. However, a large-scale demonstration should be completed to look at the real world capability of the system transporting hydrogen. Test data on pressure cycling and variations in operating temperature is needed to verify the long-term reliability to the pipe system.
- In general, good progress has been made on evaluating Polyflow Thermoflex. The hydrogen leak rate looks good, although it was not done with fittings and couplings. Delamination of the inner sleeve is a problem, and the research and development team needs to define what constitutes a piping failure in specific terms.

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

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

- This project presents good coupling of a national laboratory with industry.
- Based on the presentation, a strong degree of collaboration appeared to be present for this project.
- A fair list of collaborators and pipeline manufacturers was presented.
- Collaborations appear to be adequate and appropriate, though proposed future work may require additional collaborators.
- The project investigator is working with six different pipeline system teams as they develop different compositions of composite pipe. Review of the operational conditions found in the ditch (e.g., operating pressure cycles, temperatures, and product loss due to line leakage) by existing hydrogen pipeline operators is suggested. This will provide insight into the testing conditions to which the new composite pipes would be subjected. Also, the projected loss due to leakage was estimated at 0.5%, but based on the cost of water, that is not much revenue. However, given the cost to produce hydrogen, that becomes a much larger dollar value

considering the total volume of hydrogen projected to be stored in that composite line. The team may need to rethink this.

- Great collaboration is taking place with piping vendors.

Question 5: Approach to and relevance of proposed future research

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

- Development of codes and standards is needed for hydrogen FRP service required for safe implementation.
- The proposed work seems like reasonable next steps to build upon the previous results.
- The proposed future work to finish the screening work is fair.
- The team needs to identify the next steps to successfully establish commercial readiness of this approach.
- The proposed future work builds on past progress and is focused on the barriers. However, decision points and barriers to realization of composite pipelines in hydrogen operation were not discussed.
- No real proposed future work was suggested by the presenter. The presenter was asked about reviewing currently operating hydrogen pipelines regarding pressure and temperature along with the connectors and system gages under consideration. The presenter agreed with this idea; however, funding limitations would hinder that work. The presenter did propose a real world demonstration test of recommended designs.
- Good plans were presented for 2010-2011, but the team needs to think about testing with couplings and defining criteria for piping failure besides leak rate.

Strengths and weaknesses

Strengths

- The team used a good and balanced approach of utilizing existing oil and gas industry experience in composite pipelines.
- The project has developed useful data for evaluating the status and potential of composite pipelines for hydrogen. Relevant materials and information for cost modeling are provided by project collaborators.
- The cost of projected composite pipe appears to have been met.
- The project addresses the need for cost reduction in transmission and distribution piping for hydrogen.

Weaknesses

- The scope is a little too narrow and should be expanded to something like "establish commercial readiness of composite pipelines for transportation hydrogen application."
- No significant weaknesses were identified.
- The team needs to look at long-term pressure and temperature cycling of pipe. They also need to investigate connectors and well health monitoring of system tools. The project investigator looked at the leakage rate of system and not the cost of lost product, which could be a much larger number than the projected 0.5% loss of product over a given length of pipe.
- The team should consider retesting the composite pipe at higher operating pressure and temperature along with the cycling of pressure and the effects on the long-term life reliability of the composite pipe.
- The team needs to define criteria for piping failure and include piping junctions and couplings in durability testing.

Specific recommendations and additions or deletions to the work scope

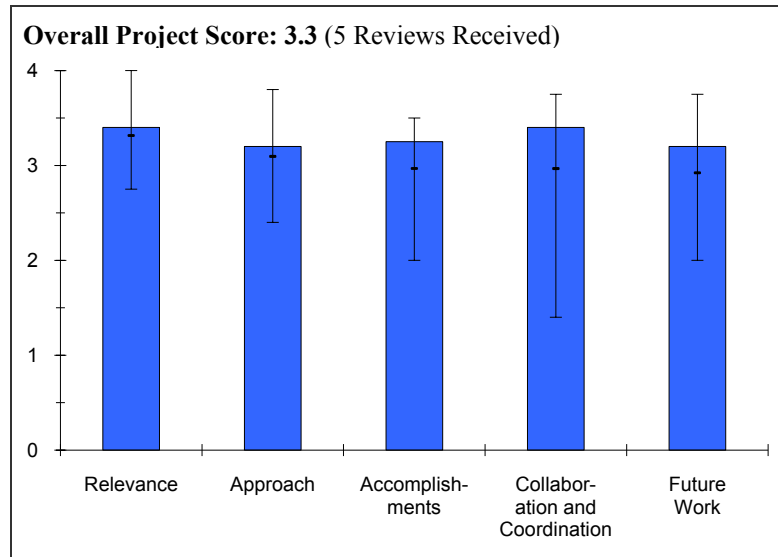
- The program needs to address the "go/no-go" decision promptly.
- The team should expand the scope to include the next step of establishing commercial readiness of the leading candidate from screening exercise.
- Testing of the composite materials under pressure cycling is an important next step in evaluating the potential for application in hydrogen delivery pipelines.
- The team should interface with existing hydrogen pipeline operators to better establish pressure cycling rates as well as operational conditions for temperature.

Project # PD-25: Hydrogen Embrittlement of Structural Steels

Brian Somerday; Sandia National Laboratories

Brief Summary of Project

The objectives of this project are to 1) demonstrate reliability and integrity of steel hydrogen pipelines for cyclic pressure by addressing potential fatigue crack growth aided by hydrogen embrittlement, and 2) enable pipeline design that accommodates hydrogen embrittlement by applying and optimizing hydrogen pipeline design code ASME B31.12 with an emphasis in FY 09-10 on measuring fracture thresholds and fatigue crack growth laws for X52 steel in hydrogen gas. The reasons for steel hydrogen pipelines are that the safety of steel pipelines is well established (e.g., third-party damage tolerance) and that hydrogen pipelines are safely operated under static pressure.



Question 1: Relevance to overall DOE objectives

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

- The embrittlement is an important issue, and while it is not in any of the critical pathways, considering the amount of resources, this seems to be an appropriate level of work.
- Pipelines are the expected low-cost delivery method. The project increases understanding of hydrogen embrittlement required for the application of steel pipe to a potential hydrogen infrastructure.
- There will likely be a need for steel pipelines to transport hydrogen. Therefore, research to understand the failure mechanisms for steel pipelines in hydrogen operation is warranted.
- The project is 40% complete.
- This project focuses on ASME code 831.12 and is attempting to address the static pressure of hydrogen and how the reduction of cyclic pressure will improve the integrity of the system.
- This project is highly relevant for the success of hydrogen infrastructure. The project goals support DOE research, development, and demonstration goals where the specific intent is to demonstrate the integrity and reliability of steel hydrogen pipelines for cyclic pressure, which is resistant to embrittlement.

Question 2: Approach to performing the research and development

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

- Improved test methods are required to develop inputs to the ASME pipeline code.
- The testing follows standard ASME B31.12, supporting pipeline design, codes, standards and permitting efforts. The approach used in this project appears to be sufficient to provide data to support and optimize the test methods referenced in standard ASME B31.12, and to better understand fatigue-related failure mechanisms of steel pipelines in hydrogen operation. Testing at different frequencies has led to test method improvements and reduced testing times.
- The project is focused on demonstrating the improved reliability of steel pipelines transporting hydrogen by reduction of cyclic pressure.
- The approach was rational toward accomplishing goals, in particular using the specified ASME code to evaluate the fracture properties of various materials.

- Milestones were clearly laid out and results were to be provided to key standard development organizations. The team also presented a secondary goal of trying to reformulate relevant standards in order to improve testing efficiency.

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

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

- In general, good progress was made on the project as compared to last year.
- The project determined properties for X52, which was identified as a potential steel of interest.
- The project has developed data and test methods that substantially contribute to the assessment of fatigue crack growth laws and pressure cycling effects on steel pipelines in hydrogen operation.
- The team made excellent progress towards showing that the embrittlement barrier can be overcome by operating in a static range of operating pressure.
- It was great to see a round-robin approach for evaluation of consistency amongst groups.
- Determination of fatigue crack growth laws was useful and highlighted the time required by current ASME code. However, the overall group should shift focus to working towards their technical goals rather than making revisions to the ASME code.

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

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

- There is a good level of collaboration among various groups. The project would benefit if it could also tie in with the validation project and acquire samples of some of the steel storage cylinders.
- This is excellent work with the DOE Pipeline Working Group and builds on use of round-robin data.
- Interactions with the DOE Pipeline Working Group and standards development organizations are appropriate.
- The project has collaboration with industry, universities and two national laboratories.
- The project has solid participation with laboratories and universities via the Pipeline Working Group and is clearly in communication with the ASME organization.

Question 5: Approach to and relevance of proposed future research

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

- This was good work on planning the development of additional data on selected X52 steel.
- Testing of the fatigue growth rates of welds is an appropriate next step. Future testing should be focused toward understanding the effects of pressure cycling on steel pipelines in hydrogen operation.
- Plans are clear for the scope of work and the overall program objectives. There is a need to focus more on newer high-strength pipeline steels that are common today and not what was common 40 years ago. Focus on X-70 thru X-100 type steels.

Strengths and weaknesses

Strengths

- The collaborations are a strength in this project. Collaborations with the National Institute of Standards and Technology, component manufacturers, and ASME are particularly important for ensuring that sufficient and relevant data is collected to support test methods and standards, as well as to understand fatigue crack growth laws of steel pipelines in high-pressure hydrogen operation. Reviewer comments from the previous year appear to have been adequately addressed.
- The project developed a sound understanding for material effects of hydrogen toward the long-term safety and integrity of steels.

Weaknesses

- The amount of reliable data that can be obtained in this project is limited because there is only one test apparatus.
- The proposed future work is to develop test methods for measuring the fracture properties of pipeline steel girth welds in hydrogen. This work has already been completed and is in use by current pipeline operators of natural gas and hazardous liquids for the Department of Transportation Pipeline Safety Administration.

Specific recommendations and additions or deletions to the work scope

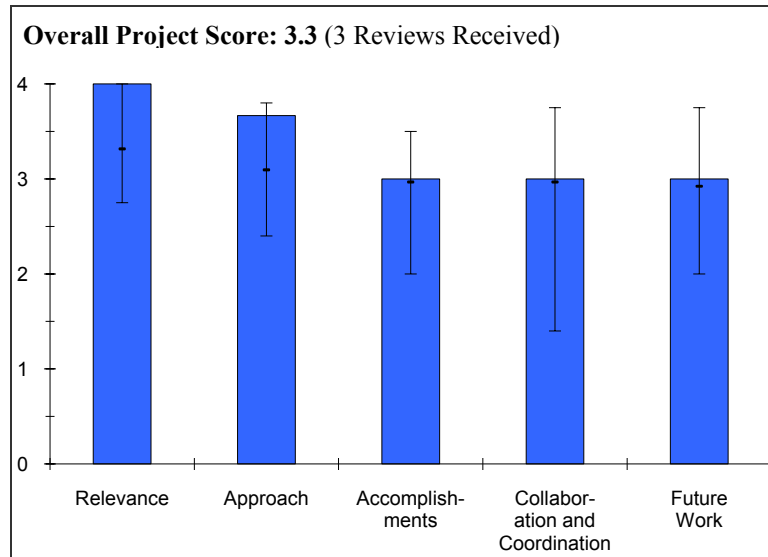
- The project should focus on the pressure cycling effects on steel pipelines in hydrogen operation. To the extent possible, determine the range of operating conditions likely to be experienced by steel pipelines in hydrogen operation, and verify that the testing parameters used are sufficient to understand the hydrogen embrittlement of these pipelines. The project should continue to generate data to determine how conservative the measurements at high frequency are and to optimize the balance between test efficiency and data reliability.
- The project investigator needs to coordinate his research and development efforts with members of the oil and gas pipeline industry.

Project # PD-26: Innovative Hydrogen Liquefaction Cycle*Martin Shimko; Gas Equipment Engineering Corp.***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) identify, design, and test the key component (i.e., continuous catalytic heat exchanger); 3) design a 50,000 kg/day plant using low/no risk development components; 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 **4.0** for its relevance to DOE objectives.



- There is a good focus on making use of off-the-shelf components, which will help to build a reliable unit with a track record for available components used.
- If efficiency improvements are realized they would provide very important benefits to the near and mid-term hydrogen infrastructure.
- This technology is clearly relevant to establishing viable hydrogen infrastructures.

Question 2: Approach to performing the research and development

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

- This is a logical approach that transitions from modeling phase to testing.
- A very good approach, with reasonable progression from the modeling through the prototype testing stages.

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

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

- It is good to see that the prototype is in the process of being built.
- The reviewer is concerned that reliance on graduate students may cause potential delays.
- It appears that technical barriers have been addressed and should be overcome.
- Technical barriers are being adequately addressed, and good progress is being made.

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

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

- The project investigator should connect with Argonne National Laboratory (Marianne Mintz) to verify the assumptions used for the DOE H2A model for liquid hydrogen and to verify that the system equipment costs are definitely approximately 40% of the H2A estimate.
- The work with partners was not outlined sufficiently. The team needs to work with hydrogen industry representatives.

HYDROGEN PRODUCTION AND DELIVERY

- Seems to be working well with partners. Some additional attention to working with partners more closely in validating assumptions in H2A models could be of benefit.

Question 5: Approach to and relevance of proposed future research

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

- The project should include work on the full-scale compressor.
- It was unclear if it will be tested on full scale with hydrogen.
- Future work plans seem adequate except for full scale testing, which is not included unless more funding is provided. Fiscal year 2011 work was not outlined.
- There is a logical progression in the work to date, and in the proposed future work. Full scale testing of this technology would be very interesting.

Strengths and weaknesses

Strengths

- It is valuable to use existing developed technologies (such as helium expanders) to bring the cost down and increase the reliability of the final product.
- The project was excellent to show progress in efficiency increases through comparison with current large-scale hydrogen liquefaction plants.
- There is a potential to use existing technology to dramatically reduce the energy for liquefaction.
- An interesting and novel approach to H2 liquefaction with potentially significant benefits to large scale hydrogen infrastructures.

Weaknesses

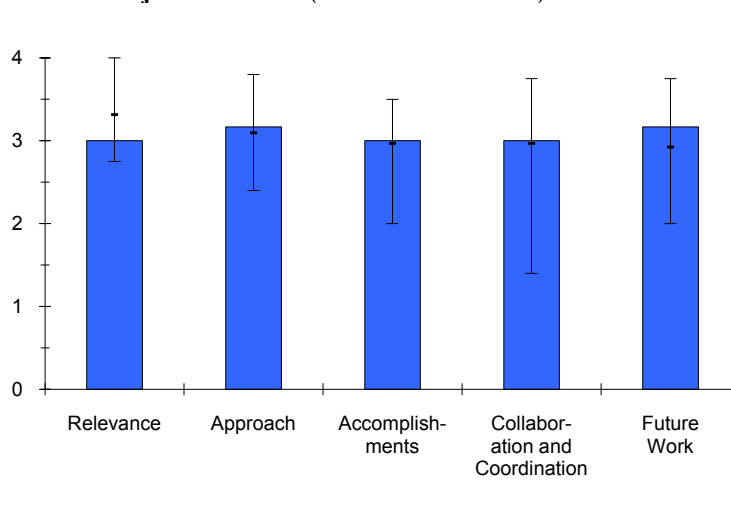
- The use of graduate students could cause delays in meeting the timeline for the final production full-scale unit.
- Continuous catalytic heat exchangers are a weakness, as the testing is not completed yet.
- The lack of an equipment test, which is scheduled, is a weakness. The project has no hydrogen providers on board.

Specific recommendations and additions or deletions to the work scope

- The project should include numbers for both the capital cost of the system and the resulting liquid hydrogen cost/kg.

Project # PD-27: Solar High-Temperature Water Splitting Cycle with Quantum Boost*Robin Taylor; SAIC/FSEC***Brief Summary of Project**

The overall objective of this project is to demonstrate the viability of a new and improved sulfur family thermochemical water-splitting cycle (i.e., sulfur-ammonia) for large-scale hydrogen production using solar energy. Project goals are to 1) evaluate sulfur-ammonia water-splitting cycles that employ photocatalytic or electrolytic hydrogen evolution steps and perform lab testing to demonstrate feasibility of the chemistry, 2) perform economic analyses of sulfur-ammonia cycles as they evolve, 3) select a cycle that has high potential for meeting the DOE 2017 cost target of \$3/kg hydrogen and efficiency goal of more than 35%, 4) demonstrate technical feasibility of the selected sulfur-ammonia cycle in bench-scale, closed-loop tests, and 5) demonstrate pre-commercial feasibility by testing and evaluation of a fully-integrated pilot-scale closed-cycle solar hydrogen production.

Overall Project Score: 3.1 (6 Reviews Received)**Question 1: Relevance to overall DOE objectives**

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

- It is hard to picture who the customer would be for this technology. Presumably the customer is someone who has a lot of desert land for the heliostat, electricity available at reasonable cost, a way to get the hydrogen to customers, and would not have to worry much about safety and pollution. There are few customers like this.
- Thermochemical cycles remain one of the most promising approaches for large-scale hydrogen production by water splitting that could meet the DOE targets for hydrogen cost and efficiency.
- This project supports the DOE research, development, and demonstration objectives.
- This is definitely in line with the DOE goals and objectives.
- The project seeks to develop a water splitting process via the use of thermochemical cycles where most, if not all, of the energy comes from a solar thermal source.

Question 2: Approach to performing the research and development

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

- The researchers are addressing issues, but more seem to pop up as the others are addressed.
- The evaluation of the sulfur-ammonia cycle is a good complement to the other thermochemical cycle programs in production and delivery. This project has an effective plan to evaluate and optimize the entire cycle.
- The team has changed their approach from last year and is now focusing on the more critical issues.
- The chemical cycle they have selected is much more complex than other thermochemical cycles. The complexity will substantially increase the capital and operations and maintenance costs, which is not reflected in their analysis. It is unclear that they will be able to lower the costs in reality.
- They do not include durability testing for any of the reactors in their approach. This is a very aggressive system and reactor life will be an issue. This is particularly important for the electrolysis stack since their approach to decrease the voltage is to raise temperature, which always results in shorter stack life.
- The project seems particularly well organized and presented.

HYDROGEN PRODUCTION AND DELIVERY

- The project appears to be working on the correct technical barriers. However, start/stop cycling needs to be addressed in much more detail.
- The investigators have shown considerable creativity in changing their approach in response to emerging issues, -such as in the use of only a thermal solar input and in eliminating the zinc oxide/sulfate based cycle.
- The overall approach seems to take for granted the catalytic high temperature sulfur trioxide to sulfur dioxide + oxygen step. In a sense it is reasonable since this unit operation is being developed by others, but there should be at least a minimal engineering design for its integration into the overall process.

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

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

- The main achievement seems to have been to get the electrolysis voltage down to 1.0 V from 1.6 V using a heliostat and a fairly complicated thermal splitting cycle that operates at temperatures up to 900° C. The reviewer expected better results than this using straight electrolysis. There are encouraging indications that the voltage can be reduced further to 0.6 V, but only for very low rate outputs. Even 0.6 V is not enough of an improvement over existing technology to justify the likely capital and safety costs of the cycle.
- There is good technical progress on improving the various sub-cycles. The modeling and economic analysis data is useful even at this early stage of the technology development.
- The lowering of the electrolytic cell potential is a good accomplishment.
- The H2A analysis underestimates the cost of water. This type of technology will be located in regions with limited water availability and water rights.
- The H2A analysis includes estimates for operation and maintenance. The project investigator should include the team's assumptions in the supplemental section. Their projected operation and maintenance costs seem low compared to the high complexity of the system and the chemicals in use.
- The project investigator is using current results in their H2A analysis, which is very good.
- More information on the oxygen evolution reactions is needed. The rate, kinetics, selectivity and catalyst durability should be described. The team obviously has much of the information (not including the durability) so it should be relatively easy to get this data.
- A hybrid cycle requires electricity that will need to be generated on-site or brought in from the grid. In order to achieve 24/7 operation, which the project investigator indicated was a goal, they will need to be connected to the grid. The assumption in the H2A models that they will be able to provide all of the electricity without purchasing from the grid is flawed since solar power is only available for a short time during each 24-hour cycle.
- The process design has come a long way since the last meeting. Bottoming cycle integration is a great idea and it would be great to see some of the process design details behind it.
- The team made excellent progress towards down-selection to an apparently more viable process cycle, using all liquid/gas systems with an electrochemical step for hydrogen generation. However, significant issues remain, including the low difference in temperature between ammonia and sulfur trioxide evolution, which could result in not only nitric oxide but also nitrogen. Ideally the temperature of ammonia release should be lowered, which may be possible by additives that increase the basicity of the melt. Secondly, the process has to be designed for continuous operation. No chemical plant, especially one operating at such high temperatures, can be efficiently turned on and off twice a day. Storage of the hot molten salt is suggested to address this issue, but keeping the sulfur trioxide to sulfur dioxide + oxygen reactor at process temperature needs to also be addressed.

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

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

- Given the issues involved, they have chosen the right academic partners.
- The critical thermochemical cycle process development is occurring at a subcontractor facility (Florida Solar Energy Center). It is important that good collaboration continues to maximize the results of the process development.
- The project has a well balanced team of industry and academia.
- The number of publications is good.

- The project includes an excellent collaborative partner on the important electrochemistry step. However, at minimum a partnership with an active developer (possibly Sandia National Laboratories) of the high-temperature sulfur trioxide to sulfur dioxide + oxygen process is critically needed.

Question 5: Approach to and relevance of proposed future research

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

- The investigators seem to be trying to improve the cycle in all the right ways. The problem with the cycle is that there is so much that needs improvement.
- The future work is well-planned and clearly focused on the key deliverables.
- The FY 11 activities seem reasonable.
- The major gap in the proposed future work would be looking at durability of the reactors, especially the electrolyzer. Lifetime testing of a minimum 1000 hours needs to be done.
- This process really needs to be a 24/7 operation. They need to include the assumptions used for the Aspen® analysis and H2A analysis for this requirement. This information should be included in the supplemental section of the presentation.
- This project is moving in a direction that has a good balance between system optimization and component development. However, more detail behind start/stop cycling as well as any thermal storage considerations would be beneficial. Steam cycles, for example, are very challenging to start/stop. A steam turbine may take most of a day just to start.
- The overall process must be designed for continuous operation beyond just a consideration of using a reservoir of molten salt. Maintaining the sulfur trioxide decomposition reactor at temperature during nighttime could (in theory) be accomplished by reversing the flow of reactants (i.e., sulfur dioxide+1/2 oxygen [air] now going to sulfur trioxide), which is an exothermic reaction. This concept is in the literature.
- A competent partner (possibly Sandia National Laboratories) for the sulfur trioxide decomposition technology should be included in the project.

Strengths and weaknesses

Strengths

- The project is unique and offers an attractive water splitting cycle.
- There is a good balance between the development of the improved thermochemical sub-cycles and the modeling/evaluation of the overall cycle.
- The project has a strong team.
- The team is focusing on the critical areas.
- This was a particularly well-constructed presentation.
- The apparent flexibility and creativity of the investigators in changing process pathways in response to technical and economic issues is a strength.
- The broad-based approach from the solar collector to the chemistry and electrochemistry of the overall process is a strength.

Weaknesses

- The cycle does not seem to work that well. It does not seem likely that this process will work well enough for practical use in the foreseeable future.
- There are still potential showstoppers in the thermochemical sub-cycles (e.g., cross contamination of ammonia and sulfur dioxide generation in the oxygen generation sub-cycle). A clear focus on solving these issues should be a priority.
- The efficiency of this process cannot be high since it can only be in the range of about 22%. The ammonia and sulfur cycle has been well studied for several decades and others have proven that it is a difficult process to optimize to get better efficiency.
- To achieve 24-hour operation in a hybrid cycle the system will need to be connected to the grid and purchase electricity from the grid.
- The chosen cycle is very complex and requires a large number of reactions and reagents. This will add capital cost and increase the operation and maintenance costs.

HYDROGEN PRODUCTION AND DELIVERY

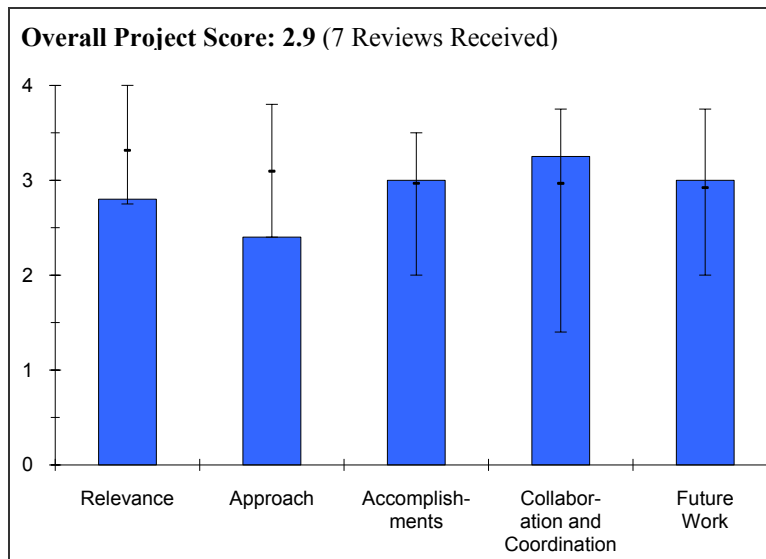
- The team is increasing the operating temperature to increase the electrolyzer performance. In water electrolyzers, this always results in decreased lifetime, and they are keeping the temperature above 80°C. The team needs to demonstrate that the electrolyzers will have a reasonable operation life at these higher temperatures.
- The diurnal nature of this project means there will be thermal cycling of the reactors and components. This needs to be addressed and is not discussed.
- The complexity of the conversion system is a weakness.
- The cost analysis is poorly described, which is a weakness.
- The project concludes that because electricity is a major contributor to hydrogen cost, voltage should be lowered to improve efficiency. The reviewer suggests doing an optimization on current density, as operation at a low(er) current density may lower electricity cost more than it raises capital cost.
- More H₂A assumptions need to be specified, for example labor requirements and basis for capital costs.
- As noted above, the overall process has to be designed for continuous operation. To accomplish this, all of the steps need to be considered, not just the molten salt cycle.
- It would be helpful to know the theoretical minimum voltage required for the electrochemical step.

Specific recommendations and additions or deletions to the work scope

- They need to plan on durability testing and thermal cycling.
- It would be beneficial to provide a table showing subsystems, capacity, cost, and maintenance for each major subsystem including the solar field, solar collector, and steam cycle, to name a few.
- More attention should be given to the sulfur trioxide decomposition step, particularly on discerning the need for its integration into the overall process.

Project # PD-28: Solar-Thermal ALD Ferrite-Based Water Splitting Cycles*Al Weimer; University of Colorado***Brief Summary of Project**

The objectives of this project are to 1) use the H2A analysis to provide guidance for a conceptual process design that is cost effective and determine feasibility, 2) conceptualize a scalable central solar reactor/receiver per H2A guidance on economics, 3) develop and demonstrate suitable materials for robust thermochemical redox cycling that will integrate easily into the solar reactor design, and 4) develop an overall plan to take the technology to the point of demonstration in five years, providing that market conditions warrant this step.

Question 1: Relevance to overall DOE objectives

This project earned a score of **2.8** for its relevance to DOE objectives.

- While this program targets the key goal of cost of hydrogen, there are basic issues about the project's ability to serve a customer. The hydrogen produced is likely to be impure and at low temperature, and the location of the facility has to be in a desert. It is hard to picture a large customer base lining up to purchase this hydrogen.
- The solar-driven thermochemical water splitting process supports the DOE objectives.
- Low carbon hydrogen is a key component of a hydrogen economy. This technology is competitive against biohydrogen production, photoelectrochemical production, and SMR with carbon capture and storage.

Question 2: Approach to performing the research and development

This project was rated **2.4** on its approach.

- The group has targeted and demonstrated rapid-cycle hydrogen generation and good (not great) material durability. The high temperature and small temperature difference between the oxidation and reforming step suggests that the overall energy efficiency of the process is low. Similarly, the high temperature of operation suggests that the costs and materials issues will always be significant.
- Oxidizing a reducing iron is likely to have a strong, negative impact on the iron structure. The hydrogen purity and hydrogen pressure are likely to remain low for this process, which limits its applicability.
- The project investigator did a good job addressing many of the weaknesses identified in last year's AMR.
- The approach assumes the ferrite is directly heated by solar power, which limits the operation of the process to the relatively few hours when appropriate sunlight is available. This will also introduce large thermal cycles, which are not addressed. The project investigator only addresses cycles between X and 1500°C.
- The project uses a simple process; there is only one reactor and only one reagent.
- The reagent is non-toxic, unlike all the other chemistries being researched.
- The new design does not lend itself to 24/7 operation. For this approach to be viable, they must be able to operate 24/7.
- The critical path needs to be in demonstrating a long cycle life of the chemicals. The project needs have more focus on this.
- The project this past year has done a very good job focusing on the critical technological issues, for example those identified by last year's review panel.
- The chemical looping approach is well established and an extension to hydrogen production is reasonable.

HYDROGEN PRODUCTION AND DELIVERY

- High temperatures (1200-1500°C) present a significant challenge for materials and energy storage.

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

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

- There are good cycling results on a five minute time scale. The small temperature difference between oxidation and reduction suggests that the hydrogen purity could not be high.
- The team was able to show that atomic layer deposition (ALD) CoFe_2O_4 can be cycled.
- It is unclear if the "ocene" cost analysis includes the price of processing to make the thin films. It seems to only include the raw material cost. ALD processing may substantially increase the cost, especially when such a large amount of the material is required.
- The number of cycle tests was not enough to demonstrate if the material is usable. The team needs to show hundreds (if not thousands) of cycles. The cycles should be between room temperature and operating temperature since they are not planning on operating 24/7.
- Operation and maintenance will be very expensive since the system is not operating 24/7. The reviewer would like to see the estimates for operation and maintenance used in the project's H2A analysis.
- The team seems to have made substantial progress towards demonstrating their goals.
- The project demonstrates a good comparison of bulk versus ALDC film performance and of considering the effect of the substrate on cycle reduction temperatures, which can lead to important conclusions.
- Temperature optimization is a significant development.

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

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

- Given the project, it is hard to imagine better collaboration.
- The team had very good collaborations.
- No evidence of collaboration.

Question 5: Approach to and relevance of proposed future research

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

- The presenter proposed to basically continue doing the current work .
- The project is ending.
- The team needs to show the cycle life.
- The team needs to modify the cycle to achieve 24/7 operation.

Strengths and weaknesses

Strengths

- This project has some interesting science.
- The project uses a simple process with non-toxic materials.
- The project has a strong team.
- The team has done a very good job of directing effort towards rectifying weaknesses identified previously.
- The team has done a very good job of experimental testing of material hydrogen flux rates at various conditions.
- It appears a tremendous amount of work has been conducted on this concept.
- The process appears to offer a promising solar-to-thermal and solar-to-hydrogen conversion efficiency.

Weaknesses

- There is a sense that this project is not likely to produce a practical option for hydrogen generation.
- It is not sufficient to use raw material cost for the ALD "ocenes" for the H2A analysis. The team needs to also include the processing cost to make the thin films.

- The system does not run 24/7; this means that there will be large thermal stresses as the system heats up and cools down each day.
- The team underestimates the operation and maintenance costs for a system operating for only a short time every day.
- The team did not address a key weakness from last year's review; i.e., high utilization of solar flux is critical for this project because the heliostat field is very expensive. The use of solar flux to heat the carrier material must be included in the economics. It is not acceptable for this project to propose high-carrier solids while doing economics on zero-carrier solids. This weakness should be addressed.
- Typically only five cycles are used to determine whether redox cycles are stable. While this is a good screening indicator, actual cycles will need to be over tens of thousands. Thus, we do not really know stability of cycling.
- While it is good of them to include an H2A analysis, no data is presented on capital costs or operating expenses. The team needs to list assumptions and corresponding basis.
- No fabrication costs of the materials seem to be included in the analysis.
- Cycle time is a critical factor for economics. However, there is no testing or assumptions listed to support the postulated five minute cycle time.
- A basic diagram of how the system would operate (in terms of the cycle) is not adequately detailed to lead the reviewer to have confidence that all cost components of the system have been included.
- The Aspen® model is not adequately labeled to make it explanatory or very useful.
- It is unclear whether or not labor is included in the analysis. Cost studies of similar systems reveal that labor can be a substantial cost contributor. Future presentations should list all key H2A assumptions.
- It is unclear how hydrogen and oxygen can be effectively separated in this solar-thermal process. It is also unclear if catalyst deterioration could be just an issue, or a serious problem.
- It is naïve to assume that ferrite is capital and will not be replaced. Material will have finite lifetime.
- The limited number of cycling experiments is a weakness. The process will undergo approximately 100,000 cycles per year. The team should perform 1,000 to 10,000 cycles at a minimum to evaluate ferrite stability.

Specific recommendations and additions or deletions to the work scope

- The project should be continued as a basic science effort since laboratory studies are needed to increase the purity and the overall efficiency. Few, if any, solar tower tests should be done at this stage.
- The above-listed project weaknesses are central to the relevance and success of the effort and they should have been addressed, especially since this project started in 2005.
- Long-term cycling experiments should be added. The economics need to be extended to consider the possibility of gas firing the system at night and during cloudy periods. The produced hydrogen will not be as "green," but

HYDROGEN PRODUCTION AND DELIVERY

- **Project # PD-29: High-Capacity, High Pressure Electrolysis System with Renewable Power Sources**

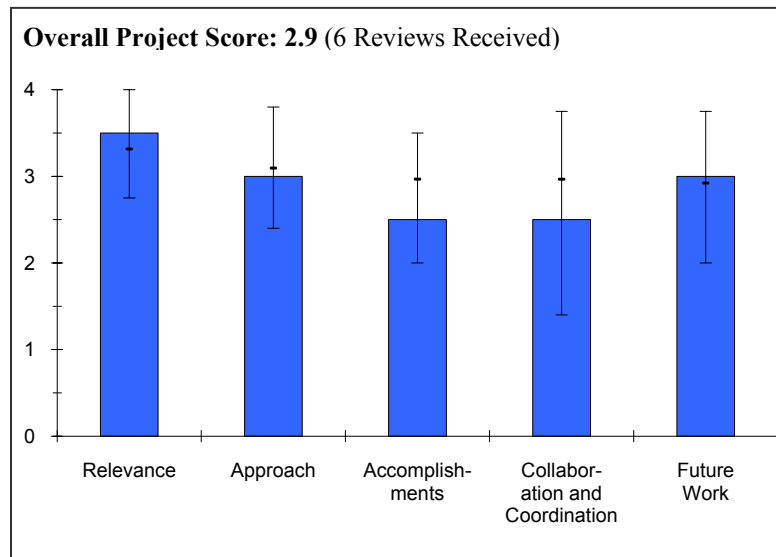
Martin Shimko; Avalence LLC

Brief Summary of Project

The electrolyzer development project goals are to 1) achieve at least a 15-fold increase in the gas production rate of a single high pressure production cell, 2) demonstrate the high pressure cell composite wrap that enables significant weight reduction, 3) build and test a 1/10th scale pilot plant, and 4) perform an economic assessment for a full scale plant (300 kg/day, 750 kW) that meets the DOE 2017 cost target of \$3.00/gge.

Question 1: Relevance to overall DOE objectives

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



- The program did meet the DOE research, development, and demonstration intent in developing a high-pressure electrolysis system that produces high-pressure hydrogen at the cell level without using mechanical compression.
- It is not completely clear what the advantages of this approach are over other types of electrolysis. While noble metals may not be needed, there are many other aspects of the cost that are driving up the capital cost of this technology.
- To achieve the DOE targets for low-cost high-pressure hydrogen production, this project focuses on the development of a unique alkaline electrolyzer cell design with the goal of generating hydrogen at a pressure of 6500 psi, thus reducing the need for mechanical compression. An emphasis is also placed on a multi-cell electrolyzer design (pilot plant scale-up) powered by renewable energy sources.
- This high-pressure electrolysis development program is fully aligned with DOE research, development, and demonstration objectives. Generation of 6,500 psi hydrogen allows direct filling of vehicle hydrogen tanks.
- Electrolysis tied to renewable resources is an important part of the DOE Fuel Cell Technologies Program portfolio.
- This is definitely a relevant project.

Question 2: Approach to performing the research and development

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

- Nested composite overwrap has shown promising results, but the team needs to further investigate the reactant mixing issue at each side of the cell.
- –The team needs a clearer pathway on where cost targets can go and how this can happen. Feasibility is also a major question, as the team is struggling to meet pressure at a safe purity level.
- The approach of using a cylindrical cell design and scaling up from a single-cell to a multi-cell “nested” design is feasible, but will require some creative engineering to complete.
- It would be interesting to see a cost study indicating the number of cells versus the length and diameter of cells during scale-up.
- The approach is very sound, with a logical progression of development. The initial work demonstrated 6,500 psi hydrogen production at a laboratory scale. The next logical steps being pursued are electrolyzer and balance-of-system scale-up. Problems identified during this scale-up work are being addressed. Success at resolving these problems will determine if continued development is warranted.

- The team is focusing on the major issue, which is whether high-pressure production can be achieved.
- The team is approaching this as an engineering problem (i.e., finding commercially available products to solve their problems). It is very likely that they will need to develop the materials themselves and it is not clear that they are prepared or planning on doing the material development themselves.
- The project is being executed with excellent efficiency given the resource level applied.

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

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

- Research did focus on a single path and understanding the design limitations, including its potential for further improvements. They are eliminating the need for a mechanical compression system by generating high-pressure reactant at the stack level.
- Significant issues were encountered in keeping oxygen purity at safe levels and it is not totally clear that these are going to be resolved. Nested cells will likely have even more issues than single cells.
- Progress demonstrating 6500 psi operation in single-cell testing has been made; however, more work towards completing the multi-cell (or nested-cell) design needs to be shown.
- A loss of cell efficiency is seen with the use of thicker membranes that are required for high pressure (6500 psi) operation. The effects of lost cell efficiency on the cost of hydrogen should be shown via the H2A model.
- Some technical and safety issues need to be resolved, including the possible accumulation of unsafe gas mixtures in the tubes exiting the electrolyzer cell.
- Significant progress has been made in terms of demonstrating the performance of the nested cell core at the laboratory scale and in demonstrating the ability to implement a composite fiber outer wrap. Reaching 6,500 psi pressure levels in larger cells remains the major obstacle, along with purity of the hydrogen and long-term operation. These obstacles are a significant challenge, and therefore progress will likely be slow. Modification of project goals should reflect this challenge.
- The progress seems modest for the time and funds spent up to this point.
- The team needs to show that they can operate at the higher pressures
- The electrolyzer efficiency is low and needs to be improved.
- The project demonstrated the membrane operation for a couple of hundred hours. The team needs to show the operation for over 1000 hours under real conditions.
- The team correctly acknowledges that their 6500 operation is not good enough. 96% oxygen purity should be end-of-life at worst, not beginning-of-life operation. The system clearly cannot last the 1000 hours of operation that is required. This was a single cell experiment and it is likely that the performance of nested cells will have higher impurities.
- The efficiency is very low and needs to be increased. The project is currently at approximately 50% efficiency, which is not close to the DOE targets (~69%).
- The project is demonstrating the high pressure operation requested by the DOE. Additionally, practical findings are being disseminated in the public forum. Full system integration up to 6250 psi is providing great practical learning for the program.

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

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

- The researcher can benefit from further collaboration with additional industry companies that specialize in sealing and hydrogen and oxygen diffusion.
- There was no real discussion of the progress of collaborators or any interaction between collaborators. The collaborators seem more like a supplier (of composite wrapping) and customer (using the National Renewable Energy Laboratory site), rather than much of a collaborative effort.
- In addition to last year's collaborations, Avalence is also working with Parker on the development of high pressure components (high-pressure hose assemblies) for the cell design.
- Some collaboration with HyperComp, Hydrogen Energy Center, and MaineOxy exists, but little information was presented to assess the degree of collaboration.

HYDROGEN PRODUCTION AND DELIVERY

- The project has a good team, but the interactions are not clear. It seems that they will really begin collaboration later.
- More collaboration between electrolysis companies would benefit the technology. For example, Giner appears to have a higher expertise in materials, while Avalence has a stronger system architecture and system optimization.

Question 5: Approach to and relevance of proposed future research

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

- Continuing on the path of developing larger cells and demonstrating scalability can support the 6500 psi reactant production without any mechanical compression.
- The project has some ideas to try, but did not really show any feasibility to date.
- A specific goal to scale-up the hardware for the pilot plant has been set. Avalence will need to demonstrate large diameter cell operation at 1000 psi, a go/no-go decision point for next year, and long-term 6500 psi operation.
- Barriers have been identified and are being addressed, predominantly in the areas of 6,500 psi operation with larger cells and reactant purity.
- The team needs to improve their membranes to increase the gas purity.
- The team needs to perform longer life testing.
- The team needs to increase their efficiency.

Strengths and weaknesses

Strengths

- Research did focus on a single path and understanding the design limitations, including its potential for further improvements. Eliminating the needs for a mechanical compression system by generating high-pressure reactant at the stack level is a strength.
- An alternative to acid-based electrolysis should allow for less expensive materials of construction, if the cost of high-pressure components does not exceed the benefit.
- Avalence has successfully demonstrated 6500 psi operation in single-cell testing. Although life-cycle testing is required, the short-term testing demonstrates the feasibility of the high-pressure cylindrical cell design.
- The core technology shows extreme promise at the laboratory scale. Some issues with respect to system scale-up have been successfully addressed, while other significant issues still remain. Avalence is very experienced and capable, with a sound project plan.
- It is an interesting concept to generate the hydrogen at 6500 psi.
- This seems to work for a single cell.

Weaknesses

- Hydrogen and oxygen diffusion through the material was not clearly addressed. The study did demonstrate eliminating the diffusion to some level by adding complexity to the balance-of-system but it did not address potential overwrap material improvements.
- The high-pressure and complex design seem to be adding more cost than benefit to the project, and safety is a serious concern.
- Polarization scans (I-V performance curves) were not given for the testing that was conducted. The stated power consumption (kWh/kg of hydrogen) for 40 and 80-mil membranes needs to be quantified by stating the specific current density operating points.
- No major weaknesses exist. There are several challenging barriers which need to be overcome, and these are being addressed.
- The efficiency is very low.
- The project is having issues with materials.
- Safety is a key concern.

Specific recommendations and additions or deletions to the work scope

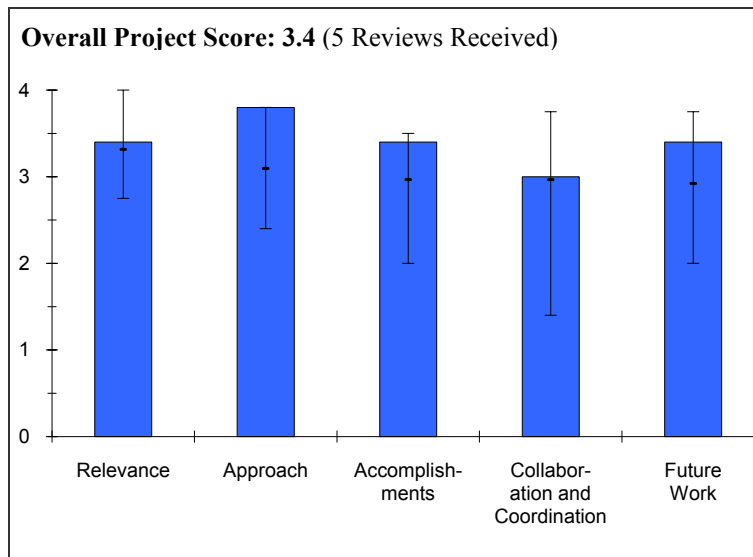
- The project would benefit from further study on reactant diffusion through the overwrap material and fabricating a larger stack, as well as demonstrating the technology scalability of any hydrogen generation at 6500 psi.
- If pressure targets cannot be reached, the team needs to look at this approach as a whole to see if there is still any benefit, including the efficiency and cost implications of compression and maintenance.
- An economic study of the system design should be conducted to demonstrate the feasibility of meeting the DOE cost targets for this program.
- Avalence should provide I-V performance curves in order to determine cell efficiency.
- No additions or deletions are recommended. The project should continue on its present path to address scale-up capable of demonstrating 6,500 psi hydrogen generation with high purity. Without this successful demonstration, further development is likely not warranted.
- The team needs to test the membranes at higher temperatures. When they operate in the nested-cell configuration, the internal temperatures will be higher. The team also needs to show that their bonding technique will work for a long period of time.
- Avalence would benefit from looking at higher reliability and efficiency compression technologies, such as the Linde ionic compressor. This may reduce their safety concerns and allow them to operate with lower-cost pressure vessels, while still capturing a high-efficiency operation. 3,000 psi may be a good "knee" in the optimum electrolysis pressure of operation. It would be beneficial to show diagrams of the system capital, operating, and feedstock costs compared with the various pressures in order to show what the optimal electrolyzer pressure might be.

Project # PD-30: PEM Electrolyzer Incorporating an Advanced Low Cost Membrane

Monjid Hamdan; Giner, Inc.

Brief Summary of Project

The overall project objectives are to develop and demonstrate an advanced, low-cost, moderate-pressure proton exchange membrane water electrolyzer system to meet DOE targets for distributed electrolysis by 1) developing a high-efficiency, low-cost membrane; 2) developing a long-life cell-separator; 3) developing a lower-cost prototype electrolyzer stack and system; and 4) demonstrating a prototype electrolyzer system at the National Renewable Energy Laboratory. Objectives for FY 09-10 are to 1) fabricate scaled-up stack components, 2) assemble and operate short stacks at Giner Electrochemical Systems for 1,000 hours, 3) complete system critical design review (CDR), and 4) begin fabrication of deliverable system.



Question 1: Relevance to overall DOE objectives

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

- The study did meet the DOE research, development, and demonstration project objectives, demonstrating an advanced, low-cost, 300-400 psi pressure proton exchange membrane water electrolyzer.
- This project contains a lot of good science that advances important principles. While the exact configurations may not be cost practical at this point, the underlying knowledge is important for setting design limits and advancing the field.
- The project is very relevant to DOE objectives in terms of cost and efficiency, but operating pressures of 300-400 psi will require a compressor to reach their ultimate goal of 6,500 psi, with its inherent cost and efficiency penalty. Stack optimization and system development exhibit a clear focus in meeting DOE goals.
- This project aligns with the DOE Hydrogen Program goals.
- This is indeed very relevant, as it provides renewable conversion to hydrogen.

Question 2: Approach to performing the research and development

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

- The dimensionally stable membrane (DSM) does show promising results and needs to be investigated further.
- All pertinent technical barriers are being addressed, often with multiple approaches. The approach includes a very feasible path toward demonstrating membrane reproducibility and durability, cell separator development, scaled-up stack design, and system development.
- The team has identified the critical path to develop a commercial product that meets the DOE targets.
- Giner is considering the complete system in optimization, including the DOE H2A values for compressor operation up to 6250 psi. However, it would be beneficial to explore the operation of all components up to ~3,000 psi or higher. This is in line with what was found by Avalence.

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

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

- A significant amount of work was spent on the characterization of the DSM and a couple of polymers, in house material, and an industry standard polymer (3M).
- Significant progress has been made in overall understanding. However, POCO graphite is very expensive and it is not likely to provide a cost savings. Some data was also somewhat misleading in that there are other failure mechanisms besides those being tested. It is not reasonable to claim 50,000-60,000 hours based on a 1000-hour test.
- Progress has been steady in all areas, with successful demonstration of DSM performance and lifetime. The remaining stack work is in the scale-up of membranes and separators, which should be challenging but not insurmountable. Successful completion of CDR will allow the initiation of system assembly and demonstration.
- The team has made very good progress.
- The stack efficiency is very impressive.
- Use of their high pressure dome increases safety and helps performance.
- The failure modes and effects analysis, as well as work on codes and standards, was included.
- The team decreased the cell assembly cost by decreasing the number of parts and changing manufacturing.
- Giner is showing good high-efficiency operation.

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

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

- The program did not show strong collaboration with industry (i.e., 3M is only a supplier). If they were a collaborating company, the presentation did not state any information except for indicating 3M as a polymer supplier.
- There was a good description of systems interaction in the safety review. The Entegris collaboration is apparent in the parts made.
- The partners are full participants and the work appears to be well coordinated. Parker Hannifin is a large-volume commercial manufacturer working on system development, Virginia Tech is a leader in hydrocarbon membrane research, 3M is a major membrane manufacturer and catalyst developer, and Entegris produces carbon cell separators with improved resistance to hydrogen embrittlement.
- The team is working with Parker Hannifin for balance-of-plant cost reduction.
- It is not clear if the team is working with 3M or just buying their catalyst.
- It would be nice to see more publications.
- More collaboration with other electrolysis companies would be beneficial. Electrolysis companies are, to a large extent, in the same boat. They would benefit significantly by pooling research resources in a manner similar to the photoelectrochemical projects.

Question 5: Approach to and relevance of proposed future research

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

- The team is developing an end-to-end system with lead industry suppliers.
- The next steps seem logical based on the work performed to date.
- Their proposed plans are logical, building on past progress to overcome the barriers of scale-up. The success of their scale-up activities will be a determining factor to warrant continued development.
- The future plans clearly push their development.
- The team is focused on the barriers.
- Mechanical pressure cycle testing would be of interest.

Strengths and weaknesses

Strengths

- The project did demonstrate technology viability and low-cost hydrogen production.

HYDROGEN PRODUCTION AND DELIVERY

- The project is aiming to develop a large-scale system and further evaluate the technology viability and durability at the system level.
- The project has a good fundamental science capability in terms of testing and approach.
- The project is very sound with demonstrated progress to date in the development of high-efficiency, low-cost membrane and a long-life cell separator. The barrier of scale-up of these components is being addressed. This barrier is challenging, but not insurmountable. The project has a highly effective and coordinated team approach.
- This is a strong team.
- The project has high efficiency and a low-cost stack.
- The titanium separator work is very good.
- The life test studies and accelerated testing experiments are well done. The team is using a good mix of experimental studies.

Weaknesses

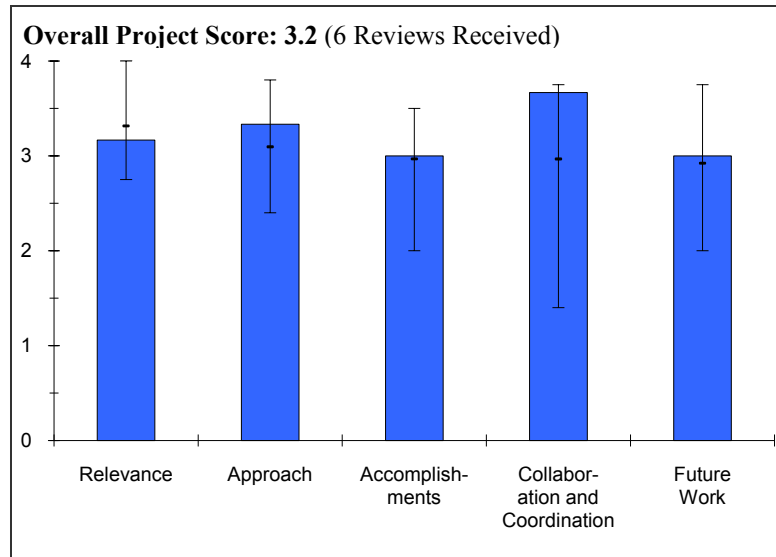
- A continuous operating run above 500 hours is needed for a true technology viability evaluation. The system durability is not there yet.
- The team has little commercial experience, or units in the field on which to base cost projections or lifetimes. Their extrapolations are very long.
- No major project weaknesses exist. Scale-up of cell hardware is the major remaining barrier, which is being addressed.
- It is unclear how the team is going to commercialize the technology.

Specific recommendations and additions or deletions to the work scope

- The project should be continuing with the end-to-end system development to demonstrate overall system efficiency, viability, durability, and cost efficiency.
- The reviewer has no recommended additions or deletions.
- The project should continue.
- As the project is exploring the pressure vessel operation, it would be beneficial to explore high-pressure operation as well, for example to demonstrate 3,000 psi operation. While H₂A-optimized hydrogen costs appear to be good with 300 psi operation, practical considerations of system reliability and distributed generation operation and maintenance would suggest that the elimination of compressors would be desirable. The Giner architecture also has a good opportunity for operating at elevated pressure. In addition, this would help them reduce parasitics associated with hydrogen drying.

Project # PD-31: Renewable Electrolysis Integrated System Development and Testing*Kevin Harrison; National Renewable Energy Laboratory***Brief Summary of Project**

The objectives of this project are to 1) identify opportunities for system cost reduction and optimization as they pertain to electric utilities; 2) characterize, evaluate and model the integrated renewable energy systems; 3) characterize electrolyzer performance with variable input power; 4) design, build and test shared power electronics; 5) develop cost models for renewable electrolysis systems; 6) quantify capital cost and efficiency improvements for wind and solar-based electrolysis scenarios; 7) perform characterization and performance testing on electrolysis systems developed from DOE-awarded projects; and 8) test electrolyzer stack and system response with typical renewable power profiles.

**Question 1: Relevance to overall DOE objectives**

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

- The system performance analysis and evaluation fall within DOE research, development, and demonstration project objective.
- The project is small-scale and it is questionable if this applies to larger-scale systems.
- This project provides a real-world demonstration of integrating renewable power sources with electrolyzers for hydrogen production, and as such it is extremely relevant to the DOE Hydrogen Program and fully supports DOE objectives. Real-world demonstrations are invaluable in addressing capital cost, efficiency, and integration with renewables to reduce the costs of generating hydrogen.
- This project supports the DOE Fuel Cell Technologies Program.
- The work aims to address cost reduction to meet the hydrogen cost goal in the area of wind and solar electrolysis. Since DOE has already funded their Technology Validation Program, it is questionable what additional value can be gained from doing the refueling station portion of the work.
- Hydrogen for storage is likely to be an early stage application for hydrogen and fuel cells, independent of vehicle success. High costs limit its practicality in the absence of a carbon tax or other policies to enable low-carbon hydrogen.

Question 2: Approach to performing the research and development

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

- The project is evaluating industry-developed end-to-end systems and/or components and technologies.
- The project is highly focused on demonstrating advanced controls, system-level improvements, and the integration of solar and wind renewable sources with electrolyzers. Their demonstrations are in the field and are real-world focused, generating valuable data.
- The energy storage cost analysis work approach is very interesting.
- The wind-to-hydrogen project approach is interesting, but the proposed integration does not seem correct. It is highly unlikely that wind towers will be dedicated to hydrogen production. It is more likely that they will do both hydrogen production and electricity production, so the power electronics would become redundant.

HYDROGEN PRODUCTION AND DELIVERY

- The power electronics work on the solar side is very interesting.
- Providing independent verification for government-funded electrolyzer development projects is very important.
- In the effort to reduce hydrogen cost, the project investigator focused on the appropriate areas that have the most influence in the overall hydrogen cost. It is a good strategy to let the grid take extra variable power from the wind and have the stack continuously run on a stable output.
- Data gathering along with close coordination with electrolyzer manufacturers provides valuable analysis.

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

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

- The project has shown excellent progress in several areas, including unattended long-duration operation of both proton exchange membrane (PEM) and alkaline electrolysis systems, electronics comparison of direct coupling with maximum power point tracking, analysis and benchmarking of hydrogen-based energy storage, and the commissioning and operation of a 350-bar refueling station. Barriers to the acquisition of more long-term test data are being addressed.
- The hydrogen station, shuttle bus, and the independent analysis are not part of this project, so it is unclear why they are discussing them. There is very limited time so the team should focus on the accomplishments that pertain to their project.
- The team finally began long duration testing, which is good.
- The power electronics for optimized solar photovoltaic (PV) electrolyzer operation was interesting, and the fact that the power electronics do not need tuning at each site is good.
- The data showed that unattended operation appears to be just a few days long. The project investigator needs to consider longer hours of unattended operation of both PEM and alkaline systems under variable wind conditions to test both stacks and power electronics under real-world conditions.
- The finding of the value of power electronics versus irradiance is significant.
- The drying energy consumption work has value.

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

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

- Numerous participants are involved in project and all seem to be fairly well coordinated. Participants include electrolysis and renewable power manufacturers, utilities, a university, and a research center.
- The work with partners and feedback to electrolyzer manufacturers is good.
- The international work is excellent. The development of international standards for electrolyzer testing is important.
- The team has excellent collaborations with various electrolyzer companies and various agencies to share lessons learned.
- The project has close ties to electrolyzer manufacturers.

Question 5: Approach to and relevance of proposed future research

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

- The team is evaluating the system performance of several vendors that are currently supported by the DOE research, development, and demonstration program.
- It is unclear if the assumptions for the cost of hydrogen produced using PEM units are realistic. Generally it is not realistic to assume PEM hydrogen cost based on a unit production number of several thousands.
- The project should try to include the cost of hydrogen for near term as well, when the number of PEM hydrogen production units is in the tens.
- The proposed future work includes comparison testing of PEM and alkaline electrolysis systems, side-by-side electrolysis stack testing, and investigation of the dynamic response differences between fuel cell, photovoltaic, and wind energy sources.
- The independent analysis and validation of the electrolyzer systems is good.

- Integration of the fuel cell is a good step to demonstrate the use of hydrogen for energy storage.
- If the intent is to compare PEM systems to alkaline systems, the project investigator needs to compare them on the same basis and have a list of appropriate evaluation criteria.

Strengths and weaknesses

Strengths

- The independent assessment of current DOE technology suppliers end-to-end systems is a strength.
- The project has a good overall systems evaluation approach.
- Renewable hydrogen production is a strength.
- The inclusion of several different technologies is a strength.
- The most significant project strength is the generation of real-world test data showing integration of renewable power sources with electrolysis systems. This test data is invaluable.
- DOE has spent a lot of money building the infrastructure for this project.
- The partners and feedback to the industry is important.

Weaknesses

- The lack of benchmark numbers from other projects is a weakness.
- It would be beneficial if there is more demand for hydrogen at hydrogen vehicle refueling stations because this would make the work more realistic due to having consistent demand.
- There are no weaknesses of note.
- The project is not focused. It wandered between wind-to-hydrogen and comparative testing, and then to activities that are not part of the project. They need to be careful that this does not turn into a “make work” project. DOE does not have the funds for a “make work” project and the project investigator is too good of a researcher to be used in this way.
- There is very little new technology, which is a weakness. The project seems to be more about the evaluation and optimization of commercialized technologies.

Specific recommendations and additions or deletions to the work scope

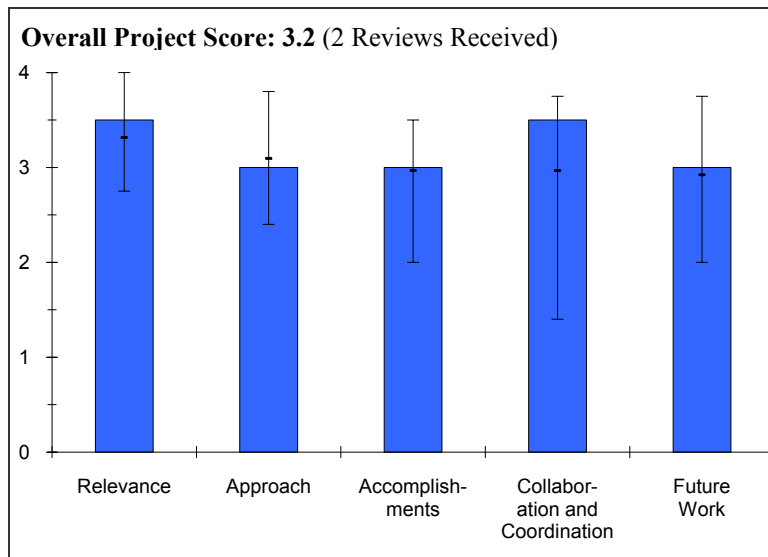
- Independent assessment of electrolysis systems helps to further understanding of this technology shortfall. The project should verify the operation of a similar, large-scale project in Stolpe, Germany. The Clean Energy Partnership (Total, Vattenfal, etc.) is involved in this project that uses a large windmill (330 kW) and electrolyzer to do similar work to this project. The presenter stated this concept was the only project of its kind in the world but it may not be. See the following resources: <http://www.hynor.no/total> (p.30-33), www.iphe.net/docs/Meetings/Norway_3-09/post-meeting/Germany/CEP.pdf (p.17), and www.netinform.net/H2/H2Stations/H2StationsDetail.aspx?ID=352.
- The team should make sure to include the production-level assumption when presenting cost targets because it was unclear what level they are based on (e.g., 1000 units produced or 1000s of units produced).
- The project should continue to expand the generation of real-world test data with even more electrolysis manufacturers and system concepts.
- As always, the team needs to continue long duration testing. They also need to show the integration with the wind.
- In the future, focus the presentation on work and accomplishments that are directly funded for this activity. The filling station and the bus, although interesting, are not part of the project and too much time was spent on them. It would have been better to spend more time on the long duration testing, the comparative testing, and the power electronics, which are key to this project. A lot of good work was done on these areas and more detail would be interesting.
- This comment is for both the project investigator and the DOE. Providing feedback to the manufacturers is very important work. NREL should continue doing this as part of the DOE electrolyzer programs (i.e., for currently active DOE electrolyzer projects) and provide independent verification of electrolyzer stack development, paid for by the DOE. It is unclear whether it is appropriate for the government to pay NREL to provide feedback to private companies to improve their technologies that are not part of a research and development project. For example, the HOGEN units being tested are not part of the development activity. This may be easily misinterpreted as consulting work paid for by the government. Perhaps some cost share from industry receiving

the feedback would be appropriate when the units tested are not directly part of a DOE-funded development activity. The concern is in the optics, not the execution.

- It is a good approach to let the grid take the extra "wild" power to keep the electrolyzer running on a steady level of power. The project investigator should consider other integration and operation options such as, (1) letting the electrolyzer run entirely on wind power to make hydrogen for point-of-use or storage (this is more feasible at remote locations without power transmission lines), or (2) sell all power to the grid at a higher price for renewable power and pull a little bit of electricity from the grid to make hydrogen. This might make more sense with limited and unpredictable hydrogen demand.
- The project should be expanded to consider hybrid electricity, i.e., wind, solar, and grid, to maximize return and minimize produced electricity costs.
- The project needs to consider the economic tradeoffs of constant utilization using grid electricity to complement wind or solar production. It is unclear whether using grid electricity offsets the capital cost to the extent that it might significantly lower the cost of peak power from stored hydrogen.

Project # PD-32: Photoelectrochemical Hydrogen Production: DOE PEC Working Group Overview*Eric Miller; University of Hawaii at Manoa***Brief Summary of Project**

The U.S. DOE Photoelectrochemical (PEC) Working Group brings together academic, industry and national laboratory leaders in the research and development of practical PEC semiconductor systems to produce hydrogen via solar water-splitting. The DOE PEC Working Group's primary objective is to develop practical solar hydrogen-production technology, using innovative semiconductor materials and devices research and development to foster the needed scientific breakthroughs for meeting DOE Hydrogen Program goals.

**Question 1: Relevance to overall DOE objectives**

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

- The technology may meet the DOE research, development, and demonstration intent, but the current state of proposed technology is at a very low technology readiness level (TRL). Each of the collaborating members is focusing on different synthesis materials, and there are many more materials for consideration.
- There are a number of good projects, especially those attempting to incorporate nanoscopic structures into their systems.

Question 2: Approach to performing the research and development

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

- Further planning of work and management of tradeoffs is still needed. More materials need to be evaluated. The current technology readiness level is very low, below TRL1. Market variability, manufacturing in a large scale, reproducibility, reliability, and durability are major issues with any new technology. Some technologies show great and promising results, but they never enter the market due to low feasibility.
- A three-pronged approach involving theory, synthesis, and analysis is promoted, which seems like a good strategy, but it needs more balance. There were only two theory projects (at approximately \$100k each?) and only one analysis (at \$100k?). Everything else is synthesis, accompanied by its own internal analysis.

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

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

- There are many other materials and experimental methods that need to be explored and evaluated, but the question is whether any of them would pan out.
- There were a few impressive reports and everyone seemed to have made some progress.

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

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

HYDROGEN PRODUCTION AND DELIVERY

- Collaboration is demonstrated among the team, in that each member is working on a different material for the same technology and sharing the results.
- A lot of good synergies have been set up. It was difficult to grade the projects, as it seemed like any given group's progress was significantly reliant on data acquired at other collaborating institutions.

Question 5: Approach to and relevance of proposed future research

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

- There are many other materials and experimental methods that need to be explored and evaluated, but the question is whether any of them would pan out.
- There is a good understanding of the technological barriers, but some of the projects are still basically hit and miss, with trying a material based mainly on chemical intuition and the presence of a decent band gap.

Strengths and weaknesses

Strengths

- Focusing on materials and evaluating their potential and viability is a strength.
- This is some really exciting work in the nanoscopic structures area. New computational power has the promise of discovering new semiconductor electrode materials.

Weaknesses

- Technology viability, scalability, and manufacturing in large scale are not addressed or recognized. Collaborating partners are all focusing on different materials, which shows how much work needs to be done.
- On the basis of simply delegating the projects among the three corners of the triangle, the program seems heavily weighted on analysis, and less on theory and synthesis. The presentation seemed to emphasize new predictive power, but the reviewer is not sure that any new compounds have been identified to date. It is unclear whether someone is going to investigate the compounds they identify. The need for large-scale manufacturing methods is recognized, but it still appears that most systems are small and require a vacuum chamber to for fabrication.

Specific recommendations and additions or deletions to the work scope

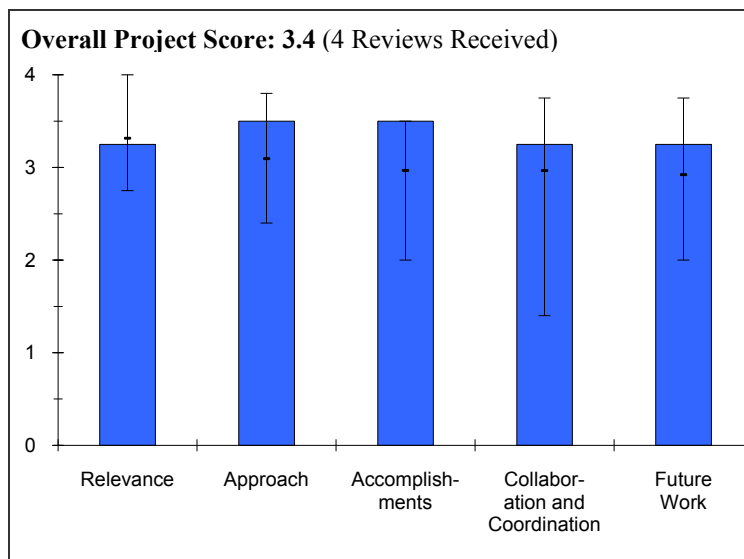
- The team should consider reevaluating technical viability and feasibility.
- The two theory groups are both at national laboratories. DOE should issue a request for proposals soliciting help from academic institutions.

Project # PD-33: Nanostructured MoS₂ and WS₂ for the Solar Production of Hydrogen*Thomas Jaramillo; Stanford University***Brief Summary of Project**

The main objective of the project is to develop new photoelectrode materials with new properties that can potentially meet DOE targets (2013 and 2018) for usable semiconductor bandgap, chemical conversion process efficiency, and durability. To date, there are no known materials that simultaneously meet these DOE targets.

Question 1: Relevance to overall DOE objectives

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



- The technology may meet the DOE research, development, and demonstration intent, but the current state of the proposed technology is at a very low TRL. Each of the collaborating members is focusing on a different synthesis material and there are many more materials for consideration.
- This is not a specific criticism of this talk versus the others, but at some point there needs to be a better cost analysis from the PEC Working Group on the entire system design. Even in PEM electrolysis the catalyst currently represents less than 10% of the entire cost. This will become more significant as the balance of plant cost is reduced, but at less than 10% of the current density for PEC the team will need a lot more benefits besides reducing the cost of platinum group metals to move forward.
- The project has a solid focus on PEC hydrogen.
- The team has a good understanding of the technical challenges to meeting targets for PEC water splitting.
- The project is investigating low-cost synthesis routes.

Question 2: Approach to performing the research and development

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

- There is still planning of work and tradeoff needs to be done.
- The team has a very well laid out experimental approach and grounding in the necessary advancements.
- The team understands the properties of nanoparticles and how they can be exploited.
- The team is applying concepts from nanomaterial literature to PEC applications.
- The team has a good understanding of materials properties and system needs.

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

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

- There is still planning of work and tradeoff needs to be done. More materials need to be evaluated. The current technology readiness level is very low, below TRL1. Market variability, manufacturing in a large scale, reproducibility, reliability, and durability are major issues with any new technology. Some technologies show great and promising results, but they never enter the market due to low feasibility.
- The proof of principle looks good, but there is a lot of work left to do. However, the approach allows a focus on demonstration of the right aspects.

HYDROGEN PRODUCTION AND DELIVERY

- It is difficult to say what has been done singularly in the last year, but what was shown looked like technical progress to me.
- The project achieved a wider bandgap, as designed.

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

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

- Collaboration is shown among the team, in that each member is working on different material for the same technology and sharing the results.
- The PEC Working Group has a lot of synergy, but there could be a little more clarity on how the work from Heske and Yan has helped guide the next steps.
- The project is fully integrated into the PEC Working Group.
- The team is working well with collaborators.
- The project is actively participating in the PEC Working Group.

Question 5: Approach to and relevance of proposed future research

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

- The team is evaluating different materials and their potentials.
- The project would benefit from input from some of the theory people.
- The project has an appropriate work plan moving forward.

Strengths and weaknesses

Strengths

- Evaluating materials viability is a strength.
- There is a good fundamental science and approach in general with a single focus, which allows for better understanding.
- The project has an excellent application of nanoscience. This may be DOE's best bang for the buck.

Weaknesses

- Technology viability, scalability and manufacturing in large scale are not addressed or recognized. Collaborating partners are all focusing on different materials, which shows how much work needs to be done.
- A practical device is a long way off, but the project could use some basic analysis to show that a system is cost feasible.

Specific recommendations and additions or deletions to the work scope

- The team should consider reevaluating technical viability and feasibility.

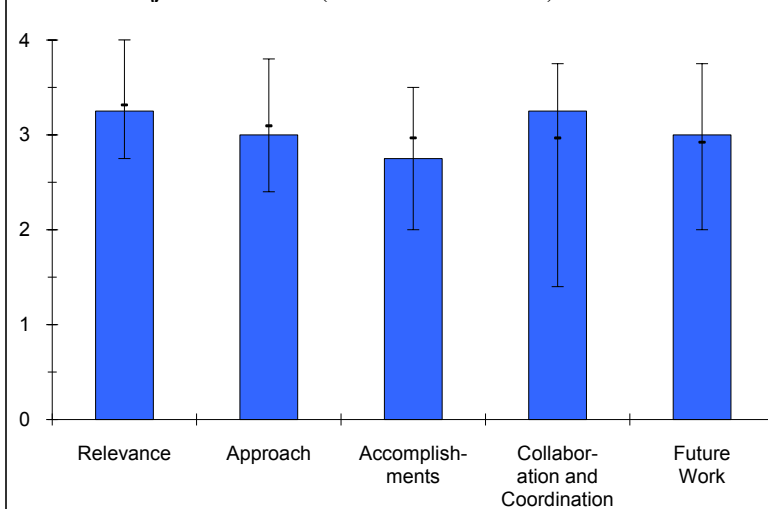
Project # PD-34: Development and Optimization of Cost Effective Material Systems for Photoelectrochemical Hydrogen Production

Eric McFarland; University of California Santa Barbara

Brief Summary of Project

The objectives for this project are to 1) develop improved materials for solar photon absorption using high throughput methods and new syntheses, with a focus on abundant and non-toxic elements; 2) use high-throughput screening to identify candidate materials with a threshold efficiency and stability that, with optimization, might meet the DOE performance and stability targets; 3) explore the effects of morphology on the PEC material system efficiency making use of nanostructures to minimize charge carrier path lengths and maximize reactive surface area; 4) explore processing and synthesis parameters to optimize efficiency through increased conductivity and minimized charge trapping and surface recombination of selected materials; 5) identify and minimize electrokinetic limits by synthesis of appropriate electrocatalysts compatible with the host, electrolyte, and reactant/product properties; 6) develop a complete “PEC unit,” combining material absorption, charge transport, stability, and electrokinetic design features; and 7) evaluate conceptual model reactor systems, theoretical and practical economic potential of alternative redox reactions, and estimate hydrogen production costs.

Overall Project Score: 3.0 (4 Reviews Received)



Question 1: Relevance to overall DOE objectives

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

- Perhaps the technology does meet the DOE research, development, and demonstration intent but the current state of proposed technology is in a very low TRL. The question is, compared to current PV technology, how superior are new materials going to be and would they improve the current PV efficiency by 50% or another level.
- As part of the PEC Working Group collection of projects, this project has the same benefits and drawbacks. It offers an interesting area for study but it is likely a long way from practical system development.
- For the hydrogen program to be a success, both cost and scale are vital components. This project keeps in mind that the use of expensive or rare materials will drive the final cost up, specifically by looking at abundant, low cost elements.
- The team is addressing barriers to efficient and cost-effective PEC production of hydrogen.

Question 2: Approach to performing the research and development

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

- The research does focus on evaluating different syntheses, and laboratory evaluations of small samples do show some promising results.
- The project investigator did not attend the poster or have a delegate, so it was impossible to ask questions on the approach. Normally indium phosphide is not stable in water. The use of alternative oxidants seems to get away from the goal of direct water splitting.
- The project shows good focus, not just on good basic science, but also on incorporation into a scaled system.
- They are using a systematic approach with go/no-go decision points.

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

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

- There is still planning of work and tradeoff needs to be done. The current technology readiness level is very low, about TRL1. Market variability, manufacturing in a large scale, reproducibility, reliability, and durability are major issues with any new proposed technology. Some technologies show great and promising results, but they never enter the market due to low feasibility.
- The budget seems large for the amount of progress made.
- Progress has been achieved in two major areas. The proposed coupling of the PEC hydrogen process with the biomass/methane coupling process gives a compelling, if complex, system to examine. This innovation in thinking has been proposed by the investigator to have side-stepped one of the more difficult challenges of PEC, oxygen oxidation, and replace it with the more facile bromide oxidation.
- The project has made good progress, especially considering there has been no funding in the past two years.

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

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

- Other members of the working group are working very well together and the reviewer did not have any comments to the contrary regarding this project investigator.
- In a project that is a confederation, rather than a fully coordinated multi-institution project, the collaborations and discussions are very good.
- The team is collaborating with key players and institutes.

Question 5: Approach to and relevance of proposed future research

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

- There are many other materials and experimental methods, which need to be explored and evaluated. The question is whether any of them would pan out.
- The proposed future work clearly builds on the successes and failures of previous work, while keeping an eye on the overall program targets.
- DOE should fund this work if they are expecting additional results.

Strengths and weaknesses

Strengths

- The project did well in out-of-the-box technical approaches, collaboration with other research labs, and focusing on the stability of materials.
- The project had strong characterization abilities.
- The synthetic capabilities to create new materials are strong, as well as the ability to formulate target compositions and then create them. The high-throughput screening capabilities enable rapid screening of compositional variations. The continued search for how to overcome barriers yields innovative proposed solutions worthy of further investigation.

Weaknesses

- Technology viability, scalability, feasibility and manufacturing in large scale are not addressed or recognized.
- No cost projections are provided, and there has been very little output from Tasks 7-9.
- It is not fully clear if the proposed particle passivation schemes will be able to keep the particles unagglomerated in the reactor without diminishing photo activity.
- The reviewer presumes there is a good understanding by the investigator, though it is not clear if there is strong understanding/collaboration regarding the engineering challenges that may be present with integration of the proposed CH₄/Br₂ cycle step.

Specific recommendations and additions or deletions to the work scope

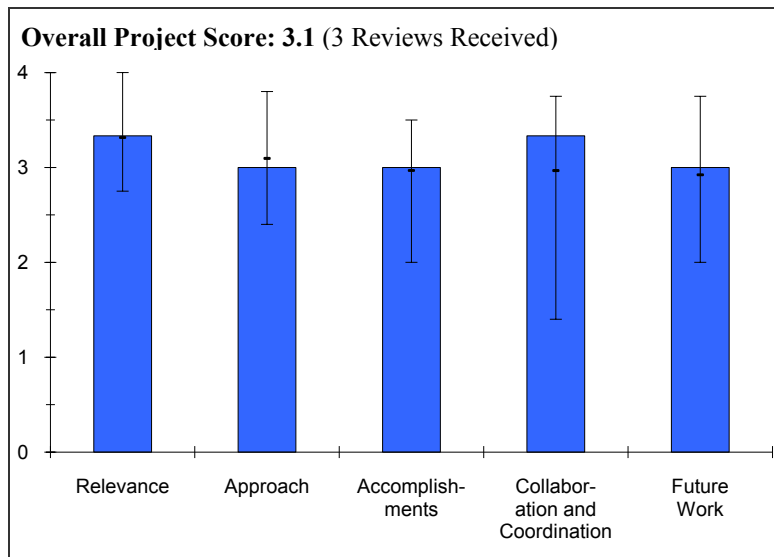
- The project should produce larger active area cells.
- The project appears to be ending this year.

Project # PD-35: Semiconductor Materials for Photoelectrolysis

John Turner; National Renewable Energy Laboratory

Brief Summary of Project

The objective of this work 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 a solar-to-hydrogen efficiency of at least 5% with a clear pathway to a 10% water splitting system, 3) exhibits the possibility of 1,000 hours stability under solar conditions, and 4) can be adapted to volume manufacturing techniques. The main focus of our work this past year has been to develop and optimize state-of-the-art materials that we have identified as promising for meeting DOE's near-term efficiency and durability targets.



Question 1: Relevance to overall DOE objectives

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

- The technology may meet the DOE research, development, and demonstration intent, but the current state of proposed technology is in a very low TRL. Each of the collaborating members are focusing on different synthesis materials, and there are many more materials for consideration.
- Materials are the best to date, in terms of direct water splitting. The reviewer would recommend specifying the project dates for this phase versus the entire field. If we have really been working on this same project since 1991, the progress is not impressive.
- This is a vital link between the storage of solar energy and hydrogen energy technology.

Question 2: Approach to performing the research and development

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

- The research does focus on evaluating different syntheses, and laboratory evaluation of small samples does show some promising results.
- The experimental approach is reasonable for the short term, although RuO₂ as a counter-electrode does not eliminate the platinum group metal (PGM) issue. It is also misleading to say that \$5.50/kg is "quite possible" based on the current status. This would require a 20% efficiency, 20-year lifetime and cost of \$80/m² of material, all simultaneously.
- The project investigator understands the technical barriers, but the project is so big it is hard to define a central theme or focus.

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

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

- There is still planning of work and tradeoff needs to be done. More materials need to be evaluated. The current technology readiness level is very low, below TRL1. Market variability, manufacturing in a large scale, reproducibility, reliability, and durability are major issues with any new technology. Some technologies show great and promising results, but they never enter the market due to low feasibility.

- It is not totally clear what work is occurring under the project investigator versus other partners. A lot of the work presented also seemed to be in specific groups' posters. However, stability mitigation strategies are an important part of the strategy, especially if they can be applied beyond the level III-V systems.
- The team tried to show technical progress by reporting projects moving ahead and others being laid aside. It was difficult to decipher whether the technical progress was occurring at NREL or elsewhere, or whether the work was funded by money flowing directly from DOE or via an NREL subcontract. In other words, a lot of results were shown, but it is unclear how much of it should have been in NREL's presentation.

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

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

- Collaboration is apparent among the team, in that each member is working on different material for the same technology and sharing the results.
- The PEC Working Group seems to be very well connected with each other and working in synergy.
- The team has excellent PEC Working Group interaction. They are clearly taking a leadership position.

Question 5: Approach to and relevance of proposed future research

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

- I would like to see the computational predictive power put to more use.

Strengths and weaknesses

Strengths

- Focusing on a single material and evaluating its potential and viability is a strength.
- This is essential work as part of the PEC Working Group, in developing reporting standards and common testing. Stabilization strategies are an important part of the project and this is the one group discussing such strategies. A long history and deep knowledge in the area of direct water splitting should provide good direction for evaluation.
- The project brings leaders in the PEC community into the DOE program. It was a good idea to establish efficiency standards.

Weaknesses

- Technology viability, scalability, and manufacturing in large scale are not addressed or recognized. Collaborating partners are all focusing on different materials, which shows how much work needs to be done.
- The project investigator should focus on making the project stand on its own merits instead of stating very broad and misleading statements about other approaches (e.g., combinatorial synthesis and electrolysis in general). The system capital cost and utilization factor is not clear, raw materials are expensive, and the system will be complex. Someone, whether this PEC Working Group or DTI, should be disclosing more of the assumptions that went into the cost model because the system design is not going to be simple in terms of compressing the hydrogen.
- The anticipated synergism between theorist and experimentalist has not quite happened yet. The reviewer is waiting for the experimentalist to try something that the theorist points to. Low-cost synthesis was listed as a secondary concern after materials, but the reviewer did not see anything on it.

Specific recommendations and additions or deletions to the work scope

- The team should consider reevaluating technical viability and feasibility.

Project # PD-36: Maximizing Light Utilization Efficiency and Hydrogen Production in Microalgal Cultures

Tasios Melis; University of California Berkeley

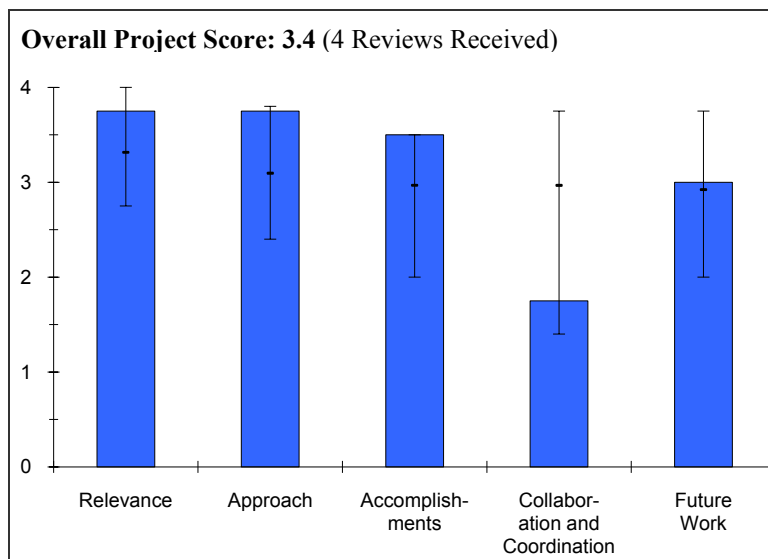
Brief Summary of Project

The objective of the project is to minimize the chlorophyll antenna size of photosynthesis to maximize solar conversion efficiency in green algae. The project will identify and characterize genes that regulate the Chlorophyll antenna size in the model green alga, *Chlamydomonas reinhardtii*, and apply these genes to other green algae, as needed.

Question 1: Relevance to overall DOE objectives

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

- Improving the light-to-hydrogen conversion efficiency by reducing antenna size fits well with the DOE Hydrogen Program mission.
- The project has a very clear relevance to the stated DOE Hydrogen Program goals for the improvement of light utilization efficiency in photobiological hydrogen production.
- The reduction of photosystem antenna size is potentially a very helpful element so that photobiological hydrogen production can work well in the long term.
- The issue of adapting the antenna size to optimize growth is key to the large-scale, inexpensive production of algal biofuels. This has been a very systematic and productive study, making clear progress each year at decreasing the antenna size and increasing the effective amount of photosynthetic electron transfer at high light.



Question 2: Approach to performing the research and development

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

- The genetic approach to antenna reduction is sensible as a start, but the project investigator did not indicate or is unaware of the limitations of this approach in terms of practical solutions. The consequences on slower growth rate were not mentioned, let alone discussed.
- This is a well-thought-out, highly targeted molecular approach that has yielded very clear results. Given the project's focus on regulatory elements, genome-enabled approaches (especially transcriptomics) could be more effectively leveraged to examine the timing of expression and relevant regulatory networks. However, this may be beyond the scope of the current project.
- The investigator used the right approach, which has been quite successful so far.
- The project involves the discovery and characterization of mutants that regulate antenna size. Three mutants have been discovered: one is completely characterized (at least in terms of physiology, though more mechanistic studies could be performed), another is partially characterized and the third awaits complete characterization. All three appear to be functionally relevant.

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

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

- The project investigator ran into some technical problems that diverted attention from the main focus. The actual data showing the relative change in rates for oxygen evolution for mutants (2) were minimal and had large errors. No data showing a comparison of rates to optical absorption were discussed, even though this was

the primary motive of the work. No hydrogen data was shown, so the effectiveness to hydrogen production was not apparent.

- The project has made impressive progress and significantly exceeds many key DOE targets in terms of the overall improvement of light use efficiency. Although there have been some issues regarding specificity of the antibodies raised against the *tla1* protein, problems of this nature are not uncommon, and the investigators appear to have successfully resolved the issue. The project has generated two publications thus far (one review and one on primary results) and, based on the work presented, several more are likely to follow.
- The investigator did excellent work in a progressive manner from mutant *tla1* to mutants *tla2* and *tlaR*, moving toward the DOE project goal.
- Progress in the project is excellent. The antenna size has been decreased, mutation by mutation, from over 600 chlorophylls to close to the theoretical size limit of just under 150 chlorophylls. Astoundingly, this has had almost exactly the predicted effect on both the rate of photosynthetic electron transfer at high light intensity and the resistance of the organisms to photoinhibition. This project is on schedule to meet all of its goals. The mutations are being used now by others both in industry and at NREL for DOE-funded research in hydrogen production.

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

This project was rated **1.8** for technology transfer and collaboration.

- The team does not have any collaboration; the project is working independently. The absence of data, as noted above, is a shortcoming. The project investigator needs to provide data demonstrating the effectiveness of the mutants and find collaborators, which should be easy since he is working at the largest bioenergy laboratory in the country.
- As stated by the lead investigator, this is a single-source project with no significant outside collaborations. If collaboration was not a requirement at the time of the project's original selection for funding, it seems somewhat unfair to give it an evaluation of "poor", but this is the only available option in the grading system though the reviewer would prefer the option of giving a "not applicable" evaluation in this case.
- If possible, it would be better to make the other antenna mutants, such as *tla2* and *tlaR*, available to the scientific community. In this way, the question of whether any of these antenna mutants can help photobiological hydrogen production could be tested by independent laboratories, which is essential as in any other scientific research.
- While it is clear that the specific goals of this work are contained within the project investigator's laboratory, it would be good to see more formal collaboration in the characterization of the mutants. Characterization could be tested both in terms of mechanism of the proteins involved and in terms of the efficacy of the mutations in a real-world application. Some of this is happening without formal collaboration, which is great, but the rate of implementation could be increased with a more concerted effort in this regard.

Question 5: Approach to and relevance of proposed future research

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

- The project has a minimal description of priorities. It is difficult to know what the project investigator will do next or what his understanding is of the problems that need to be overcome.
- Since the project is nearing the end of its funding period, it is somewhat difficult to assess future work. Having said that, the investigators have identified a promising new avenue of research with *tlaR* mutants and would no doubt apply many of their previously developed techniques to characterize the functional properties of this protein and its role in antennae formation.
- The proposed future work is mainly to finish up with mutants *tla2* and *tlaR*, which looks reasonable.
- The remaining work is clear in terms of characterization of the mutants and is well laid-out.

Strengths and weaknesses

Strengths

- The project did well in the creation and screening of antenna mutants.

HYDROGEN PRODUCTION AND DELIVERY

- There has been impressive progress from a highly productive research group. In addition to its relevance in photobiological hydrogen production, the results of this work will have very clear relevance to considerations of algal systems for bioenergy production, regardless of the target fuel compound.
- This reviewer in general agrees with the comments made by last year's reviewers: the investigator has demonstrated superior progress toward well-defined goals; the investigator has a collection of mutant organisms with truncated antenna sizes and, based on these mutants, novel genes were identified; the outcomes reveal how chlorophyll antenna sizes are regulated for the first time in *Chlamydomonas*; the investigator's laboratory is well equipped to determine chlorophyll antenna size; the team has a good project investigator and demonstrated accomplishments; this project has a well-defined problem to solve that is directly applicable to large scale growth; the project team has demonstrated that mutations that result in decreased antenna size can be found and can also improve photosynthetic efficiency and stability to high light levels; and the investigator is an expert in photosynthetic systems of *Chlamydomonas*.
- The greatest strength of the work is the systematic manner in which mutants have been developed, characterized and shown to behave in predictable ways.

Weaknesses

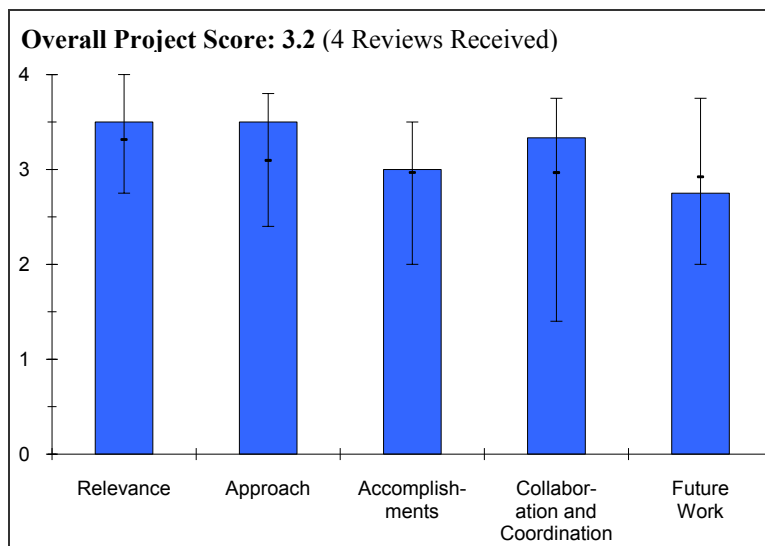
- The project had weaknesses with its limited characterization of mutants, old recycled data, a lack of independent corroboration of data, and no established collaborations established.
- This reviewer in general agrees with the comments made by last year's reviewers: even though mutants with truncated antenna sizes displayed higher photoconversion efficiency (oxygen evolution), it is not yet determined if hydrogen production is similarly improved; the project has insufficient data and descriptions on advanced mutants; ultimately, this project needs to be coupled to hydrogen production values in order to be critically evaluated; no data was presented to show increased hydrogen production in the *tla1*, *tla2*, and *tlaR* mutants; and the investigator should have made the *tla1*, *tla2*, and *tlaR* mutants fully available to the scientific community for independent tests.
- There are no serious weaknesses in this project. As stated above, more formal collaborations with industry and other laboratories could now be formed to accelerate the pace of implementation.

Specific recommendations and additions or deletions to the work scope

- If the project were to receive renewed funding, it would be significantly strengthened by establishing partnerships with groups more focused on photobioreactor design and evaluation. These partnerships would provide an important test bed for generated strains and allow the investigators to examine potential scaling issues.
- As stated above, expansion of the genome-enabled approaches would benefit this approach.
- One general concern is that, based on growth rate and other properties, these mutants would presumably be at a significant competitive disadvantage relative to wild-type algae and other phototrophes. Although it may be beyond the scope of this project, the question of whether photobioreactors can be maintained over time, with engineered algal strains remaining the dominant population, would seem to be an important consideration in scaling and eventual deployment.
- Overall, the investigator has made excellent progress with a quite reasonable project scope. This project effort should be funded when possible if the investigator could agree to make the antenna mutants such as *tla2* and *tlaR* available to the scientific community.

Project # PD-37: Biological Systems for Hydrogen Photoproduction*Maria Ghirardi; National Renewable Energy Laboratory***Brief Summary of Project**

The overall objective of project is to develop photobiological and integrated photobiological/fermentative systems for large-scale hydrogen production. Task objectives are to 1) address the oxygen-sensitivity of hydrogenases, which prevents continuity of hydrogen photoproduction under aerobic, high solar-to-hydrogen (STH) conditions; 2) utilize a limited STH hydrogen-producing method (sulfur deprivation) as a platform to address other factors limiting commercial algal hydrogen photoproduction; and 3) integrate photobiological and fermentative systems in different configurations for less costly hydrogen production in the short term.

**Question 1: Relevance to overall DOE objectives**

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

- All tasks have high relevance to the DOE Hydrogen Program mission.
- The project's objectives are highly attuned to the DOE Hydrogen Program objectives and this was clearly described in the presentation materials.
- The main goal of the NREL photobiological hydrogen project is to create an oxygen-tolerant hydrogenase mutant, which (if successful) could be a very helpful component for photobiological hydrogen production to work well in the long term.
- The three tasks address important elements of both continuity of biological hydrogen production and feedstock costs. The first task is the oxygen sensitivity of the hydrogenase. The second task is working with the sulfur deprivation approach to increase product yield in immobilized systems, in particular looking at ATPase mutants that all proton leakage and reduced antenna size mutants. The final task is integrating photobiological and fermentative organisms to improve the total yield of hydrogen. Each task has shown progress towards reducing risk though some have more than others, as described below.

Question 2: Approach to performing the research and development

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

- The project approach uses a combination of the development of previous research and development and some very clever new ideas.
- The research approaches (discussed in more detail below) are clearly focused on addressing key barriers in the development of scalable hydrogen production using phototrophic organisms.
- The project uses a rational scientific approach of using computer simulation of hydrogenase coupled with site-directed mutagenesis, although there has been no luck so far in the team's attempts to create a desirable oxygen-tolerant hydrogenase mutant. The expression of an oxygen-tolerant bacterial hydrogenase in *Chlamydomonas* is a reasonable alternative approach. The team also has a good approach of creating fusion between hydrogenase and ferredoxin to improve reductant flux to the hydrogenase.
- The first task met some difficulty. The hydrogenase mutants designed to block oxygen from entering the active site actually had the opposite effect, presumably due to folding issues. This aspect of the project now awaits further modeling to determine if it is possible to design mutants that can both block oxygen and avoid protein

destabilization. The reviewer wonders, in fact, if design mutants to stabilize the protein might have the desired effect, simply because it may be the protein dynamics that best lends itself to oxygen entry. The focus of task 1 has turned to the expression of a bacterial oxygen-tolerant hydrogenase in *Chlamy*. The constructions have been made and inserted, but it is not clear if this has resulted in protein expression or activity at this point and additional work is ongoing to understand the limits to expression. Finally, progress has been made towards creating a system for random mutagenesis, including an expression system for hydrogenase in *E. coli* that has been developed. This system will be used to screen libraries of random mutants for oxygen tolerance. A special high-throughput assay has been developed. While there were no home runs in task 1, each of the subtasks has shown progress or answered an important question about feasibility and therefore risk assessment.

- Task 2 has shown more progress. In particular, the ATPase mutants designed to allow some leakage of protons in the chloroplast, and thus keep the gradient from limiting the rate of photosynthetic electron flow, appear to have had a positive effect on overall hydrogen production on the order of a third greater. This is both an interesting scientific observation, as it suggests that the rate of the photosynthetic electron transport chain really is rate limiting as expected, and it provides some hope for further improvement of the hydrogen production rate by increasing photosynthetic rates. They also took advantage of the mutants being prepared by Mellis (also part of this program) that decrease antenna size and thus allow denser cultures at higher light levels. Again, the rate of hydrogen production was clearly much higher in these mutants, particularly in the early time after sulfur deprivation. The fact that this works as predicted suggests that we are really beginning to get a handle on what the limiting issues are, which bodes well for further improvement. Overall, these are probably the most interesting and potentially useful results in this project.
- Task 3 also showed some promising results. In this task, the concept is to couple biomass utilization with algal hydrogen production. By fermenting biomass to acetate and related materials, the biomass is available for uptake by photosynthetic organisms that can use this as an energy source, along with light, for making hydrogen. Apparently the two separate reactions, acetate with the photosynthetic organisms and fermentation of potato wastes to form organic acids (and to make hydrogen), have both worked. It remains unclear whether there is really any great advantage of using photosynthetic organisms rather than just making the hydrogen anaerobically, given the complications of having to illuminate the cultures and the oxygen made by the cultures interfering with hydrogenase action, but the concept is interesting.

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

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

- Multiple types of data were presented, which indicates a high degree of characterization. One issue could be the limited value in some proof of concept ideas like hydrogenase-ferredoxin fusion that would be unlikely to be applicable in vivo or lead to a practical in vitro system, in the reviewer's opinion.
- For Task 1, it is difficult to assess progress due to recent shifts in objectives. Expression of alternate hydrogenases, such as *Chlamydomonas*, is at a very early stage of development, and although the goal of developing hydrogenase-ferredoxin fusions seems interesting and relevant to Hydrogen Program goals, it is unclear how this will be pursued further at NREL. If funding is not available, will this be handed off to the Massachusetts Institute of Technology? Other subtasks appear to be at transitional stages, and further study is needed to assess potential impacts.
- For Task 2, the studies on immobilized algal films have yielded interesting results on the tradeoff between optimal hydrogen production rates versus oxygen protection. These studies should inform the development of future production platforms as the work moves forward. The construction of ATP synthase is at too early a stage to meaningfully assess progress.
- For Task 3, the project has made good progress in terms of optimizing conditions for hydrogen production by bacterial consortia and determining whether growth on algal biomass would be feasible (the presentation implies that it is feasible). However, the real test of this system will be integrating the fermentative subsystem with the photobioreactor. Although it appears that connections have been completed, no further information was presented, but it would have been helpful to see even preliminary data. I am less clear on how the potato waste fermenter fits into this project; is this a necessary sub-element?
- Although there is clear progress on the various subtasks, there are many points listed where project elements are either a transitional stage or have been just been initiated, making it somewhat difficult to assess the progress of the project as a whole.

- Overall, this project is making quite reasonable progress, although the project team so far (for nearly 10 years, since FY 00) seems unable to create a desirable oxygen-tolerant hydrogenase mutant. This probably just reflects the challenging nature of the research project. This reviewer believes the project investigator and the team are quite talented and are working hard with decent effort. Therefore, their effort should be appreciated. They are making an effort also in somewhat different areas, such as the sulfur-deprivation platform and other research aspects.

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

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

- The team has multiple effective collaborations.
- Although there are extensive collaborations with other institutions, it is not always clear how these fully integrate into the project's overarching objectives or future goals, which may contribute to the somewhat scattered sense of objectives (discussed in more detail below).
- The collaboration of the NREL team with other institutions is excellent. It seems intended to reach out to others in the field and rightly so.
- The team has significant and viable collaborations on each task. It was particularly nice to see the collaboration between this group and Mellis on the antenna mutants, as it points to the importance of interactions between DOE-funded researchers in this area.

Question 5: Approach to and relevance of proposed future research

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

- Multiple tasks are planned with a clear justification for most, though one issue is how the priorities are established. There was limited justification in terms of quantitative expected improvements for each task. The reviewer questions, if fewer funds were available, which tasks would be prioritized first and why.
- Several of the sub-tasks are at critical points where viability will need to be demonstrated in the coming year. Although the majority of the specific research objectives are appropriate, the reviewer would have liked to hear more discussion on how effort will be directed if a given element does not perform to expectations.
- The proposed future work looks reasonable.
- For task 1, some hard decisions need to be made, particularly about moving forward with the site-directed work, but also about the likelihood that a truly random mutagenesis approach is going to achieve the kind of results desired. This task could simply go on forever trying to determine what might be a better approach without the ability to make some sort of clear prediction based on structure/function understanding. While the transfer of the oxygen-tolerant bacterial gene is a possibility, there are many complexities in such a system that go well beyond just the hydrogenase and it is difficult to see how the different factors are going to be sorted out.
- As described above, task 2 is making better progress and the proposed studies seem more logical.
- Task 3 is confusing to this reviewer. The team needs to determine what value is added from using photosynthetic organisms if the only real objective is to go from potato starch to hydrogen. It seems that other non-photosynthetic organisms would be better suited for this purpose and would be much easier to grow.

Strengths and weaknesses

Strengths

- The team has a strong record of accomplishments, publications, invitations, and scholarship. This is an interactive group that educates the community and shares information to advance the field.
- The project is clearly attuned to the goals of DOE's Hydrogen Program and nicely leverages resources available at NREL and the collaborating institutions.
- This reviewer in general agrees with the comments made by last year's reviewers: this is a long-term project that is relatively well funded and has many partners; the project team is exploring the fundamental understanding of hydrogenase structure and function, particularly with regard to oxygen tolerance; and the team is also characterizing the conditions that allow hydrogen production, particularly when some oxygen is present.

HYDROGEN PRODUCTION AND DELIVERY

- The major strengths of the project have been in better defining some of the parameters that can be productively changed. It appears that decreasing oxygen sensitivity by blocking oxygen pathways through design is more complex than expected. On the other hand, making it possible for the photosynthetic system to run faster does seem to increase hydrogen evolution rates, as does decreasing the antenna size, and this is valuable knowledge.

Weaknesses

- The status of attaining hydrogen production benchmarks was not made clear. It was also unclear how dead-ends are identified (i.e., go/no-go decisions). It seems that some projects get carried forward with no closure.
- The project's tasks and subtasks, although individually interesting and appropriate, in many cases seem scattered across a wide range of goals and objectives. It is sometimes unclear how these subtasks form an integrated project where the whole is greater than the sum of the parts. This should not be read as a criticism of the newly developed project elements, which are interesting and appropriate (and were apparently requested in a previous review). However, as the project moves forward, it would be appropriate to evaluate the performance of various subtasks (both new and old) and redirect effort and resources to a more streamlined set of well-integrated goals.
- This reviewer in general agrees with some of the comments made by last year's reviewers: progress in this project seems slow or at least unclear. For example, the team has been working on developing high-volume throughput screening tests for several years and it is not clear what progress has been made. Other comments from last year include the following: the challenges and progress should be better identified; there is no indication, at this point, how this work could be scaled and no real understanding of how to increase the hydrogen production to a point that will be useful at scale; and this project is early stage exploratory work, which is not a weakness, but it makes extrapolation to any kind of useful system essentially impossible.
- The logic associated with task 3 is a bit unclear. They need to quickly answer the question about whether involving photosynthetic organisms in this case really makes sense.

Specific recommendations and additions or deletions to the work scope

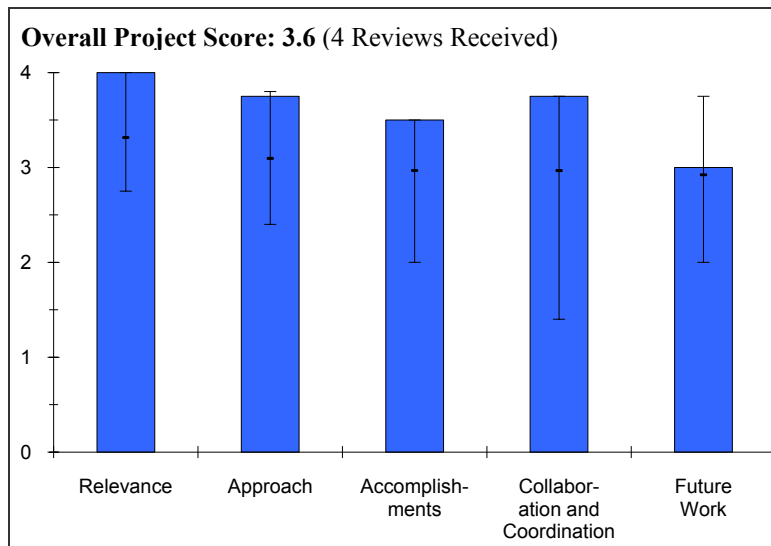
- Overall, the project team has made a reasonable effort towards the project goal and should receive continued funding support if possible. The NREL team effort should continue to focus on achieving the main goal of the project (i.e., to create a desirable oxygen-tolerant hydrogenase mutant), which is really what they were funded to do. Although the team's approach of computer simulation with site-directed mutagenesis seems to not be working, expression of an oxygen-tolerant bacterial hydrogenase in *Chlamydomonas* is a likely alternative pathway to achieve the goal (especially since the NREL team has already worked out some of the required accessory genes to express a functional hydrogenase, so this is likely doable). It could be viewed as a sign of failure to jump on something else without achieving the major project goal. Therefore, the project team should make sure to achieve the main goal of the project before spending time on something else.
- It is worthwhile to note that photobiological hydrogen production research is a quite challenging and long-term research and development area, which may or may not fit the time scale of a typical EERE program. Program-wise, the currently EERE-funded projects are not sufficient to address the (at least) six known problems (technical barriers) in algal hydrogen production. As reported in 2010 U.S. Patent Number 7,642,405 and PCT application number WO 2007/143354, these six problems are proton gradient accumulation, carbon dioxide inhibition, bicarbonate binding requirement, electron-drainage by oxygen, hydrogenase oxygen sensitivity, and oxygen/hydrogen separation and safety issue. Without solving these six problems, the photobiological hydrogen production technology will not work. The EERE photobiological hydrogen program seems to need additional innovative project teams to overcome these technical barriers. Perhaps this type of project effort is better to be supported through DOE's Office of Basic Energy Sciences program, where the program funding is relatively more stable, so that the investigators such as the NREL team could focus on their research rather than worrying about funding year by year.
- It is time to take a hard look at task 1 and consider reallocating personnel and resources to the other tasks, particularly to task 2.

Project # PD-38: Fermentation and Electrohydrogenic Approaches to Hydrogen Production*Pin-Ching Maness; National Renewable Energy Laboratory***Brief Summary of Project**

The overall objective of the project is to develop direct fermentation technologies to convert renewable, lignocellulosic biomass resources to hydrogen. Task goals are to 1) determine effects of substrate loading on rates and yields, 2) develop genetic tools to improve hydrogen molar yield, and 3) develop a continuous flow microbial electrolysis cell reactor to improve hydrogen molar yield.

Question 1: Relevance to overall DOE objectives

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



- All tasks have high relevance to the DOE Hydrogen Program mission.
- The project's objectives are clearly aligned with specific technical goals of DOE's Hydrogen Program. The emphasis on conversion of lignocellulosic plant material lends additional relevance to current DOE efforts in the development of biomass feedstocks for bioenergy production. The collaborative development of fuels cells for the conversion of organic acids produced during primary fermentation addresses one of the key barriers of fermentative hydrogen production (i.e. comparatively low hydrogen yield).
- The objective of the project is to develop direct fermentation technologies to convert renewable, lignocellulosic biomass resources to hydrogen, which addresses feedstock cost and hydrogen molar yield barriers to improve the techno-economic feasibility.
- The work is highly relevant to hydrogen yield, waste accumulation, and feedstock costs (particularly the first objective). The ability to directly process lignocellulose sources with a high hydrogen yield is very valuable.

Question 2: Approach to performing the research and development

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

- The project has a technically sound approach that complements other work going on elsewhere.
- At each step, the approach to accomplish the stated objectives of the project is well thought-out and clearly justified. In some cases, more foundational work (such as the development of better genetic tools for relevant hydrogen producing microorganisms) is being pursued, but this is reasonable and necessary to achieve the long-term goal of increasing hydrogen production. The project has an appropriate focus on mixed culture hydrogen production systems operating under high temperatures given that these systems should provide greater flexibility in the conversion of a range of substrates. The production systems should also be more robust in maintaining hydrogen-producing community structure during growth on necessarily non-sterile feedstocks.
- One of the approaches is to use corn-stover lignocellulose and cellulose-degrading bacteria to address feedstock cost. The second approach is to redirect metabolic pathways to maximize hydrogen production via the development of genetic methods. Another approach is to improve the hydrogen molar yield (mole hydrogen/mole hexose) by integrating dark fermentation with the microbial electrolysis cell (MEC) reactor to convert waste biomass to additional hydrogen.
- The combined approach of enhancing the fermentation process and coupling this with MEC technology is novel and has been very productive. Task 1 focused on adapting the bioreactor technologies for the direct fermentation of corn stover and Avicel, which are both available at NREL. In particular, *Clostridium thermocellum* has been employed in this work with significant success. Task 2 has focused on improving the

HYDROGEN PRODUCTION AND DELIVERY

Clostridium metabolism of cellulose through genetic engineering. They have started by investigating the effects of known inhibitors on the hydrogen production. In this way, they have identified blocking acetaldehyde production as a major contributor to increased production. Inhibiting formate production from pyruvate also gave a significant improvement. The development of a genetic system is in progress. They have managed to find appropriate growth conditions on plates and locate an appropriate plasmid for expression. Initial conjugation attempts from E. coli were unsuccessful, and they are now using S-17-1 E. coli to attempt conjugation again. This strain has worked well with related photosynthetic organisms like rhodobacter and thus is a promising avenue. Task 3 is being run in Pennsylvania State University (PSU) laboratory and involves processing the material left over after fermentation using an MEC. In this case, a voltage is applied to provide a driving force and the hydrogen is evolved at the cathode of the cell. Bacteria at the anode serve to metabolize the material in the waste stream and provide the electrons to the anode. The integration of these methods appears very promising.

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

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

- Multiple types of data were presented, which indicates a high degree of characterization. The project investigator exhibits high versatility in working on both biomass conversion and molecular biological approaches. Co-culturing work has some practical limitations, which the investigator did not make clear, and the results indicated limited improvement in hydrogen yields thus far. It is still worth pursuing, but predictions of the expected gains to be realized with co-culturing remain unclear and prior literature results were not made apparent. There appears to be some good progress on the CBS expression.
- There has been very good progress on Task 1. It will be important to further development of the system to make a determination of hydrogen production characteristics under different substrate loading conditions and with varying microbial community compositions (small caveat on the latter, see below).
- Task 2 presents some challenges in terms of developing improved transformation systems for C. thermocellum. The electroporation approach comes with its own difficulties (especially for anaerobes). This task appears to be at a transitional phase, and more results will be needed to meaningfully assess the progress. The integration of this task with the work in tasks 1 and 3 is a bit more tenuous.
- Overall, this project seems to be making very good progress, including the following: determined the effects of substrate loading on hydrogen molar yield and rates; established a co-culture (C. thermocellum and a Clostridium consortium) and improved substrate utilization (both hemicellulose and cellulose); performed a hydraulic test and achieved steady hydrogen performance in the reactor using a continuous flow system; and achieved up to $0.53 \text{ m}^3/\text{m}^3\text{-d}$ at a cathode surface area of $0.15 \text{ m}^2/\text{m}^3$.
- Task 1 has met its objective of measuring the molar stoichiometry between hydrogen evolved and hexose units consumed. Molar yields in the 1.5 region were generally detected. Task 2 has also met its twin objectives of first using known metabolic inhibitors to determine which pathways to genetically engineer and then developing and evaluating some of the basic tools required for genetic engineering. That said, conjugation has not yet been demonstrated, although the team seems to be taking a reasonable approach to developing a conjugation system in that the plasmids and E. coli strains being used have worked in similar cases previously. Task 3 has shown considerable progress in that the PSU group has been able to demonstrate that, using the effluent left over from lignocellulose processing at NREL, they can obtain almost seven moles of hydrogen per mole of hexose, bringing the total to over eight. What is not clear in what was presented is exactly how scalable this is. During questions at the presentation, it became clear that it takes roughly a day to clear one of their reactors, which could ultimately be the rate limiting aspect of the system.

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

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

- The team has multiple effective collaborations. The project investigator seeks input from other experts when needed to advance the project.

- The collaborative aspects of this project, including those being conducted with other groups supported by the DOE Hydrogen Program, appear to be well coordinated and are consistent with the overarching goals of the work.
- The collaboration of the NREL team with other institutions is excellent. They seem to intend to reach out to others in the field, and rightly so.
- Obviously, there is an interaction between NREL and PSU. In addition, there are collaborations within NREL to provide the biomass sources, and there is a collaborator in Canada helping on the development of the genetic system.

Question 5: Approach to and relevance of proposed future research

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

- One issue is how the priorities are established. There was limited justification in terms of quantitative expected improvements for each task. The team should determine which tasks would be prioritized first if fewer funds were available.
- The future work that was presented represents logical next steps that build on current efforts. The reviewer has some concerns regarding the lack of plans to perform any characterizations on the microbial consortia being used in this project; this is more fully described below.
- The proposed future work looks quite good.
- For each of the tasks, the proposed work seems generally appropriate. Task 1 appears to be mostly complete. For task 2 the big issue is whether they will be able to generate a working conjugation system for *Clostridium*, and the plans for doing this seem reasonable. Task 3 is also essentially complete. This was a bit confusing as the downloaded presentation did not specifically call out future work to be performed.

Strengths and weaknesses

Strengths

- The project investigator is highly collaborative, interactive, and technically versatile.
- This is a generally well considered approach that addresses many of the major challenges in the development of fermentative hydrogen production.
- This reviewer in general agrees with the comments made by last year's reviewers: the team has meaningful milestones, which indicate substantial thought being put into the process and, as a result, the team has developed a plan to achieve its goals; the project's integrated process better utilizes the feedstock; the project has a very good combination of novel fermentation with MEC technology; and the project results in terms of molar yields are quite impressive.
- The project demonstrates good integration of fermentation and MEC approaches and strong collaboration. Good progress has been made towards improving hydrogen per hexose ratios.

Weaknesses

- Fewer reviews and more primary research publications are needed, particularly on the expression work.
- This reviewer pretty much agrees with some of the comments made by last year's reviewers: this project requires a relatively expensive feedstock; maintaining the feed mixtures will be a significant challenge for this team; hydrogen gas produced could be consumed by methanogens, which could be a show stopper; MEC requires external supply of electricity and the energy efficiency of the MEC system is not very clear; and it would be good for the team to start working on predicting the effects of scaling output and considering the roadblocks involved in the scaling process.
- Future work plans were not very clear.

Specific recommendations and additions or deletions to the work scope

- I find the undefined nature of the microbial consortium being used here somewhat problematic. Given the amount of effort being put into developing this as an inoculum source for biomass conversion bioreactors, having some information on community composition would give a better sense of metabolic potential, likelihood of ability to convert different carbon substrates, presence of strict versus facultative anaerobes, and

ability to determine if organisms performing competing processes (e.g., spore-forming acetogens, heat resistant methanogens) remain in the culture. Conducting a 16S-based phylogenetic characterization of the consortium should be relatively straight forward, especially given the limited microbial diversity likely to present in the sample after the heating enrichment step to select for spore-forming organisms.

- Given the recent emphasis on development of dedicated biomass feedstocks such as switchgrass and poplar, it may be appropriate to consider these as potential carbon sources for future testing.
- Overall, the project team seems have made some very good progress towards the project goal and should continue to receive funding support to explore the work if possible. The MEC part is quite interesting, but it needs to provide clear and objective analysis on the energy efficiency since it consumes electricity. Economic assessment of the proposed process is another issue. They need to also pay attention to the issue of methanogens that could eat hydrogen because sterilization of large amounts of waste biomass for energy production would unlikely be feasible.

Project # PD-39: Hydrogen from Water in a Novel Recombinant Oxygen-Tolerant Cyanobacterial System

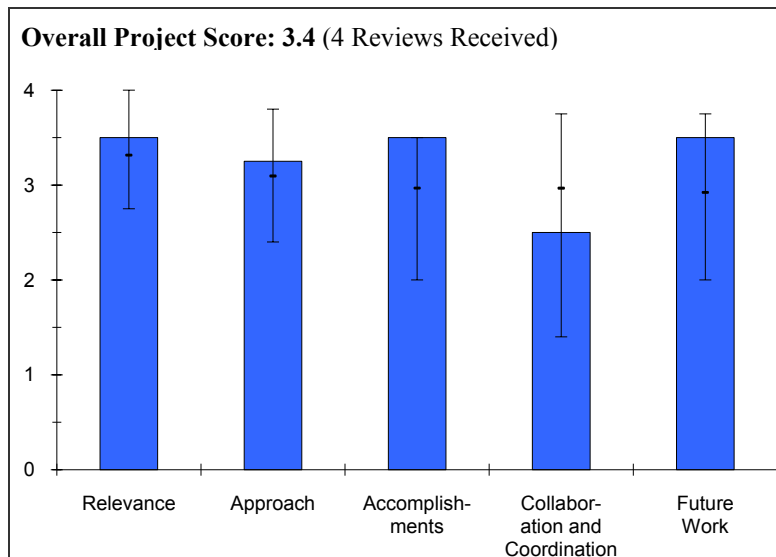
Qing Xu; J. Craig Venter Institute.

Brief Summary of Project

The overall objective of project is to develop an oxygen-tolerant cyanobacterial system for continuous light-driven hydrogen production from water. The target for 2011 is to produce one cyanobacterial recombinant evolving hydrogen through an oxygen-tolerant nickel-iron-hydrogenase. The target for 2018 is to demonstrate hydrogen production in air in a cyanobacterial recombinant.

Question 1: Relevance to overall DOE objectives

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



- Most tasks in this project are relevant to the DOE Hydrogen Program mission.
- The project effectively addresses a key barrier to biological hydrogen production in microbial phototrophs, namely the oxygen sensitivity of hydrogenase enzymes.
- The goal of this photobiological hydrogen project is to develop an oxygen-tolerant cyanobacterial system for continuous light-driven hydrogen production from water.
- Finding new oxygen-tolerant hydrogenases and transferring them into cyanobacteria is highly relevant to DOE goals in terms of the continuity of hydrogen production.

Question 2: Approach to performing the research and development

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

- The project approach involves a heterologous expression of an oxygen-tolerant hydrogenase in a model host. The same approach is underway in many laboratories with limited success, which leads to the conclusion that new ideas are needed.
- This project attempts to address two barriers to hydrogen production by the cyanobacterium *Synechococcus* sp PCC 7942 through elimination of the putative uptake hydrogenase present in the wild type and provision of more oxygen tolerant hydrogenase derived from a different organism. The selection of *Synechococcus* sp PCC 7942 as a platform is reasonable, given the sequenced genome and availability of genetic tools for this organism (with a caveat noted below). The nickel-iron hydrogenase of *Thiocapsa roseopersicina* has similarly been well characterized in previous studies. A parallel project with similar experimental logic is being performed by collaborators at NREL working on *Synechocystis* sp. PCC6803 and a hydrogenase from *Rubrivivax gelatinosus*.
- Although this approach is appropriate and reasonable from a research perspective, there is not a great deal of justification as to why these organisms in particular should be developed for hydrogen production or how they might perform in anything other than bench-scale conditions.
- The approach is to transfer a known oxygen-tolerant nickel-iron-hydrogenase from *T. roseopersicina* into cyanobacterium *Synechococcus* sp PCC79423, to identify novel oxygen-tolerant hydrogenases through metagenomic analysis of marine microbes in the global ocean, and to transfer the hydrogenases into cyanobacteria.
- There are two tasks. The first is a parallel effort by J. Craig Venter Institute (JCVI) and NREL to transfer known oxygen tolerant hydrogenases into cyanobacteria. JCVI is transferring the hydrogenase of *T. roseopersicina* into a *synechococcus* strain and NREL is transferring the hydrogenase of *Rubrivivax gelatinosus*.

into a synechocystis strain. Both efforts involve the expression of the gene followed by isolation and characterization of the hydrogenase and determination of the activity in vivo. All of these efforts seem like solid approaches.

- The second task is performed entirely by JCVI and involves discovering new oxygen tolerant hydrogenases from a broad sampling of oceanic species, as well as the cloning and expression of this system in cyanobacteria. This is a very ambitious but potentially high payoff approach to solving the problem and again involves the same basic types of processes as described above, with the addition of the initial screening to find likely candidates. Again, this all seems very solid.

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

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

- The evidence given was not always convincing. Qualitative data on hydrogen activity was reported and only in vitro assay is currently reported. The team could improve the quantitative determination of their activity.
- The team at JCVI has successfully introduced the necessary genes for hydrogenase expression and assembly into *Synechococcus* and is able to detect low-levels of activity in cell extracts. This has been accomplished for the nickel-iron hydrogenase gene from *R. gelatinosus*, as well as a hydrogenase derived from a marine metagenomic database. Although this is an impressive accomplishment (especially the latter), the reviewer remains concerned that expression has not yet been demonstrated in vivo. This may reflect improper assembly of the enzyme, incorrect presentation of the enzyme in the native cell environment, or any number of other factors that could prove extremely challenging to correct.
- Although the current results may represent 80% progress in terms of milestones, the success of the project very much hinges on introducing detectable activity into intact cells, and the reviewer would reserve judgment until this can be unambiguously demonstrated.
- The presentation of enzyme assay data in crude extracts was somewhat confusing and difficult to interpret; this should be presented in a much clearer fashion in the future.
- The project has thus far generated two publications of primary data (one released, one accepted) and has several others in preparation.
- Overall, this project seems to have made very good progresses including the following: at JCVI the genes of the *Thiocapsa* oxygen-tolerant hydrogenase were transferred into *S. PCC7942* and activity from the heterologously-expressed hydrogenase was detected; a novel nickel-iron-hydrogenase was cloned from the Sargasso Sea environmental DNA, expressed in *T. roseopersicina*, and showed activity in the presence of low levels of 1% oxygen; and the genes of this novel hydrogenase were transferred into *E. coli* and *Synechococcus*, and activity from the heterologously-expressed hydrogenase was detected.
- The NREL team has developed two different expression systems, expressed at least three CBS hydrogenase subunits and one maturation subunit in *Synechocystis*, and purified a CBS native hydrogenase.
- The JCVI group first characterized the isolated hydrogenase, then cloned the required hydrogenase genes in cyanobacterium, expressed it, and demonstrated activity in the expressed strain. Similarly, the NREL group has cloned the genes, expressed them, and isolated the hydrogenase from cyanobacteria.
- The JCVI group has also identified a new oxygen-tolerant hydrogenase from their broad sampling of the ocean, which is a nickel-iron hydrogenase. They have cloned the needed genes and expressed them in *roseopersicina*. The genes were very heat tolerant and moderately oxygen tolerant. The entire gene cluster required was then cloned into cyanobacterium lacking hydrogenase, and weak but definite hydrogenase activity was demonstrated.
- This project has had excellent progress.

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

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

- It seems like the work at NREL and JCVI is done independently, rather than collaboratively. Different organisms are done at different sites, and evidence of true interaction is not so apparent. JCVI is not using NREL's extensive facilities.
- No results from collaboration with Kovaks at Szeged given.

- Although the collaboration with researchers at NREL was discussed in detail, the presented material suggested that this exists as a largely parallel project, and it was unclear whether there was a significant degree of integration and collaborative work being conducted between the two groups. Minimal information was provided on collaborations with the three other institutions, other than that they share a similar approach.
- The collaboration of the JCVI and NREL seems very good.
- The collaboration with NREL adds substantially to the activity with two opportunities for expression and comparison of oxygen-tolerant hydrogenase. In addition, they are collaborating with two other laboratories involved in the expression of hydrogenase.

Question 5: Approach to and relevance of proposed future research

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

- The arrival of a new person, Dr. Weyman, to replace Dr. Xu in leading this effort indicates a change in personnel that was not explained at the outset, could indicate a good future for new developments.
- As was mentioned above, demonstrating in vivo expression of hydrogenases in the non-native hosts remains the most critical milestone that this project must meet. The proposed future work is appropriately focused on this goal.
- The proposed future work looks reasonable.
- The future work revolves around both characterizing the strains with heterologous hydrogenases and improving them by adding additional genes and manipulating the metabolic pathways. These are sound approaches with significant promise.

Strengths and weaknesses

Strengths

- The project has strong expertise for metabolic engineering of this type, and the ability to effectively leverage metagenomic libraries is a significant advantage.
- The project has a well-defined work plan.
- JCVI has very good microbial (cyanobacterial) molecular genetics and genomics expertise to contribute.
- JCVI is making an excellent effort to identify novel oxygen-tolerant hydrogenases through metagenomic analysis of marine microbes from the global ocean.
- The project has made consistent progress in transferring oxygen-tolerant hydrogenases from several sources into cyanobacteria and demonstrating activity.

Weaknesses

- The strong genomics/bioinformatics capabilities at JCVI are not apparent in the results presented. The heterologous expression approach that is used is redundant with other efforts elsewhere that also have not yet been successful.
- The parallel nature of the collaborations seems to be a weakness, and the reviewer is unclear on why the project resources would be divided in this way. A clearer demonstration of integrative effort is needed.
- Expression of an oxygen-tolerant hydrogenase is unlikely to result in a practical cyanobacterial system for continuous light-driven hydrogen production from water, because the oxygen sensitivity of hydrogenase is merely one of the (at least) six known problems (technical barriers) in photobiological hydrogen production. For example, there is a very different type of oxygen sensitivity that has nothing to do with the hydrogenase, but sucks electrons away from the hydrogen-production pathways even at an oxygen concentration as low as 1000 ppm, whereas the in-vivo hydrogenase is completely active. Therefore, this electron-draining oxygen sensitivity (reported in 2003 Applied Biochemistry and Biotechnology, Vol. 105-108, pg 303-313) is a far more serious issue that needs to be addressed in photobiological hydrogen production than the oxygen sensitivity of hydrogenase per se.
- There are no significant weaknesses.

Specific recommendations and additions or deletions to the work scope

- If possible, localization of introduced hydrogenases within the cell could prove very informative.

HYDROGEN PRODUCTION AND DELIVERY

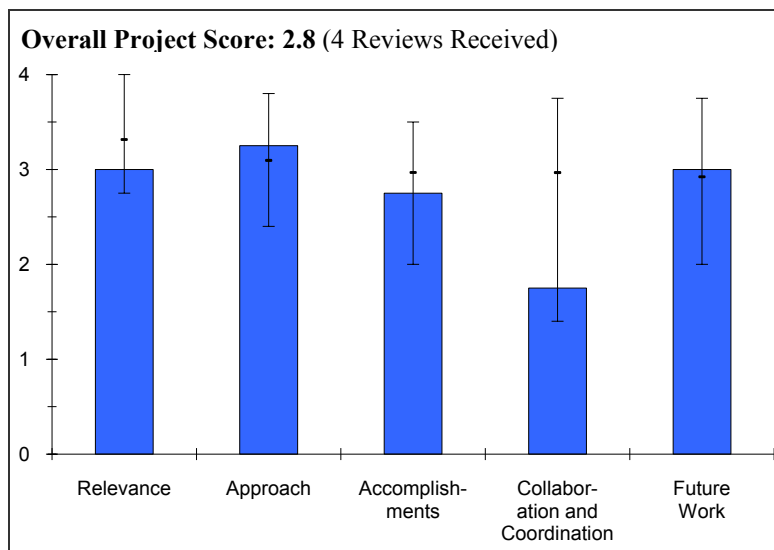
- Overall, the project team has made some very good progress toward the project goal and should receive continued funding support to explore the efforts, if possible. The involvement of JCVI could benefit the DOE photobiological hydrogen program by contributing to its expertise on microbial (cyanobacterial) molecular genetics and genomics. JCVI's effort on searching for novel oxygen-tolerant hydrogenases through metagenomic analysis of marine microbes from the global ocean is also potentially valuable.
- One must also understand that photobiological hydrogen production research is a quite challenging and long-term research and development area. Program-wise, the current EERE-funded projects are not sufficient to address the (at least) six known problems (proton gradient accumulation, carbon dioxide inhibition, bicarbonate binding requirement, electron-drainage by oxygen, hydrogenase oxygen sensitivity, and oxygen/hydrogen separation and safety issue) in algal hydrogen production. Expression of an oxygen-tolerant hydrogenase by the JCVI-NREL project would help solve only one of the six technical problems that are reported in 2010 U.S. Patent Number 7,642,405 and PCT application number WO 2007/143354 A2. Without solving the remaining five problems, the photobiological hydrogen production technology will not work. That is, the EERE photobiological hydrogen program seems to need additional innovative project teams to overcome these technical barriers. Perhaps this type of project effort is better to be supported through DOE's Office of Basic Energy Sciences program, where the program funding is relatively more stable so that the investigators, such as the JCVI-NREL team, could focus on their research rather than worrying about funding year by year.

Project # PD-42: Catalytic Solubilization and Conversion of Lignocellulosic Feedstocks*Troy Semelsberger; Los Alamos National Laboratory***Brief Summary of Project**

The overall objective of the project is to develop novel low-temperature chemical routes and catalysts to produce hydrogen/syngas from lignocellulosic feedstocks. The 2012 target is to reduce the cost of hydrogen produced from biomass gasification to \$1.60/gge at the plant gate (less than \$3.30/gge delivered). By 2017, the target is to reduce the cost of hydrogen produced from biomass gasification to \$1.10/gge at the plant gate (\$2.10/gge delivered).

Question 1: Relevance to overall DOE objectives

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



- The project aims to develop a low-temperature catalytic aqueous phase reforming (APR) process to produce syngas from lignocellulosic feedstocks, which is the type of biomass that is most available. The project is very challenging, but it may have an important impact in the future production of renewable hydrogen from the most abundant biomass and wastes.
- Hydrogen production does not have a very high yield from this process. However, it appears that they may be getting an insoluble phase of hydrocarbons, which could be a useful fuel. The researcher did not investigate this potential, and it may be worth revisiting some key tests. Lignin is a difficult feedstock to digest, and the concept that is proposed would be useful for integrating with a traditional digester.
- This project supports the programmatic goals to produce hydrogen from renewable sources at costs competitive with fossil sources.
- This project was not sufficiently funded to move the technology forward to address the barriers.

Question 2: Approach to performing the research and development

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

- The low-temperature catalytic APR process has a number of advantages over the pyrolysis-based processes. The proposed research is directed towards solving the fundamental problems associated with the solubilization of lignocellulosics and hydrogen-selective APR.
- The approach could have been more thorough in analyzing yields of various species. The mass and energy balance was not pursued to a sufficient extent to track the full conversion of potential fuel species.
- The work accomplished is of high quality and the approach is well defined.
- The team has not been able to demonstrate if this technology can accomplish the stated goals, but the problem is due to funding constraints. The results look interesting and the chemistry appears to be feasible, but the results are very limited and the economic analysis is at too high of a level because there is not enough data to accurately represent the technology.

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

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

HYDROGEN PRODUCTION AND DELIVERY

- The project only had one year of work during which the team established an experimental apparatus and performed initial APR and solid phase biomass conversion with interesting observations in the chemistries of these systems.
- It is my understanding that the technical results shown are from previous years. It is not surprising that they have not made recent progress since they have not had any funding for 2009 and 2010.
- \Again, the reviewer would like to have seen a full spectrum of product species and any hydrophobic phases.
- For the work performed, the progress is good and the results are encouraging that this technology may be practical for certain applications.
- The issue with this project is that there is no indication of how much funding was provided against the original project budget. Only \$500k was made available from 2007 to the present. The results of the work presented should have allowed it to proceed, but since the budget was cut it was not continued.

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

This project was rated **1.8** for technology transfer and collaboration.

- The team does not have any partners.
- The reviewer did not see much, if any, collaboration.
- This program was done without significant collaboration.
- The team has is no collaboration, but it may have been because the budget was cut in 2009.

Question 5: Approach to and relevance of proposed future research

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

- The team's system concepts and explanations of future work are very good.
- The future work looks interesting and logical. However, I am not sure if this is the right presenter for the work. The future work would propose to augment traditional digestion.
- The proposed work plan is reasonable based on the accomplishments. However, more bench-scale work should be carried out on actual wood, both hard and soft, to validate if the cellobiose is a good model compound.
- Due to the high cost of the catalysts in the preliminary economic model, the additional work should validate the rare earth options to cut the \$19 million cost more quickly, and if it is not possible, then the project should not be continued.

Strengths and weaknesses

Strengths

- The project tackles one of the most important challenges in developing technologies for hydrogen production from renewable and low-cost biomass (i.e., the utilization of lignocellulosic feedstocks). The APR system proposed here is extremely challenging but, if successful, it would be a viable alternative to the traditional pyrolysis or high-temperature gasification methods.
- The team has a good vision of what they want to achieve.
- The project has a good research and development team at Los Alamos National Lab.
- The project uses a good technical approach that has not been attempted in the past.

Weaknesses

- The plans are reasonable, but currently there is not enough data to evaluate the technical approaches.
- While the team has a good vision of what they want to achieve, they have had very limited good results.
- The project does not have any teaming with universities or companies that may have more expertise on catalyst systems for aqueous phase reactions.

Specific recommendations and additions or deletions to the work scope

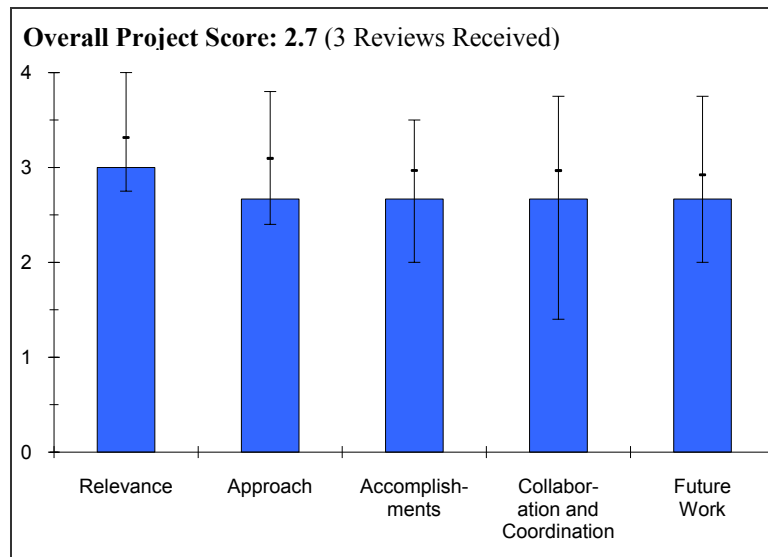
- It would be valuable to revisit some of the original tests and check for an insoluble phase in the product. The off-gassing of significant amounts of carbon dioxide and a little hydrogen would suggest that there could be hydrocarbon chains remaining after lignin digestion, which could be a useful fuel or chemical feedstock.
- DOE should continue the funding and establish a stage gate review once the project has achieved more data.

Project # PD-45: Distributed Reforming of Renewable Liquids Using Oxygen Transport Membranes

Balu Balachandran; Argonne National Laboratory

Brief Summary of Project

The overall objective for this project is to develop a compact, dense, ceramic membrane reactor that meets the DOE 2017 cost target of less than \$3.00/gge for producing hydrogen by reforming renewable liquids. The reactor would use oxygen transport membrane (OTM) to supply pure oxygen for reforming renewable liquids. The initial focus on reforming natural gas was changed to ethanol reforming in FY 08. Objectives during the past year were to use OTM to reform ethanol at less than or equal to 700°C and generate data for detailed analysis to identify benefits of the approach.



Question 1: Relevance to overall DOE objectives

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

- The success of this project would support the DOE objectives for the DOE Hydrogen Program by reducing the costs and energy requirements for reforming of ethanol.
- Technology is a contributing factor to enabling a hydrogen economy, but not crucial.
- The project objectives are aligned with the DOE Hydrogen Program goals, and the barriers listed are also appropriate. However, considering the budget and the objectives, it appears to be an overly ambitious project.

Question 2: Approach to performing the research and development

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

- The research approach for this project is logical and well thought-out. The approach addresses the technical barriers to reduce the capital costs for ethanol reformer technology, which increases efficiency, selectivity, and durability by using an oxygen transport membrane.
- The project plan is good.
- The approach is poorly defined. Other than stating the obvious, there is no clear definition of how the objectives will be accomplished.
- Oxygen transport membranes are well known, and there have been significant efforts in this area with multi-million dollar projects led by Air Products and Praxair. In light of this, it is not clear what is unique about the approach.
- The milestone description is very weak and—there are no quantitative measures that define the milestones. Simply stating "perform ethanol reforming studies..." does not constitute a milestone. It would be useful to have some targets in terms of conversion, efficiency, cost, and other similar metrics.
- On slide 8, no criteria are established for a go/no-go decision, e.g., a go/no-go decision is not possible just based on the "testing of catalysts."

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

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

- The accomplishments to date have been limited by the lack of funding. Note that this should not be considered a shortcoming of the researchers. It was not clear if the air stream will be pressurized to improve oxygen flux rates. The cost of increased air pressure versus the benefits may need to be detailed.
- The team needs to address steam effects because, in SMR processes, the steam ratio is one of the most important variables in determining costs and energy efficiency.
- The team's progress appears to be reasonable given the low funding level. However, several plots comparing OTM versus blank are unnecessary, as these are expected results and not novel. Also, the use of rather low ethanol concentrations (7-13%) does not serve any practical purpose.
- It would be helpful to present the data in the form of commonly used parameters that can be compared with other studies, such as conversion, instead of a production rate in cm^3/min , without mentioning the feed rates of ethanol and air.
- The comparison of different material compositions on slide 13 is meaningful. However, these flux results are not verified with the use of these membranes in ethanol reforming.
- The results of economic analysis are abruptly presented in slides 14-15 and cannot be appreciated or judged in the absence of any mention of assumptions with respect to membrane performance and cost.

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

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

- This project has well-developed collaborations with other institutions, including a potential end-user.
- Investigators should consider collaborations with commercial catalyst providers, as well as practitioners of steam methane reforming.
- The collaborations are reasonable at this stage. However, the interactions among them are not apparent and it is not clear from the results if any collaboration is leveraged.
- A key problem appears to be the absence of an industrial partner who can provide direction with respect to commercial aspects.

Question 5: Approach to and relevance of proposed future research

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

- The proposed future work is clearly laid out and will address the technical barriers necessary to make this project a success.
- The proposed plan should work to acquire kinetic data and develop an engineering model of the process, which will allow the investigation of parameter space including space velocities (reactor size and cost), steam ratio, etc.
- The future work plan is stated in rather vague terms. It is first necessary to establish that the proposed approach can significantly reduce the ethanol reforming cost. This would help to establish specific performance targets and corresponding go/no-go decision points. At present the project seems to have been poorly structured.

Strengths and weaknesses

Strengths

- This project is very focused on improving the ethanol reforming process, and the experimental design clearly addresses the technical barriers.
- The project builds on strong OTM efforts and the team has good expertise in membrane fabrication.
- The team has good knowledge of OTM materials and past experience with synthesis and testing of such materials.

Weaknesses

- There has been a lack of consistent funding to date, which is not a fault of the researcher.
- The project does not address sealing issues. This is always a major issue in OTM and other high-temperature membranes.

HYDROGEN PRODUCTION AND DELIVERY

- The team needs to clearly show the advantage of oxidative reforming over steam reforming. The investigator claims OTM advantages in methane reforming, but it has not been commercialized.
- The team has a lack of understanding of commercial aspects.
- The project has poorly defined objectives, targets, and milestones.
- There is an insufficient basis for the proposed approach and benefits.

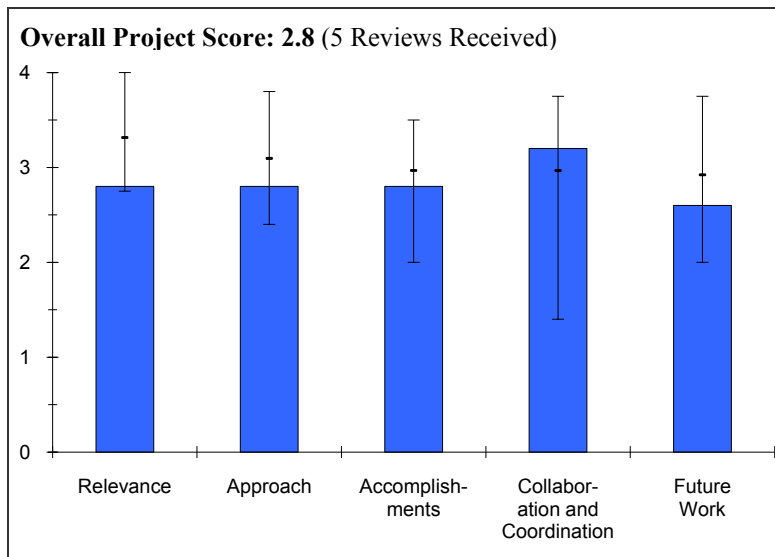
Specific recommendations and additions or deletions to the work scope

- The team should perform an engineering analysis (and supporting experiments) to show how much better OTM-assisted reforming must be in order to be economically superior to steam reforming. This may be a function of scale.
- As stated above, the project needs to first establish a clear baseline, improvement potential, specific targets, and a corresponding clear pathway.
- The work seems to emphasize material compositions to improve performance. Based on the prior work in this area, it is known that the real issues with this approach are with respect to fabrication, integrity, and durability, which are not addressed in the project.

Project # PD-46: Reversible Liquid Carriers for an Integrated Production, Storage and Delivery of Hydrogen
Alan Cooper; Air Products

Brief Summary of Project

The overall objective of this project is to develop a conceptual design and fabricate an initial 0.1 to 1-kW prototype of a dehydrogenation reactor/heat exchange system to deliver hydrogen via liquid carrier materials. The project is divided into three tasks: 1) liquid phase hydrogen carrier raw materials sourcing and processing, 2) develop a conceptual design and fabricate an initial 0.1 to 1-kW prototype of a dehydrogenation reactor/heat exchange system to deliver hydrogen, and 3) conduct an economic evaluation of the delivery and storage system for the liquid carrier hydrogen delivery concept.



Question 1: Relevance to overall DOE objectives

This project earned a score of **2.8** for its relevance to DOE objectives.

- This program evaluates a novel approach where hydrogen is absorbed and desorbed from an organic liquid. The concept is similar to an oil change; change the system with fresh liquid, extract the hydrogen from the liquid, drain the spent liquid, then recharge with the fresh liquid. The concept, if viable, is intriguing. The process and the status of the activity is very clear.
- The reviewer is not sure this pathway shows the potential to achieve much lower delivery cost and widespread adoption.
- The project seems highly attuned to DOE Hydrogen Program objectives.
- This is very relevant, as delivery cost dominates the overall hydrogen fuel cost.
- The liquid organic hydrogen carriers (LOHC) concept can be a game-changer for the transportation hydrogen economy and infrastructure requirements.
- This process is important to enabling a hydrogen economy, but not critical.

Question 2: Approach to performing the research and development

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

- The approach to this task is focused. It is unclear which activities are occurring on the to-be-determined working fluid. The presentation did not clarify if it is to be Perhydro-nitrogen-ethylcarbazole or if this fluid is being used as an example for the modeling.
- The reviewer found the approach to be interesting, novel, and highly focused on the development of solutions to long-term needs in hydrogen fuel distribution.
- The approach is fair, it demonstrates reaction productivity to meet the system volume targets.
- It would be better if the focus first is on identifying the LOHC that is cost effective and safe, as the key limitation for this concept is to identify a working LOHC. A model LOHC does not have benefit.
- It is better to directly collaborate with the hydrogen original equipment manufacturer (OEM), BMW, on a timeline and criteria for the demonstration and acceptance of this concept.
- The forecourt dehydrogenation solves only half of the problem and onboard hydrogen storage remains one of the key bottlenecks. It is better to focus on onboard dehydrogenation.

HYDROGEN PRODUCTION AND DELIVERY

- Advanced reactor concepts are required to achieve high conversions with the high rate of gas generation. The novel reactors, such as the suspended slurry being investigated, have the potential to raise conversion.

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

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

- The program seems to be adequately focused and directed.
- It appears that the testing and results have improved, though long-term benefits from the method may need to be evaluated.
- It seems that significant progress had been made on a challenging set of barriers.
- The team has not made much progress since last time. The only progress is test reactors with measurements of productivity.
- The work should be directed to focus on identifying a practical LOHC carrier as all of the reactor and other development applies to the current carrier, which is not practical.
- The projected delivery cost range is too wide. It should be more specific at this point.
- The team's progress is very good considering the short time the project has actually been funded in 2010.

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

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

- The collaboration with other parties appears to be adequate.
- OEMs are critical to the adoption of this process and yet are missing from project.
- The project appears to be an effective collaboration between industry, academic researchers, and DOE national laboratories.
- The project has a good number of relevant partners.
- The reviewer would like to see a timeline by the OEM (BMW in this case) to deploy a test version in one of their vehicles.
- The team has a good list of collaborators. Pacific Northwest National Laboratory's experience in microreactors is a good complement to the investigator's expertise.

Question 5: Approach to and relevance of proposed future research

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

- The future work plan, while detailed, might consider additional ancillary issues that would need a plan to institute the concept.
- The exact future work for the project was not clear. The team needs a more developed plan of next steps and potential improvements.
- The reviewer found the logic of the proposed future work somewhat difficult to follow, but did not have an engineering background and would defer to more qualified reviewers.
- The project has a fair list of items for future work
- As mentioned before, future work should include deployment in the vehicle (through BMW).

Strengths and weaknesses

Strengths

- The concept appears sound, and the effort is working towards a set of functional requirements for the reactors.
- The project has good safety aspects and delivery simplification of hydrogen-to-vehicle from a production facility.
- The team has good partners with the right relevance and technical strength.
- Air Products and chemicals are the right choice for the lead in this work area.

Weaknesses

- The definition on the infrastructure details required to implement this concept appears to be lacking.
- It is unclear if there is an assurance of hydrogen quality for fuel cell vehicles. Critical project partners are absent, such as large OEMs (besides BMW).
- The project has a poor approach. They need to first identify and establish the candidate LOHC material, look at its economics, and then do the reactor development.
- The project needs better co-ordination with an OEM on vehicle deployment plans.

Specific recommendations and additions or deletions to the work scope

- The project should define what other things need to happen to institute this concept, for example, how to distribute, collect and reprocess the material.
- The project should examine the allowable toxicity of the working fluid and the personal protection equipment required to transfer the charged and depleted fluids.
- It is unclear if the general public will be doing the fueling, or if certified technicians will be required.
- The project needs to either bring on board more vehicle manufacturers, or consider working on a fleet application for this method. The project needs to have a more detailed analysis of the future cost advantages versus conventional (or proposed) hydrogen delivery methods.
- The project should search for a practical, safe and cost effective LOHC material.
- The team needs to establish the protocols and approach for material recycling at the station.
- Forecourt dehydrogenation should be deleted from the scope because it only solves half the problem.

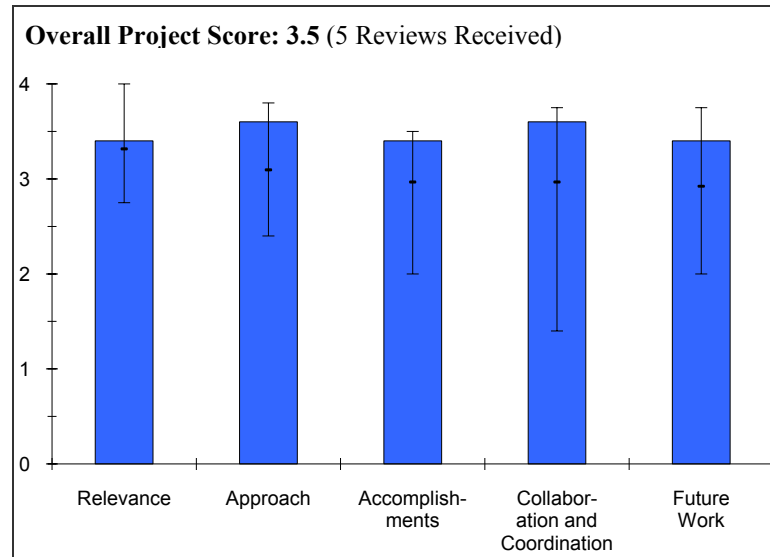
Project # PD-47: Materials Solutions for Hydrogen Delivery in Pipelines

Todd Boggess; Secat, Inc.

Brief Summary of Project

The overall objective of this project is to develop materials technologies to minimize the embrittlement of steels used for high-pressure transport of hydrogen. The objectives are to 1) identify steel compositions and processes suitable for construction of a new pipeline infrastructure or potential use of the existing steel pipeline infrastructure and 2) understand the economics of implementing new technologies. The objective to develop barrier coatings for minimizing hydrogen permeation in pipelines and associated processes is on hold per DOE.

Question 1: Relevance to overall DOE objectives



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

- Hydrogen pipeline materials are very relevant to the delivery of hydrogen over long distances. The reviewer would like to see work done on weldments, and not just unwelded material.
- The need to evaluate the effects of hydrogen embrittlement for existing pipeline steels is very important.
- The project seemed well attuned to DOE objectives.
- This project demonstrates important work on a metallurgical testing of steels for hydrogen pipeline service.
- This is a project whose objective is to deliver material microstructures that are hydrogen compatible. The reviewer thinks it is the only program in the DOE that explores the metallurgical aspects of the material microstructure relative to hydrogen embrittlement. Amongst four originally proposed microstructures, the project has down-selected two low-alloy steels that were found to exhibit the best performance in gaseous hydrogen tensile testing. One of these alloys, designated as steel B, is an X70/X80 polygonal ferrite with coarse acicular ferrite at 10%. The other steel microstructure, designated as steel D, is an X52/X60 polygonal ferrite. Fracture toughness results for these microstructures indicate that they are extremely resistant to hydrogen degradation up to pressures of 3000 psi with fracture toughness values greater than $80 \text{ MPa}\cdot\text{m}^{0.5}$. The fatigue properties of these steels were also studied. The da/dN curves indicate that hydrogen increases the growth rates for both steels B and D in the intermediate stress intensity factor range. On the other hand, it seems that the near-threshold fatigue crack growth rates are similar to those in air. It remains to be seen how these hydrogen-induced crack growth rates are affecting the life of a pipeline. In summary, the project is showing outstanding progress toward ascertaining the hydrogen resistance of two promising material microstructures.

Question 2: Approach to performing the research and development

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

- The project is doing good, standard work.
- The project uses a tried and true industry approach to evaluating materials.
- Although the project is considerably outside of my area of technical expertise, the need to evaluate the potential of existing pipeline infrastructure to serve in hydrogen distribution seemed reasonable and was convincingly presented.

- The project is relating steel microstructures, as characterized by microscopy, to performance at high hydrogen pressures using American Society for Testing and Materials (ASTM) test procedures for tensile strength and fracture stress (e.g., the appearance of cracks).
- The project has been asking the right questions and, as a result, it concluded that the polygonal ferrite/coarse acicular ferrite (steel B) provides the best performance in high-pressure hydrogen environments. The latest tests on fracture toughness in gaseous hydrogen and fatigue crack growth are precisely the tests needed to ascertain the compatibility of these microstructures (steels B and D). The project is also planning to explore the relationship between performance and the fraction of acicular ferrite. This is indeed the right approach, as it will provide further insight into how we should tailor the microstructure to achieve better resistance.

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

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

- The project has some nice results. The reviewer would have preferred more metals to be included and some weldment tests performed. Without these additional data, one might carry out pipeline design based on limited test results.
- The progress to date is excellent.
- From admittedly a very limited number of samples, alloys of two microstructure types were selected as potentially the best performers.
- This work has provided an important knowledge base on the relationship between the pipeline steel's microstructure and its compatibility with hydrogen.
- The project has identified that the presence of acicular ferrite in low-alloy steels provides increased resistance to hydrogen degradation. In fact, the measured fracture toughness is very high (greater than $100 \text{ MPa}\cdot\text{m}^{0.5}$ for alloy B) and this is an excellent result. The project also found that the fatigue resistance is independent of the fraction of the acicular ferrite (steels B and D). This is a result that needs further investigation given the fact that both steels B and D were found to exhibit increased crack growth rates in fatigue at the intermediate stress intensity factor range regime. The growth rates near the threshold stress intensity factor range are not different from those in air, which is an intriguing result that holds great promise for future developments.

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

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

- The team has some collaboration but nothing special, either good or bad.
- The collaboration to date is good. The team should discuss this project with the Department of Transportation (DOT) Pipeline and Hazardous Materials Safety Administration. There may be a synergy there that would identify additional alloys of interest and potential funding sources.
- The project exists as part of a well-integrated consortium of industrial, academic, and national laboratory personnel.
- The project has very close collaboration with a number of industry partners and academia for obtaining characterization data.
- The project's collaborations with the Sandia National Laboratories are outstanding. The project managed to obtain fracture toughness data and fatigue crack growth rates, which is a direct result of this collaboration.
- Collaboration with Oak Ridge National Laboratory (ORNL) is good, as long as it aims at addressing alloy development for enhanced hydrogen resistance, such as the effect of the acicular ferrite content. The in-situ tensile testing at ORNL, although a screening procedure, is not reliable for assessing materials against hydrogen embrittlement. By way of example, it is reported on slide #24 that for pressures greater than 800 psi alloy D is more resistant than alloy B under strain rates of 10^{-5} . This contradicts the fracture toughness results shown in slide #29 whereby alloy B is more resistant than D. The point is that hydrogen-induced loss of reduction in area in tensile tests is not a reliable index of embrittlement. In fact, for the same two alloys and pressures greater than 800 psi, the ORNL result at a strain rate of 10^{-4} is exactly opposite to the result at a strain rate of 10^{-5} .
- Collaborations with the American Society of Mechanical Engineers Codes and Standards division for the development of B31.12 is also good for the project because it helps place the project's results under a proper industrial perspective for pipeline design.

Question 5: Approach to and relevance of proposed future research

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

- They have a plan to fill in the needs, but unfortunately they plan to do this after the money runs out.
- The proposed work is very good. It would have been nice if the scope was larger, but it is likely limited by funding.
- The presenter mentioned that the project is in its final stage of DOE funding and is unlikely to be renewed. The future work presented seems a logical next step in securing future support from relevant private sources.
- The team proposes the examination of a greater number of samples. It is not clear what is meant by in-situ testing of the steels under hydrogen.
- The project's future work plan to investigate the relationship between embrittlement and the fraction of acicular ferrite is a very well-thought-out approach.
- It is an intriguing result that the fatigue crack growth rates at near-threshold stress intensity factor changes for steels B and D are the same as that in air. Its validity needs to be understood at various pressures.

Strengths and weaknesses

Strengths

- This is a good, solid project and well done. The team has decent collaboration and the project is relevant.
- This project has a clear, direct, applied science approach.
- The project is providing a valuable knowledge base on the effect of hydrogen on pipeline steels, which is important for any development of a hydrogen economy that will require the conveyance of hydrogen at much higher pressures than are currently employed.
- The strength of the project is the collaboration between Sandia National Laboratories and DGS Metallurgical Solutions. They both provide complementary expertise for the success of the project.

Weaknesses

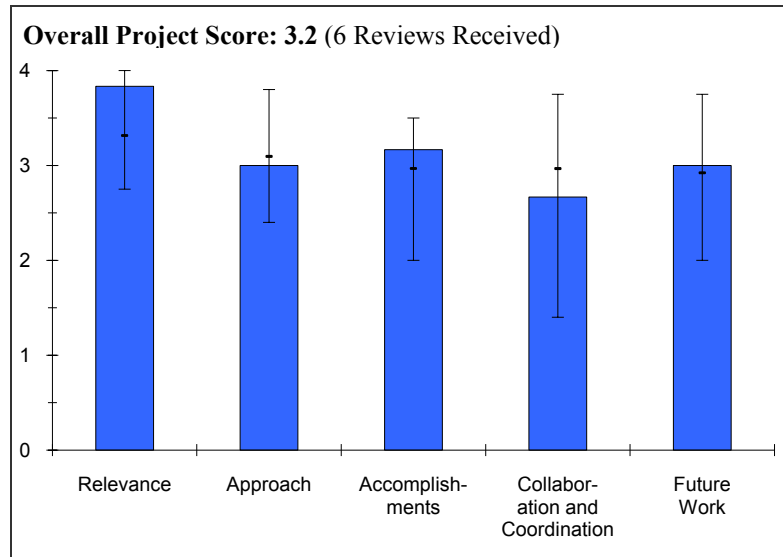
- No effect on welds measured, and these are often the weak points. The steels that were looked at are fairly old school.
- The project had a lack of breadth of the testing. The reviewer would have liked to see a dozen or so alloys evaluated.
- The number of evaluated samples and microstructure types is still very limited for gaining a desirably broader knowledge base of the effect of hydrogen on pipeline steels.
- It is not productive to focus resources on tensile testing. The project should continue with fracture toughness testing and fatigue crack growth testing. The reviewer does not believe that reduction in area can be used to evaluate suitability for service, as mentioned in slide #43. In fact, as the project has found, and the reviewer discussed above, reduction in area frequently yields contradictory results to those from fracture toughness.

Specific recommendations and additions or deletions to the work scope

- The project should look at welds as soon as possible.
- There are a number of questions posed on other alloys currently used for hydrogen storage. It would be interesting if the scope of the task were extended to include the evaluation of existing DOT cylinders steel alloys. These alloys are being considered for fuel storage on mobile material-handling equipment like fork trucks.
- Given that hydrogen-induced corrosion of steels depends on a dissociation of the hydrogen molecule into H atoms, the team should consider if a hydrogen and deuterium isotopic exchange rate into HD (as can be readily followed by mass spectroscopy) could possibly be utilized as a diagnostic for the onset of such corrosion.
- The project should focus on 1) quantifying the effect of the acicular ferrite content on fracture toughness, and 2) why the presence of acicular ferrite is not influential on decreasing fatigue crack growths.
- The project should explore other possible microstructural details that can be tailored to enhance fracture toughness and fatigue resistance.

Project # PD-48: Development of Highly Efficient Solid State Electrochemical Hydrogen Compressor (EHC)*Ludwig Lipp; FuelCell Energy, Inc.***Brief Summary of Project**

The objective of this project is to 1) develop designs and materials to increase EHC pressure capability from 2,000 to 6,000 psi, 2) improve the cell performance to reduce power consumption, 3) reduce the EHC cell cost by increasing operating current density, and 4) study thermal and water management options to increase system reliability and life. When compared to current mechanical compressors, an EHC will increase reliability and availability, prevent the possibility of lubricant contamination, increase compression efficiency, and potentially reduce hydrogen delivery cost to less than \$1/gge.

**Question 1: Relevance to overall DOE objectives**

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

- Using the "hydrogen pump" as a compression option is novel and promising.
- This project has the potential to demonstrate great results and the potential for improving the energy efficiency of hydrogen compression that is so critical to a hydrogen roll out
- Achieving hydrogen compression pressures between 5,000 and 10,000 psi is critical to successful on-board hydrogen storage for fuel cells (or internal combustion engines) used in transportation.
- High-pressure hydrogen compression, using an electrochemical system (with no moving parts) is very attractive.
- The project objectives involve improving performance and durability and reducing costs for EHCs, which are goals that support the DOE research, development, and demonstration mission.
- The project is clearly focused on developing this EHC technology to the point where it is competitive with state-of-the-art compressors with further improved reliability, availability, and efficiency.
- The project is aimed at developing a novel hydrogen compression technology, and it is addressing critical issues such as reliability, efficiency, and cost. Hydrogen compression is an important aspect of hydrogen fueling under various scenarios.

Question 2: Approach to performing the research and development

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

- The approach being taken is sound and focused.
- The approach has been on the safe side should push the boundaries faster. For example, it was stated that the team completed 20 cycles to 3000 psi in a 10-cell stack, but they did not test beyond that. It would be helpful to understand the number of cycles before failure.
- The project uses a unique approach to compress hydrogen that does not require the conventional mechanical compression dependence on moving components. The approach comes close to achieving its near-term goals of 5,000 psi.
- Current scoping research has seemed to demonstrate the concept, but it remains focused on improving technology for higher pressure. Equally important, if not more so, is increasing capacity beyond two pounds of hydrogen per day.

HYDROGEN PRODUCTION AND DELIVERY

- The approach appears reasonable at the broadest level, but lacks detail. Project milestones and progress towards them were highlighted and demonstrated tracking to the requisite metrics.
- The approach is well defined with appropriate key parameters such as current density, catalyst loading, and cell design.

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

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

- The technical accomplishments to date are very good.
- Accomplishments such as compression ratio and hydrogen recovery are good, but the energy consumption of the current prototype was unclear. For example if the heating value for EHC 100A-1-9 is approximately 4.1 kWh/kg lower, what is it being compared to?
- There is good progress in achieving the compression goals of 5,000 psi.
- Good technical review of accomplishments and progress on demonstrating capability to deliver higher pressures. One key item missing is cost estimates for a fully operational commercial system. It is unclear whether this system will be competitive with conventional compression systems.
- Project milestones, including increasing pressure (i.e., to 5,600 psi), efficiency, and stack scale-up, appeared to be demonstrated. However, the efficiency and cycling data that were highlighted were at lower pressures than those of interest. The overall progress has been good. The capacity of a single cell is approaching the target of 6,000 psi, although the same needs to be accomplished with a multiple-cell stack.
- The energy consumption, which is a critical parameter, has been improved significantly. However, it is not clear if the values reported are for a single cell or a cell stack.
- It appears from the milestones table that hydrogen recovery is reduced when the number of cells in a stack is increased. This reduction could be a drawback when this system is compared to a mechanical compressor, where there is no loss of hydrogen.
- Current density and catalyst loading are mentioned as critical parameters to cost and efficiency targets, however no improvements are reported with respect to these parameters.
- The team needs to conduct a cost estimation to demonstrate that the cost target can be met. Also, the capacity needs to be improved significantly to be of practical value; 2 lb/day is too small.

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

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

- The collaboration with others is good. If the concept, or rather the industry needs, had been discussed with the OEMs it would have been better. The usefulness of a 6,000 psi compressor is limited when considering hydrogen-fueled commercial and personal vehicles.
- While collaboration partners (FuelCell Energy, Inc. and Sustainable Innovations, LLC) and academia partners (University of Connecticut), were included, the overall collaborations were not sufficiently described.
- Collaboration with Sustainable Innovations and University of Connecticut were noted, but there was little acknowledgement of their contributions. It would be helpful to have more detail than one line on one slide to determine the extent of collaboration.
- Two subcontractors are listed, but their specific contributions and the extent to which they participate in this project is unclear. The reviewer would encourage additional collaborations with other entities focused on novel compressor technologies and/or electrochemical processes, particularly for validation.
- The team has appropriate partners and the team members are well qualified to conduct the proposed work. Nevertheless it would be helpful to add an end-user as a partner as the product development gets closer to real-life situations.

Question 5: Approach to and relevance of proposed future research

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

- The proposed work is focused for the 6,000 psi application, though the present 5,600 psi may be adequate for existing needs assuming the efficiencies are improved to a point nearing the goal levels.
- Future work should push the boundaries to determine competitiveness with current technology, such as demonstrating 2 lb/day at 6,000 psi, increasing the pressure capability of a single stage EHC cell from 5,600 psi to 12,000 psi, and reducing the power consumption to that of mechanical compressors (or lower).
- The goals to increase pressure capacity (5,600 to 6,000 psi), improve long-term durability, and increase output (at 3,000 psi) will be addressed and are a logical progression to achieving long-term goals.
- They have an acceptable target for future work, but the program ends in two months. The reviewer would like to have seen economic analyses of expected costs for this system at full scale deployment and comparison to conventional systems, including both CAPEX and OPEX.
- The team is focused on moving to a higher-pressure capability, yet durability and efficiency work is at lower pressures. There seems to be a disconnect in conditions and operation between these tasks.
- The plans are in line with the goals. However, it would be more desirable to achieve the lifetime and cycling performance, as well as hydrogen recovery at the maximum target pressure of 6,000 psi and not 3,000 psi. Also, it should include at least conceptual design for a higher capacity, for example to match a fueling station.
- The plan mentions "Update estimates of capital and operating costs," but there is no mention of any cost results to date.

Strengths and weaknesses

Strengths

- The strengths of the project are the focused applied science and the near-term goal of 6,000 psi. This pressure level is adequate for the fueling of 250 bar systems. (The 250 bar systems are often used with hydrogen-powered material handling systems (e.g., fork trucks)).
- A strength of the project is the ability to use this technique to separate non-reactive compounds like nitrogen, argon, and helium.
- The project has a clear, concise development process and outline of goals. The project lead's experience is also a strength.
- The novel approach to compress hydrogen without the use of mechanical/moving components is a strength.
- The project is novel and technologically elegant.
- Direct conversion of electrical energy to hydrogen compression is an appealing approach and the team members have the technical capabilities required for the tasks. With no moving parts, there is the potential for a higher efficiency machine with lower maintenance costs than a mechanical compressor.

Weaknesses

- The current scope limits the use of this equipment. It is suggested that if the goal were extended to 7,200 psi, it would cover 350-bar fueling (for buses and trucks). If the goal could be extended to 14,000 psi, it would cover 700-bar fueling, which is the current DOE car fleet goal.
- The water content of the compressed hydrogen is a weakness. The present car fleet fuel requirements limit water to approximately 5 ppm to avoid sublimation of ice on the valve and instrument operating surfaces.
- The goals need to be higher, and future cost estimates are not provided. The presentation made no mention of failure modes or development barriers, but these need to be known in order to facilitate collaborations (e.g., materials failure and transport reduction).
- While this concept is successful in avoiding mechanical devices and issues regarding parasitic mechanical energy losses and gradual wear of components, it does not deal with potential parasitic losses arising from internal resistance and degradation/poisoning of membrane properties.
- The concept goal of 2 lbs/day of hydrogen seems rather low. The team needs to address and discuss concepts to scale up the system to a larger throughput.
- The team did not present any economics to show if this would be viable as compared to conventional compression technology.
- Practical system designs are challenging and have not yet been addressed.
- With a futuristic view, cost and performance should be compared with emerging technology options (e.g., ionic liquid and metal hydride-based compressors) as well and not just with conventional mechanical compression.

HYDROGEN PRODUCTION AND DELIVERY

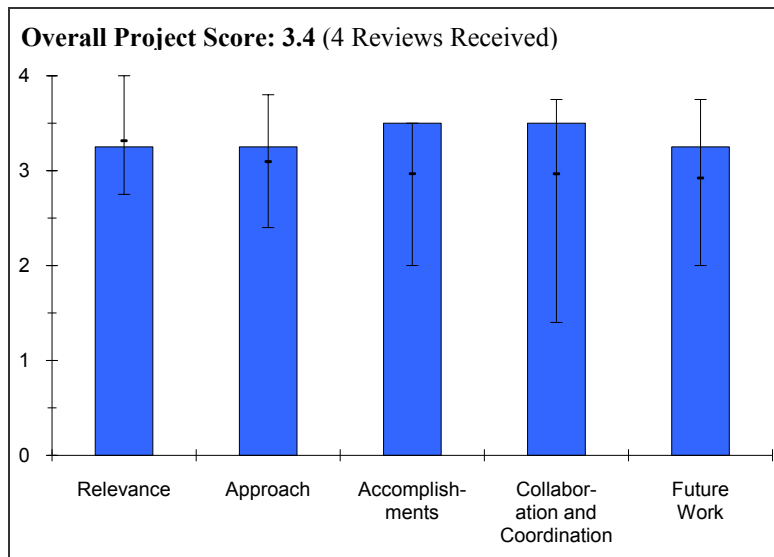
- The milestones table is confusing with different pressure levels, different cell structures (number of cells), lifetime and cycling targeted. The progression from a single-cell to a multiple-cell stack, the number of cycles, and lifetime testing should be better aligned with the final product configuration in mind.
-

Specific recommendations and additions or deletions to the work scope

- This is an excellent project. The team should consider a post-compression drier and pressure level (possibly by staging cells) approximating the needs of 350 and/or 700-bar systems to open market potential. It may be useful to have discussions with either a fuel provider or specialty gas company.
- The team should increase the project goals to allow the determination of future competitiveness with current methods of compression.
- The project should add a task to address the impact of internal resistance on system efficiency and provide some level of characterization of performance degradation as a function of compression cycles.
- The team should do the scoping economics and a comparison to conventional compression systems.
- The project should include a detailed cost estimation to show that targets can be met at practical flow rate capacities and under practical operating conditions.
- Key barriers to scale up should be identified up front and addressed to make sure that they will not be showstoppers.
- The final report should include a discussion about key parameters, such as cell density and catalyst loading, and their impact on cost and performance.

Project # PD-51: Characterization of Materials for Photoelectrochemical Hydrogen Production (PEC)*Clemens Heske; University of Nevada Las Vegas***Brief Summary of Project**

The overall objective of this project is to compile experimental information about the electronic and chemical properties of the candidate materials produced within the PEC Working Group to determine status-quo, find unexpected results, propose modifications to partners, and monitor the impact of implemented modifications. The project objectives are to 1) use a world-wide unique “tool chest” of experimental techniques; and 2) address all technical barriers related to electronic and chemical properties of the various candidate materials, in particular, bulk and surface band gaps, energy-level alignment, chemical stability, and impact of alloying/doping.

**Question 1: Relevance to overall DOE objectives**

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

- The technology may meet the DOE research, development, and demonstration intent, but the current state of proposed technology is at a low technology readiness level.
- This sub-project supplements the family of investigators on this joint project by providing the characterization of materials and a fundamental understanding of the materials being studied, both before and after electrolysis testing. This understanding is essential for providing much needed direction on the mechanisms and limitations of these photoactive materials for the design of improved materials at the molecular level.
- The work performed in this project is vital to understand the mechanisms of in-situ energy-level alignments, as well as the subtle changes that occur to the materials over time.
- The project is addressing the pertinent barriers to PEC production of hydrogen.

Question 2: Approach to performing the research and development

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

- The research focuses on evaluating and characterizing the synthesized iron oxide behavior.
- As a stand-alone project, this project does not have a lot of strategic direction. The sub-team seems to be at the mercy of the other investigators in terms of what materials are being studied. However, the materials characterization approach is excellent and provides good direction back to the team.
- The work uses state-of-the-art techniques and provides quantitative insight into areas which used to be primarily speculative or qualitative.
- The project is applying characterization skills to a number of materials.

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

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

- There is still planning of work and tradeoff needs to be done. The current technology readiness level (TRL) is very low, about TRL1. The major issues with any new proposed technology, such as this, include market

HYDROGEN PRODUCTION AND DELIVERY

variability, manufacturing in a large scale, reproducibility, reliability, and durability. Some technologies show great and promising results, but they never enter the market due to low feasibility.

- Work has been completed on all of the materials of interest from the other PEC Working Group teams, and feedback was given with guidance on mechanisms.
- This project does not directly address the barriers outlined in the DOE program. Instead, the progress here is graded as excellent for the insight that this project provides for the variety of materials systems examined. The work here can greatly accelerate the success of materials and systems iterations.
- The project has characterized a number of materials for a variety of collaborators.

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

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

- Collaboration is apparent among the team in that each member is working on a different material for the same technology and sharing the results.
- It is not clear how much the other investigators are leveraging this work to set their next direction. It would be helpful to have one of the team members describe the overall roadmap and interactions.
- All of the work is collaborative in nature; the investigator provides analytic services to other DOE-funded PEC projects.
- The team has excellent interaction with key players in the PEC community.

Question 5: Approach to and relevance of proposed future research

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

- The team is evaluating different materials and studying the impact of material modifications.
- The team is continuing to provide the same type of analytical results for new systems and newer collaborators will continue to provide important inputs for guiding the next iterative steps.
- Work should continue as long as there is a need for these characterizations within the PEC community.

Strengths and weaknesses

Strengths

- The project has good out of the box technical approaches, collaboration with other research labs, and focus on the stability of material.
- The team has excellent materials characterization capability and thoroughness in the experimental approach.
- The project provides important data to guide the design of the next materials iteration, in both synthetic and theoretical approaches. This helps the collaborators understand better what works and what does not work.

Weaknesses

- Technology viability, scalability and manufacturing in a large scale are not addressed or recognized.
- The team is somewhat at the mercy of other teams, in terms of the materials to be evaluated.

Specific recommendations and additions or deletions to the work scope

- The team should produce larger active area cells and evaluate the viability and feasibility of the technology.

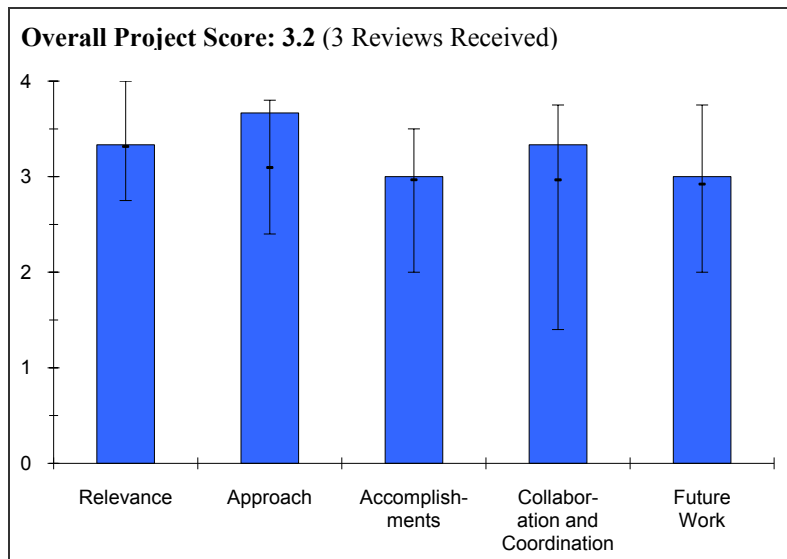
Project # PD-52: PEC Materials: Theory and Modeling*Yanfa Yan; National Renewable Energy Laboratory***Brief Summary of Project**

The main focus of the project is to 1) understand the performance of current PEC materials, 2) provide guidance and solution for performance improvement, 3) design and discover new materials, and 4) provide theoretical basis for go/no-go decisions to DOE PEC hydrogen projects.

Question 1: Relevance to overall DOE objectives

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

- The technology may meet the DOE research, development, and demonstration intent, but the current state of the proposed technology is at a very low technology readiness level. Each of the collaborating members is focusing on different synthesis materials, and there are many more materials for consideration.
- The project has a very good theoretical approach, which is needed for this area.
- A fundamental understanding of how the various properties of PEC materials can be tuned is important. Additionally, a quick way to screen various doped compositions without risking false negatives from non-optimally processed materials is a valuable tool.

**Question 2: Approach to performing the research and development**

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

- The research focuses on evaluating different syntheses, and the laboratory evaluation of small samples show some promising results.
- The approach can help to determine the limitations and advantages of different material structures if it is used by the rest of the team.
- The approach slide (slide 5) outlines the strategy of using theory to investigate band structure, optical absorption, defect and doping effects, surface chemistry, and structural stability. However, the last two items are not addressed in the presentation, though the contributions of understanding the first three on the list are very valuable.

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

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

- There is still planning of work and tradeoff needs to be done and more materials need to be evaluated. The current technology readiness level is very low, below TRL1. The major issues with any new proposed technology, such as this, include market variability, manufacturing in a large scale, reproducibility, reliability, and durability. Some technologies show great and promising results, but they never enter the market due to low feasibility.
- The team as a whole has a long way to go to prove the feasibility of direct PEC. All of the systems to date require voltage assist to produce photocurrent in water. This sub-team, however, is providing good progress.

- It is not clear whether the delafossite optical absorption coefficients shown on slide 15 are calculated or measured. Slides 8, 10 and 11 underscore one of the primary pitfalls of theory work, which is that the theory only holds if the proposed structure is actually formed. It is refreshing to see that pitfall called out explicitly.

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

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

- Collaboration is apparent among the team, in that each member is working on different material for the same technology and sharing the results.
- This sub-team is somewhat dependent on the other team members in the PEC Working Group, but less so than Heske since they are modeling instead of measuring. The reviewer would like to see continued direction setting.
- The collaborations listed are very useful, including synthesis groups for materials creation and properties and an analytical group (Nevada) for the confirmation of band structures. During the reporting period, it appears that most of the collaboration was with University of California, Santa Barbara.

Question 5: Approach to and relevance of proposed future research

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

- Many other materials and experimental methods need to be explored and evaluated, but it is unclear whether any of them would provide desired results.
- It would be helpful to discuss why the next generation materials were chosen.
- Continuing to support the PEC efforts through the theory work is an important component to the overall discovery process. There appears to be a good mix of stages of materials (i.e., early-stage work, such as the BiVO_4 , and work that is further along such as the iron oxide and the delafossites). The stability of nitrides and carbides is interesting, and it will be interesting to see if theory can really help identify materials' stability.

Strengths and weaknesses

Strengths

- The project is focusing on a single material and evaluating its potential and viability.
- The project has strong theory and calculation competency, thus providing a good explanation of data.
- The theory component is important to help understand the results observed and to help guide promising areas of research, especially in light of limited resources. The project seems to be taking "physical realities" into account, such as the formation of different phases and the possibility for a dopant to dope into different sites.

Weaknesses

- Technology viability, scalability, and manufacturing in large scale are not addressed or recognized. Collaborating partners are all focusing on different materials, which shows how much work needs to be done.
- The project needs to take a stronger direction-setting role on the synthesis of materials from other members.
- There is no indication that the theory is developed enough that it can give any predictions regarding the final phase of the materials or which of the multiple sites a dopant will prefer. Such capabilities would enhance the screening value of the simulation work.

Specific recommendations and additions or deletions to the work scope

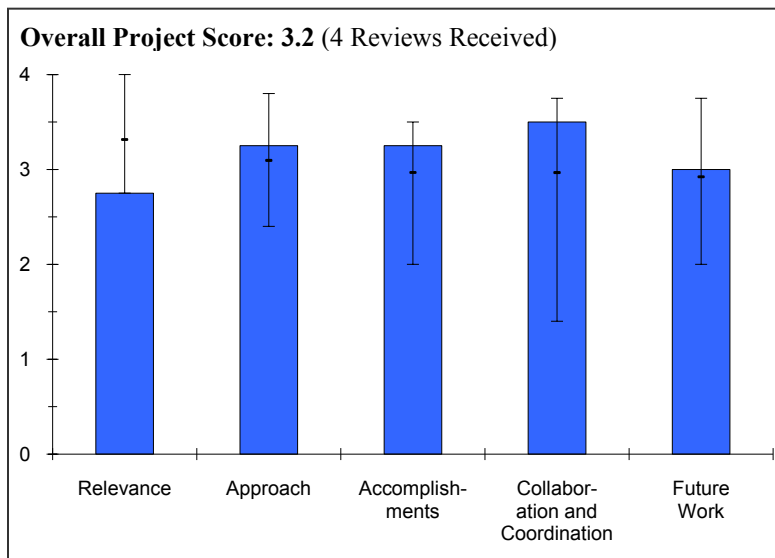
- The team should consider reevaluating technical viability and feasibility.

Project # PD-53: Photoelectrochemical Hydrogen Production: Progress in the Study of Amorphous Silicon Carbide as a Photoelectrode in Photoelectrochemical Cells

Arun Madan; MVSystems

Brief Summary of Project

The overall objective of this project is, by December 2010, to fabricate a hybrid a-Si tandem solar cell/amorphous silicon carbide photoelectrode device which exhibits a photocurrent greater than or equal to 4 mA/cm² and durability in electrolyte of at least 200 hours. Advantages of amorphous silicon carbide photoelectrode are: 1) lower bandgap (E_g) in comparison with tungsten oxide, produces more photocurrent; 2) bandgap can be increased/tuned with carbon inclusion into amorphous silicon material; and 3) amorphous silicon carbide uses same plasma-enhanced chemical vapor deposition technique (PECVD) as amorphous silicon photovoltaic (PV) cells.



Question 1: Relevance to overall DOE objectives

This project earned a score of **2.8** for its relevance to DOE objectives.

- The technology may meet the DOE research, development, and demonstration intent, but the current state of proposed technology is at a very low technology readiness level. Each of the collaborating members is focusing on different synthesis materials, and there are many more materials for consideration.
- It is not clear why one would want to degrade the efficiency of a solid state device by burying it with an over layer and using it to split water. While this is an elegant solution to the problem of not having good materials for splitting water directly from the sun, it seems that this approach adds significant complexity and cost, making the comparison to PV plus electrolysis even less attractive.
- The project is in line with the DOE goals and targets.
- The project effort is aligned with the DOE program objectives.

Question 2: Approach to performing the research and development

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

- The research focuses on evaluating different syntheses, and laboratory evaluation of small samples shows some promising results.
- It is not clear how these devices are going to get to the 10% target, but even the 5%-7% that has already been reached is fairly impressive.
- The approach of leveraging PV technology is highly valuable.
- The team has a systematic approach, which is making good use of analytical equipment and evaluation.

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

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

- There is still planning of work and tradeoff needs to be done and more materials need to be evaluated. The current technology readiness level is very low, below TRL1. Market variability, manufacturing in a large scale,

HYDROGEN PRODUCTION AND DELIVERY

reproducibility, reliability, and durability are major issues with any new proposed technology. Some technologies show great and promising results, but they never enter the market due to low feasibility.

- Good progress has been made against the milestones laid out in the project.
- The analysis of work function and differing surface modification/catalytic sites was well done and looks to have been fruitful. The analytical work in collaboration with Professor Heske helps to point out potential degradation pathways, which will relate to durability of the systems.
- Good progress has been made in several key areas.

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

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

- Collaboration is apparent among the team, in that each member is working on different material for the same technology and sharing the results.
- The project is well integrated with the PEC Working Group.
- Sample exchange for testing and analysis has led to very useful information regarding both performance and durability.
- This is a collaborative project with appropriate partners.

Question 5: Approach to and relevance of proposed future research

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

- Many other materials and experimental methods need to be explored and evaluated, but it is unclear whether any of them would yield desirable results.
- There seems to be a lot of future work for a project with a go/no-go decision later this year. A better plan may be to focus on how to get the information that is needed for the decision.
- The results seem to indicate that elimination of the silicon oxide (via Hydrofluoric Acid [HF] etch) improves performance, but that silicon oxide forms again during PEC testing. If this affects the durability significantly, prevention of the formation of silicon oxide should be considered. Incorporation of nitride materials looks like a good avenue to pursue from a materials stability standpoint.
- A go/no-go decision is to be made by the end of 2010.

Strengths and weaknesses

Strengths

- Focusing on a single material and evaluating its potential and viability is a strength.
- The project has an elegant solution to the problem of band mismatch for water splitting. The partners have good materials characterization capability.
- The project leverages an existing knowledge base of PV very well and supplements the PEC knowledge base. The project leverages collaborations for testing and analysis.

Weaknesses

- Technology viability, scalability, and manufacturing in large scale are not addressed or recognized. Collaborating partners are all focusing on different materials, which shows how much work needs to be done.
- The cost of this approach compared to other options is a concern and should be addressed. The project should determine what counter electrode will be looked at long term and how much that will hurt efficiency, how the system will be designed, and if these electrodes can be made in a large active area.
- The project has a PV approach to PEC. However, the collaborations bridge the knowledge gap, just as the investigator's knowledge of PV bridges some PEC knowledge gaps.

Specific recommendations and additions or deletions to the work scope

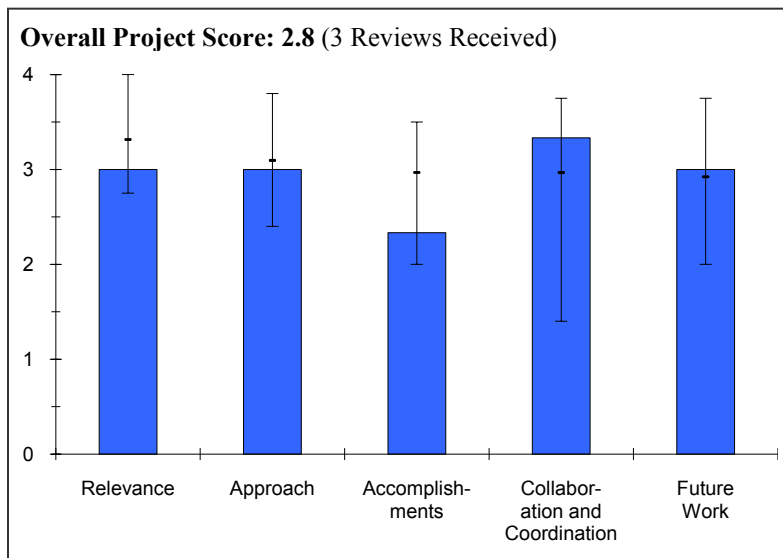
- The team should reevaluate technical viability and feasibility.

Project # PD-54: Progress in the Study of Tungsten Oxide Compounds as Photoelectrodes in Photoelectrochemical Cells

Nicolas Gaillard; Hawaii Natural Energy Inst.

Brief Summary of Project

The overall objective of this project is to study tungsten oxide in PEC cells. Advantages of tungsten oxide include 1) good performance has been demonstrated in several applications, 2) film can be deposited using low-cost processes, and 3) tungsten oxide satisfies the main criteria for water splitting. A tungsten oxide PEC device has shown 3.1% solar-to-hydrogen efficiency demonstrated in a mechanical stack configuration (using MVSysystems' solar cell). However, this material suffers from 1) its bandgap value (2.6 eV) that limits light absorption and 2) the position of the valence band versus oxygen half-reaction potential.



Question 1: Relevance to overall DOE objectives

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

- The technology meets the DOE research, development, and demonstration intent, but the current state of proposed technology is at a very low technology readiness level. Each of the collaborating members is focusing on different synthesis materials, and there are many more materials for consideration.
- The project uses an interesting idea, but the reviewer does not completely see the advantages compared with other options. The reviewer would like to see a more detailed cost and efficiency comparison.
- The project is aligned with DOE objectives.

Question 2: Approach to performing the research and development

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

- The research focuses on evaluating cost effective fabrication methods and different processes; laboratory evaluation of small samples shows some promising results.
- The team's testing approach is generally sound and the project is well-designed for the goals laid out.
- The project addresses DOE-appropriate barriers.

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

This project was rated **2.3** based on accomplishments.

- There is still planning of work and tradeoff needs to be done and more materials need to be evaluated. The current technology readiness level is very low, below TRL1. Market variability, manufacturing in a large scale, reproducibility, reliability, and durability are major issues with any new proposed technology. Some technologies show great and promising results, but they never enter the market due to low feasibility.
- Significant data from the last year was in the poster. The progress on milestones seems to be at the same point in 2010 as it was in 2009.
- The project research is progressing towards the performance objectives.

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

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

- Collaboration is apparent among the team, in that each member is working on different material for the same technology and sharing the results.
- The project is very well coordinated with other related posters. The PEC Working Group in general seems to be collaborating well. The team could potentially use characterization and modeling more effectively.
- The team is a participant in the PEC Working Group and is collaborating with appropriate technical partners.

Question 5: Approach to and relevance of proposed future research

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

- There are many other materials and experimental methods that need to be explored and evaluated. The question is whether any of them would produce desired results.
- There is a good plan focused on addressing material issues.

Strengths and weaknesses

Strengths

- Focusing on a single material and evaluating its potential and viability is a strength. The project also does well in economic viability studies.
- The team has good science and a good approach, with collaboration across many groups.

Weaknesses

- Technology viability, scalability and manufacturing in large scale are not addressed or recognized. Collaborating partners are all focusing on different materials, which shows how much work needs to be done.
- The cost of this approach compared to other options is a concern and should be addressed. It is unclear what counter electrode will be looked at long term and how much it will hurt efficiency, how will the system be designed, and if these electrodes can be made in a large active area. The project seems to be at a lower point than the other teams in terms of efficiency.

Specific recommendations and additions or deletions to the work scope

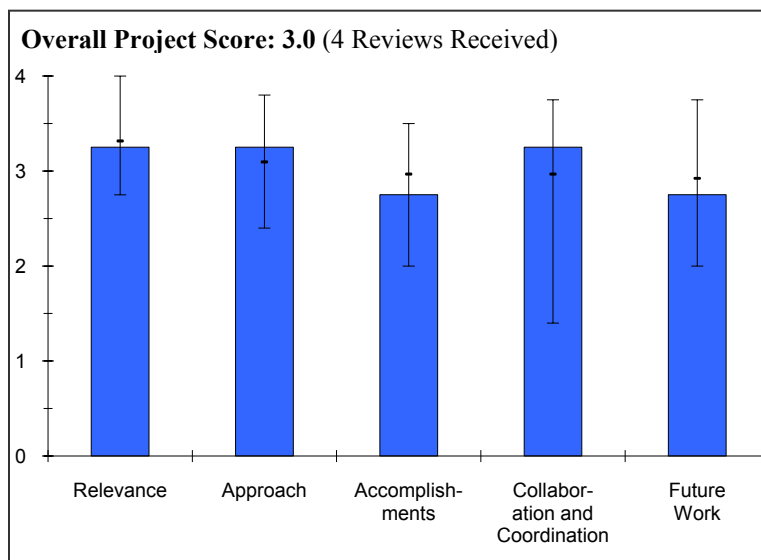
- The team should consider reevaluating technical viability and feasibility.

Project # PD-55: Progress in the Study of Copper Chalcopyrites as Photoelectrodes in Photoelectrochemical Cells

Jess Kaneshiro; Hawaii Natural Energy Inst.

Brief Summary of Project

The overall objective of this project is to develop copper chalcopyrite materials for incorporation into a hybrid photoelectrode (HPE) device capable of splitting water for hydrogen production when immersed in a suitable electrolyte and illuminated by sunlight. Material development objectives are to 1) identify methods of increasing the bandgap of copper chalcopyrite films to pass more light to an underlying solar cell; 2) perform surface modifications, including decreasing required voltage bias, improving surface kinetics, and increasing durability; and 3) identify methods to move the valence band maximum lower, including using silver in place of copper, using sulfur in place of selenium, and surface treatments.



Question 1: Relevance to overall DOE objectives

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

- The technology may meet the DOE research, development, and demonstration intent, but the current state of proposed technology is at a very low technology readiness level. Each of the collaborating members is focusing on different synthesis materials, and there are many more materials for consideration.
- It is not clear why one would want to degrade the efficiency of a solid state device by burying it with an over layer and using it to split water. While an elegant solution to the problem of not having good materials for splitting water directly from the sun, it seems that this approach adds significant complexity and cost, making the comparison to PV plus electrolysis even less attractive.
- Without a single material in existence that meets all criteria, it is important to examine multiple materials avenues to meet the targets.
- The project is aligned with DOE objectives.

Question 2: Approach to performing the research and development

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

- The research focuses on evaluating different syntheses, and laboratory evaluation of small samples shows some promising results.
- The reviewer is not sure why the team does not just use copper indium gallium (di)selenide (CIGS) PV technology with electrolysis, since that seems easier than trying to do band matching.
- Different facets affecting the ultimate performance of a device have been isolated, and approaches to the improvement of performance, as measured by the DOE targets, have been identified for investigation.
- The project addresses appropriate barriers to cost-effective and efficient PEC production of hydrogen.

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

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

HYDROGEN PRODUCTION AND DELIVERY

- There is still planning of work and tradeoff needs to be done and more materials need to be evaluated. The current technology readiness level is very low, below TRL1. Market variability, manufacturing in a large scale, reproducibility, reliability, and durability are major issues with any new technology. Some technologies show great and promising results, but they never enter the market due to low feasibility.
- The team has made some progress, but they do not show much traction towards milestones since 2009 and there appear to be limitations to getting farther. The team should try to use modeling to see if this is intrinsic or if in theory these issues can be overcome.
- Various pieces seem to be coming together, and the path forward is clear. The phase segregation seen in AlGaSe is not entirely unexpected. The segregation does raise some questions regarding the usefulness of the preliminary data shown.
- The project is making good progress in achieving goals.

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

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

- Collaboration is apparent among the team, in that each member is working on different material for the same technology and sharing the results.
- Collaboration in general between the groups seems very good in terms of information sharing. They need leverage information to determine the pathways forward.
- The exhibited ties to and use of collaborators are good.
- The team is a participant in the PEC Working Group.
- The team is collaborating with appropriate partners.

Question 5: Approach to and relevance of proposed future research

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

- There are many other materials and experimental methods that need to be explored and evaluated. The question is whether any of them would pan out.
- The team did not really answer a reviewer question from last year on the go/no-go decision. Slide 6 is not a "milestone plan," it is the end goals for each year. The team needs to describe the science that is proposed to meet these milestones.
- The proposed future work addresses the work needed to reach targets and to overcome barriers in a way that is not redundant with other work going on in DOE-sponsored projects.
- There is a structured approach that meshes well with other partners in the activity.

Strengths and weaknesses

Strengths

- Focusing on a single material and evaluating its potential and viability is a strength.
- The material has very high photocurrent, which the team would like to leverage in this project.
- This project approaches system challenges in novel ways. These paths have basis either in theory or in correlation to PV systems, showing good rationale for the choices made. Their progress appears to be good, despite uncertain funding during the course of project.

Weaknesses

- Technology viability, scalability, and manufacturing in large scale are not addressed or recognized. Collaborating partners are all focusing on different materials, which shows how much work needs to be done.
- The cost of this approach compared to other options is a concern and should be addressed. It is unclear what counter electrode will be looked at long term and how much will that hurt efficiency, how the system will be designed, and if these electrodes can be made in a large active area.
- While all of the work is interesting and useful, of the three main facets, surface treatment and back contact work seem to be a different general scope than the silverization. Ultimately, there should be some focus on cost of

materials. Although some digging shows that silver is likely to be cheaper than indium, it is probably still more expensive than copper.

Specific recommendations and additions or deletions to the work scope

- The team should consider reevaluating technical viability and feasibility.
- The team consider separating the silverization into a separate project, if the segregation cannot be easily overcome.

Project # PD-56: Critical Research for Cost-Effective Photoelectrochemical Production of Hydrogen

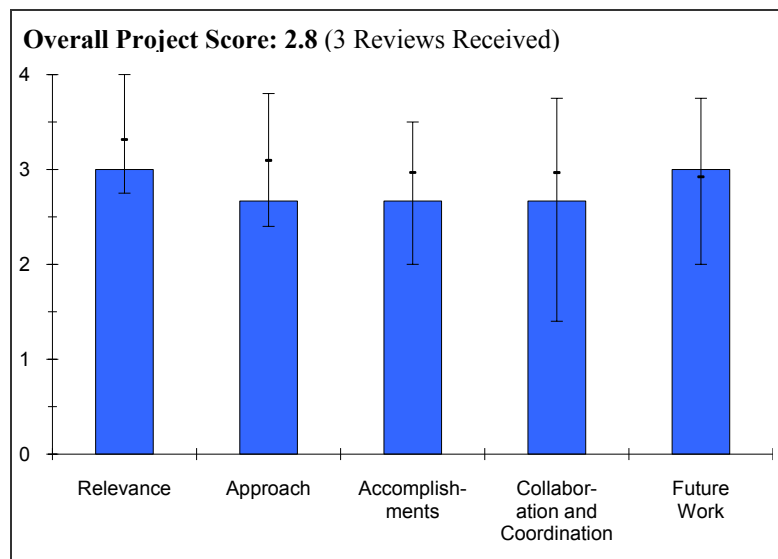
Liwei Xu; Midwest Optoelectronics, LLC

Brief Summary of Project

The overall objective of this project is to develop critical technologies required for cost-effective production of hydrogen from sunlight and water using thin film silicon-based photoelectrodes. Two approaches are taken for the development of efficient and durable PEC cells: 1) an immersion-type photo electrochemical cell in which the photo-electrode is immersed in electrolyte, and 2) a substrate-type PEC cell in which the photoelectrode is not in direct contact with electrolyte.

Question 1: Relevance to overall DOE objectives

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



- The study may meet the DOE research, development, and demonstration intent, but the current state of proposed technology is at a very low technology readiness level. Each of the collaborating members is focusing on different synthesis materials, and there are many more materials for consideration.
- The comparison approach is attractive, although this project requires a lot of engineering. The reviewer likes the idea of directly comparing immersion versus substrate, rather than being limited to one.
- The objectives are aligned with DOE.

Question 2: Approach to performing the research and development

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

- The research focuses on evaluating different materials, and laboratory evaluation of small samples shows some promising results in lowering the cost and increasing the efficiency.
- This project has some good work, but it seems a little scattered in terms of laying out an organized experimental pathway.
- If the project is successful, the work will contribute to overcoming barriers.

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

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

- There is still planning of work and tradeoff needs to be done and more materials need to be evaluated. The current technology readiness level is very low, below TRL1. Market variability, manufacturing in a large scale, reproducibility, reliability, and durability are major issues with any new technology. Some technologies show great and promising results, but they never enter the marketplace due to low feasibility.
- Progress has been made despite no FY 09 funding. The chemistry seems reasonable; although, as stated above, the device engineering is difficult and seems a little outside the expertise of the team.
- The team is making good progress in the fabrication of materials.

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

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

- Collaboration is apparent among the team, in that each member is working on different material that would apply to the same technology.
- Interaction between partners is not very clear. The presentation did not describe, for example, when the team is meeting and how tasks are coordinated.
- The team has active collaborations with appropriate partners.

Question 5: Approach to and relevance of proposed future research

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

- There are many other materials and experimental methods that need to be explored and evaluated. The question is whether any of them would pan out.
- The project is leveraging partner research and expertise.

Strengths and weaknesses**Strengths**

- Focusing on additional potential materials and evaluating their potentials and viability is a strength.
- The team is learning from issues and making progress. Direct comparison between the substrate and immersion approach is refreshing, compared with teams that ignore direct electrolysis.

Weaknesses

- Technology viability, scalability, and manufacturing in large scale are not addressed or recognized. Collaborating partners are all focusing on different materials, which shows how much work needs to be done.
- There is substantial industry knowledge on the alkaline electrolysis side that could be better leveraged. It might be worth consulting with GE or another company with technology in this area. It seems like there is a lot of work left to cover in the remaining time and budget.

Specific recommendations and additions or deletions to the work scope

- The team should consider reevaluating technical viability and feasibility.

Project # PD-58: Characterization and Optimization of Photoelectrode Surfaces for Solar-to-Chemical Fuel Conversion

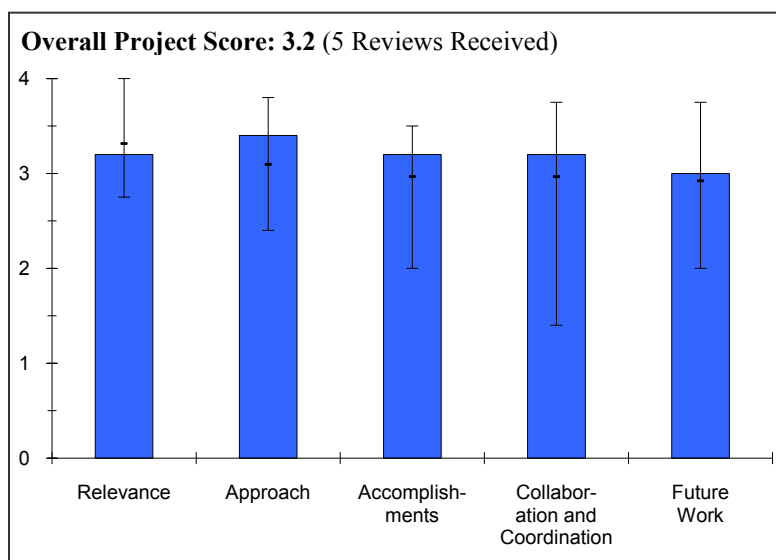
Tadashi Ogitsu; Lawrence Livermore National Laboratory

Brief Summary of Project

The objectives of the project are to 1) understand the underlying mechanism of surface corrosion of semiconductor-based PEC cells, 2) understand the dynamics of water dissociation and hydrogen evolution at the water-photoelectrode interface, 3) understand the electronic properties of the water-electrode interface, and 4) understand the relationship between corrosion and catalysis.

Question 1: Relevance to overall DOE objectives

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



- The technology may meet the DOE research, development, and demonstration intent, but the current state of proposed technology is at a very low technology readiness level.
- This project is doing very important background work for understanding what materials will work and what will not work. The reviewer would like to see this applied to more relevant semiconductors.
- The team is studying some interesting phenomena, but somebody with a background in the catalysis of hydrogen evolution should be advising them.
- Understanding the surface chemistry of the system, both intended and side reactions, is an important facet to being able to tailor robust materials.
- Understanding the fundamental properties of materials could be helpful to other members of the working group.

Question 2: Approach to performing the research and development

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

- Surface corrosion of semiconductor-based PEC materials is important for further understanding of the corrosion effect on different materials and how it impacts their performance.
- The project has a nice capability in modeling and demonstration of the role of water structure. It is challenging to get to this level of detail and good progress is being made.
- The reviewer is not sure what the full limits are of what they can calculate. Certainly there is a fundamental problem in that semiconductors are not very catalytic as electrodes, and so understanding adsorption energies of hydrogen, oxygen, water, and their intermediate species is of interest. It is unclear if the team can model energies if we put a few nanoclusters of platinum on the indium phosphide (InP) surface. The reviewer was a little concerned by the remark that they "can't simulate excited states."
- The work here provides important information on the decomposition pathway of a material that shows promising properties before decomposing. It is always important to properly understand the failure modes before trying to design a solution.
- The simulation results could lead to new directions for experimental work.

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

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

- The research did evaluate the surface corrosion effect on several oxides in depth.
- The project has made impressive progress in a short time. Despite a reviewer question about only being a surface model, their animations seem to show propagation of a corrosion mechanism already (one can see underlying bonds starting to break apart). It will be important to extend the model to a longer term.
- The team is just getting started and has many interesting calculations ahead of them. The reviewer was not too excited seeing water adsorption on InP and is unclear why modeling a few picoseconds of dynamics teaches us anything about catalysis or corrosion. Those surface oxygens eventually begin to work their way into the lattice, oxidizing the entire electrode. The team should clarify if the lattice oxygen diffusion is going to be modeled.
- In the short time that the project has been active, it seems that good progress has been made towards establishing a baseline model from which to work, including observation in the simulation of the degradation mechanism.
- The team has interesting computer simulations.
- The team needs to corroborate calculated behavior with experimental data.

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

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

- Collaboration is apparent among the team, in that each member is working on different material on the same technology and sharing the results.
- Real collaboration is not clearly demonstrated. It is unclear what feedback is being given to other partners or being taken into the model.
- The reviewer hopes the team will have a lot to say and that the experimentalists will listen to them. However, it would help if they crunch numbers on the materials that the experimentalists are making.
- Although it is not clear that the collaborative exchange had begun at the time the project was started, it is clear that the lines of communication are now identified and open.
- The interactions with the PEC Working Group are very useful.

Question 5: Approach to and relevance of proposed future research

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

- The team seems to be aware of logical next steps in the project and limitations to be addressed. They could use discussion on what other materials will be addressed, as well as an overall map of the project.
- Most of what the team has proposed has yet to be performed, so the reviewer's comments are basically the same as the Approach section.
- The future work appears well laid out to build upon the work reported here and addresses several potential avenues to model improving the system.
- Collaborations with experimentalists will be helpful to the understanding of calculated and observed responses of materials.

Strengths and weaknesses

Strengths

- Focusing on surface corrosion characteristics is a strength.
- The project has made good progress in understanding and technique.
- The team has a potentially powerful method for understanding catalysis of the water-splitting/hydrogen-evolving reaction.
- The project fills a hole in the overall research portfolio.

Weaknesses

- There is still planning of work and tradeoff needs to be done and more materials need to be evaluated. The current technology readiness level is very low, below TRL1. Market variability, manufacturing in a large scale, reproducibility, reliability, and durability are major issues with any new technology. Some technologies show great and promising results, but they never enter the market due to low feasibility.

HYDROGEN PRODUCTION AND DELIVERY

- The project still has a way to go on the model to extend below the surface and apply to less expensive semiconductors that will have more relevance.
- The reviewer thinks there are more relevant systems than InP that the team could be looking at and that they could at least put some platinum on the surface.

Specific recommendations and additions or deletions to the work scope

- The team should consider reevaluating technical viability and feasibility.
- The project should evaluate the photoanode also. It would be useful to have a good semiconductor for oxidative water-splitting to evolve oxygen.
- The team could add work to examine modified electrode materials