2011 — Hydrogen Production and Delivery
Summary of Annual Merit Review of the Hydrogen Production and Delivery Sub-Program

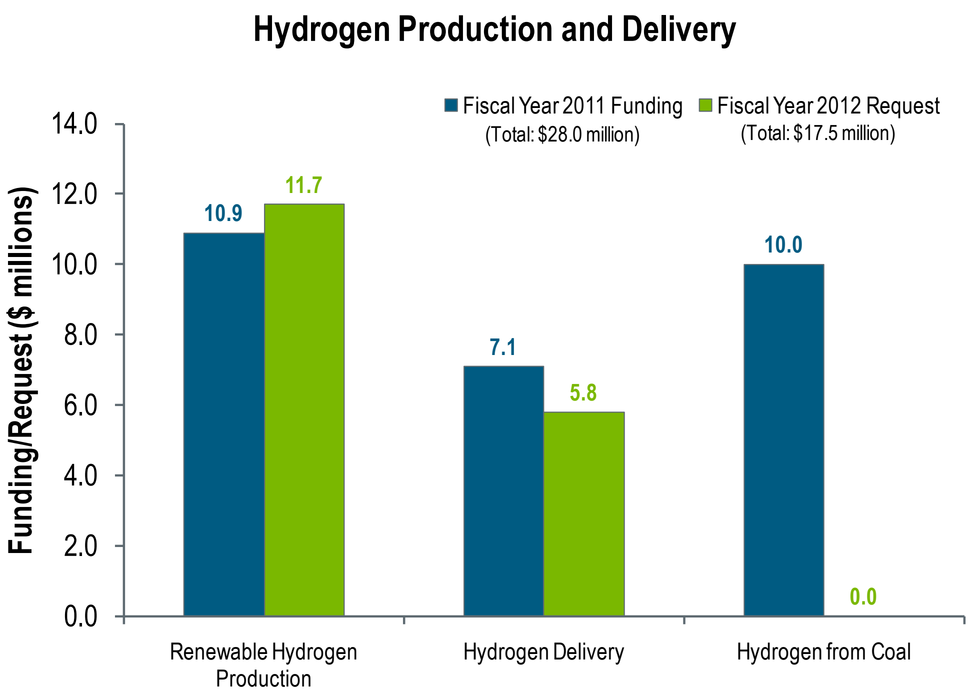
Summary of Reviewer Comments on the Hydrogen Production and Delivery Sub-Program:

This review session evaluated hydrogen production and delivery research and development (R&D) activities in the U.S. Department of Energy (DOE) Fuel Cell Technologies (FCT) Program in the Office of Energy Efficiency and Renewable Energy (EERE) and in the Hydrogen and Clean Fuels Program in the Office of Fossil Energy (FE). The hydrogen production projects that were reviewed represented a diverse portfolio of technologies to produce hydrogen from renewable energy sources, as well as coal with carbon sequestration. Production project sub-categories included water electrolysis, bio-derived renewable liquids reforming, biomass gasification, solar-driven thermochemical cycles, photoelectrochemical (PEC) direct water splitting, biological hydrogen production, hydrogen production from coal, and separations technologies. The hydrogen delivery projects reviewed included research and development in advanced composite tube trailer vessels, low-cost pipeline materials, pipeline and forecourt compression, electrochemical compression technology, liquid hydrogen production and pumping, and delivery cost analyses.

The production and delivery projects were considered by reviewers to be well aligned with DOE goals and objectives. In general, the reviewers found that these projects have made considerable progress in reducing both projected capital and operating costs and in improving material properties. Reviewers stressed the importance of continued improvement in the stability, durability, and performance of materials for components such as membranes and catalysts; devices and structures for splitting water; and tube trailers, pipeline, and compressors for hydrogen delivery. Reviewers also emphasized the need for continued analysis and modeling of production and delivery technologies and pathways to aid in the optimization of cost and performance.

Hydrogen Production and Delivery Funding by Technology:

The fiscal year (FY) 2011 appropriation for the Hydrogen Production and Delivery sub-program includes $18 million from EERE's FCT Program and $10 million from FE. In the FCT Program, approximately 61% of the sub-program funds were for production and about 39% were for delivery; this is similar to the 64% to 36% distribution in FY 2010. Funding for hydrogen production in the FCT Program is increasingly focused on early development, long-term, renewable pathways such as PEC, biological, and solar-thermochemical hydrogen production. This trend is expected to continue in FY 2012 with a $17.5 million request, when projects focused on separations will have ended. Hydrogen production R&D efforts in FE continued to focus on development of separation membranes and catalysts for hydrogen from coal. Emphasis in FY 2011 was on demonstration of performance through long-term bench scale and slip stream tests. In FY 2011 and FY 2012, hydrogen delivery activities in the FCT Program are focusing on reducing pipeline and forecourt compression cost, increasing tube trailer capacity, and identifying viable low-cost early market delivery pathways. A chart showing sub-program funding for FY 2011 and 2012 (requested) is included on the next page.



Majority of Reviewer Comments and Recommendations:

In general, the reviewer scores for the production and delivery projects were above-average to high, scoring in the range of 2.4–3.7, with an average score of 3.1. The scores are indicative of the technical progress that has been made over the past year.

Electrolysis: Five electrolysis projects were reviewed, with an average score of 3.3. Projects in this topic area tended to score favorably, with some receiving high marks for exceeding efficiency and capital cost targets for this year. The major emphasis of electrolysis projects was on cost reduction through cell and stack optimization. Specific efforts were directed toward increasing the stack efficiency by reducing the cell potential. Independent testing and integration with renewable power sources was another emphasis. Reviewers noted that all projects demonstrated good progress and they commended them for their effective collaborations and quality of design. The reviewers emphasized that future work should continue to focus on cost reduction, stack efficiency, and long-duration stack testing.

Bio-Derived Liquids Reforming: Two projects in bio-derived liquids reforming were reviewed, with an average score of 2.8. Projects in this area included development of catalytic steam reformation of oil for producing hydrogen, as well as investigation into aqueous phase reforming, a process producing hydrogen from bio-oil at moderate temperatures. In general, the projects reviewed consisted of a straightforward approach, focusing on optimizing the components of the process. Reviewers noted that the projects appear to be well aligned with DOE objectives and that the projects demonstrated increased hydrogen yields and catalyst durability, although costs were still high. Reviewers stressed that improving the catalyst was a critical next step, as well as addressing issues of capital cost and feedstock. They also stated that critical barriers must be overcome before this technology can be applied at the forecourt. One reviewer cautioned that liability issues associated with storage of potentially toxic, water soluble organic liquids is a critical barrier to deployment of this technology at the forecourt. This issue is being addressed by the project teams.

Biomass Gasification: One biomass gasification project was reviewed, receiving a score of 2.6. This project was focused on the development of high-temperature metallic or glass membranes for close coupling with a biomass gasifier for direct production of hydrogen from syngas. Reviewers found the proposed use of a membrane within the gasifier or after the first cyclone to be an interesting challenge, and they stated that it would likely lead to a

commercially viable process for biomass-derived hydrogen. Reviewers suggested a comparison of the benefits and potential drawbacks (e.g., concerns regarding sulfur contamination, biomass tars, biomass feed variability, thermal shock, stress, and durability of metal/glass/ceramic membrane modules) be performed for different membrane development approaches.

Solar-Driven High-Temperature Thermochemical Production: Four projects in solar-driven high-temperature thermochemical hydrogen production were reviewed, with an average score of 2.9. Efforts in these projects were directed toward simplifying the cycles, lowering the temperature, and developing materials durable enough to withstand extremely high temperatures. There was also ongoing investigation into thermal energy storage via molten salts, which would allow for continuous operation of the systems. Projects reviewed in this topic area were rated favorably for their solid technical approaches and for effective domestic and international collaborations. Reviewers observed that there has been reasonable progress, including improvements in efficiency. They suggested that future work should focus on advanced materials research, which is critical to the success of this technology. Reviewers also recommended longer durability tests and continued economic analysis.

Photoelectrochemical Hydrogen Production: Six projects in PEC hydrogen production were reviewed, with an average score of 3.4. Reviewers felt that projects in this area were generally well aligned with DOE objectives, with a universal focus on developing viable PEC materials and prototypes. They also observed that significant milestones were met by these projects, including the achievement of new performance benchmarks for crystalline systems and thin-film material systems. These projects also received praise for other notable accomplishments, including a valuable analysis of materials and semiconductors. Projects were rated highly for improvements to materials and catalytic activity, team leadership, and collaborations with the PEC Working Group. The reviewers' recommendations for future work included the suggestion that further development of component materials and stable catalysts should be included as teams look into scaling-up prototypes. Reviewers also emphasized that some projects will need to focus on narrowing their number of candidate materials for the PEC cells.

Biological Hydrogen Production: Four projects in biological hydrogen production were reviewed, with an average score of 3.3. Projects in this area encompassed a portfolio of photobiological and fermentative production methods using various micro-algal, cyanobacterial, and bacterial microorganisms for splitting water and using biomass resources to produce hydrogen. Although the improvement in oxygen tolerance was moderate, reviewers observed that the approach to modify the redox potential of the ferredoxin has yielded significant results. They also noted that moderate progress was made with continuous hydrogen production and light utilization, but they expressed concern that there could be trouble with scaling-up the projects. A key recommendation was that future work should focus primarily on increasing oxygen tolerance and attaining continuous hydrogen production.

Hydrogen from Coal: Six projects in hydrogen production from coal funded by FE were reviewed, with an average score of 2.9. The main focus of coal-based hydrogen production R&D was working toward the goal of zero-emission production, and the majority of projects were also working to reduce their use of expensive catalysts in order to reduce costs. Projects included bench-scale testing of purification and separation technologies as well as efforts to improve system efficiencies. Reviewers noted progress in all areas, including flux, selectivity, cost, and durability. Reviewers also consistently recommended testing membranes in the presence of all contaminants found in coal, not just sulfur. They suggested that future work should focus on further development of the membranes by increasing the durability, flux, and stability without sacrificing one to achieve another.

Separations: One project in separations was reviewed, with a score of 2.4. The project focused on the development and fabrication of several types of hydrogen separation membranes, and on reducing cost through design by decreasing the use of expensive materials. According to reviewers, good progress was made. Reviewers noted that membranes were generally well designed and innovative, although the trade-off between flux and selectivity was a recurring issue and further development of membranes would be required. Reviewers recommended additional long-duration tests and expanded collaborations with industry partners.

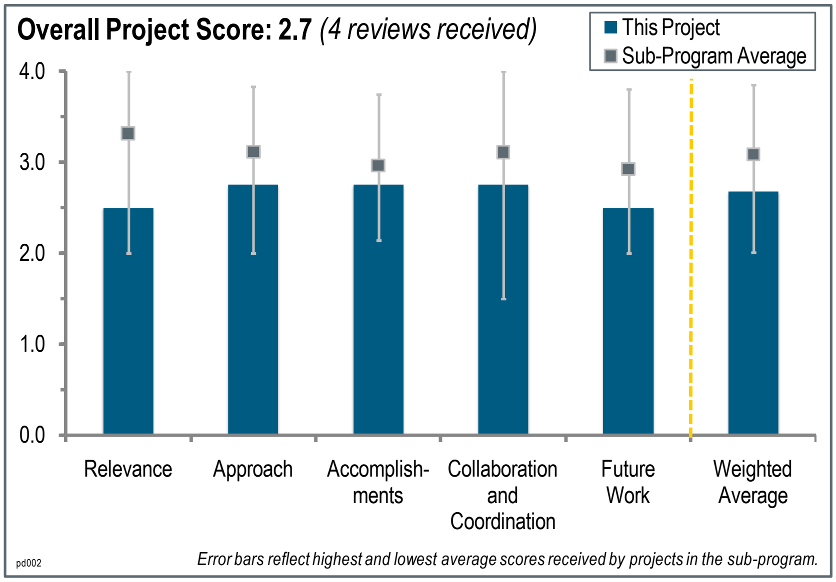
Hydrogen Delivery: Thirteen projects in delivery were reviewed, with an average score of 3.1. Projects reviewed in the Delivery sub-program portfolio continued to receive high marks from reviewers for the sound progress made toward the sub-program's cost goals, particularly the work on high-capacity tube trailer vessels, pipeline materials, and pipeline compressors. Reviewers highlighted the level of expertise in this broad topic area and were impressed with the degree of collaboration within many of the projects. While recommendations for improvements tended to

be project-specific, there was a general consensus that future work should be strongly focused on reducing costs on a per-kilogram-of-hydrogen basis; that estimates or projections of cost reduction should be vetted through analysis; and that synergies between various delivery technologies (e.g., storage and compression) should be considered and, when possible, evaluated for potential minimizations of pathway cost.

Project # PD-002: Biomass-Derived Liquids Distributed (Aqueous Phase) Reforming

David King; Pacific Northwest National Laboratory

Brief Summary of Project:



The objective of this project is to develop bio-derived liquids aqueous phase reforming technology for hydrogen production that can meet U.S. Department of Energy's (DOE) efficiency and cost targets. Objectives are to reduce reformer capital cost by: (1) maximizing catalyst activity and hydrogen selectivity to reduce reactor volume and associated purification steps; (2) developing new techniques to characterize the catalyst, especially under operating conditions, in order to understand catalyst functions and improve performance; and (3) developing an understanding of competing reaction pathways to guide the design of improved catalysts. The project will address feedstock issues by examining the efficacy of aqueous phase reforming of (aqueous soluble) bio-oil as a means to significantly reduce feedstock costs for hydrogen production.

Question 1: Relevance to overall U.S. Department of Energy objectives

This project was rated **2.5** for its relevance to DOE objectives.

- Aqueous phase reforming offers a potential pathway to lower the cost of hydrogen and aligns with DOE objectives.
- The project supports DOE's objectives because the efforts are focused on the two key issues: capital cost and feedstock.
- The results presented on aqueous phase reforming of bio-oils indicate monumental hurdles will have to be overcome to meet DOE goals in the near term.
- Distributed reforming of bio-oils is a non-starter due to liability issues surrounding the storage of toxic or potentially toxic water-soluble oxygenates at forecourts (i.e., consumer fueling stations). As a result of the legal issues arising from methyl tertiary butyl ether, no energy company will consider storing toxic oxygenates at the forecourt, even methanol. Ethanol is an exception because it is non-toxic and rapidly metabolized by soil organisms.

Question 2: Approach to performing the work

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

- The approach is reasonable and the examination of bio-oil is a good step. Conducting experiments on each of the 10 representative compounds in bio-oil is a good approach.
- The project is well designed. The barriers lie in the chemistry and nature of bio-oil. The cost analyses are based on the full conversion of all components. The full conversion of readily reactive components showed promise, but the cost analysis based on current conversion results is about six or seven times higher. It is not clear how the chemistry can be changed to make this a more cost-effective process. The reviewer's overall impression was that aqueous-phase reforming is not a viable technology.

- The approach appears to be adequate; however, the current choice of feedstock, namely bio-oil, could still experience significant barriers for forecourt application. Nevertheless, the outcome of the work should be useful for central reforming.
- The catalysts in this project have very high (3%) platinum loadings. At this loading, the catalyst has to last a very long time. The economic impact of low catalyst life is compounded by the high cost of replacement at this small scale. Therefore, catalyst lifetime tests are imperative. Any decline in activity on a weekly time scale is likely to make the process non-viable. These tests need to be carried out with real bio-oil. While model compound studies are valuable for mechanisms, catalyst poisons are often found in very small concentrations in uncharacterized fractions. Parallel testing with real pyrolysis oil needs to be carried out, especially for lifetime testing. Economic analysis needs to be performed to assess the impact of a catalyst lifetime on hydrogen costs. Analysis should also include sensitivity to biomass price (money divided by dry ton). The investigators should test several "real-world" bio-oils, including stabilized materials. Real bio-oils are likely to be two-phase systems.

Question 3: Accomplishments and progress towards overall project and DOE goals

This project was rated **2.8** for its accomplishments and progress.

- The technical results were impressive. The identification of acetic acid as an unreactive component and its deactivating effect on glycerol reforming was very good. It is clear that the team has expert knowledge.
- Good work was done characterizing the reactivity of bio-oil model compounds.
- The researchers have conducted the tests according to schedule and achieved solid performance data on which to base their Hydrogen Analysis (H2A) production cost calculations. The problem is that current projects are for \$25 per kilogram (kg), vastly exceeding the \$3.80/kg target. They need to be near 100% selectivity, but offer no specific pathways to achieve this goal.
- No conclusions are provided for the fiscal year 2010 work reported on sorbitol. This reviewer asks if the lower space velocity, which is required to achieve reasonable conversion, is practical from a cost perspective. The H2A results for bio-oil on slide 19 show the annual utilities cost as the highest cost component. It is not clear what these are. There is also no indication of an effort to reduce these costs, which should have a greater impact. An explanation would be helpful. It is clear that the current results are far from meeting the target. This should be addressed in a more focused manner.

Question 4: Collaboration and coordination with other institutions

This project was rated **2.8** for its collaboration and coordination.

- The project's collaborative efforts were very good.
- Work with collaborators on characterization was mentioned but not described in any detail in the presentation.
- It is not clear how the collaboration with Virent is leveraged.
- It is recognized in the industry that conventional bio-oil is of poor quality due to high oxygen and water content, which is detrimental to hydrogen production. Efforts should be directed to consider better quality bio-oil. In view of this, it is important to collaborate with a bio-oil company or organization. In order to meet the main cost goal, there needs to be collaboration with an entity with expertise in process development and engineering to complement the Pacific Northwest National Laboratory group's strength in fundamental catalytic research.

Question 5: Proposed future work

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

- Inclusion of real bio-oil is a good addition.
- The plans are focused on catalyst improvements and more fundamental work in terms of understanding reaction mechanisms. While this is useful, there needs to be complementary efforts on process development.
- Finding an improved catalyst should be a top priority for the researchers.
- There was no timeline for go/no-go decision point two. Reducing the hydrogen production cost from more than \$25 to \$3.80 requires a credible time plan to meet the targets, and this was not presented.

Project strengths:

- A strength of this project is obtaining experimental results on the 10 individual representative components of bio-oil.
- Excellent technical knowledge is evident in this project.
- This project has good catalyst characterization, strong reactor studies with model compounds, and strong applications.
- Catalyst development is the major strength of the group. The researchers also have a good fundamental understanding of reaction pathways, mechanisms, and kinetics.

Project weaknesses:

- The overall low hydrogen selectivity is leading to a very high projected hydrogen cost.
- This project does not appear to be a viable technology in the near term. The bio-oils would have to undergo considerable separations, which would be costly.
- There is a lack of insight on the process and engineering aspects of this project. For example, it is unclear if the high cost of utilities can be reduced. Feedstock selection is critical and additional external input on this would be helpful.

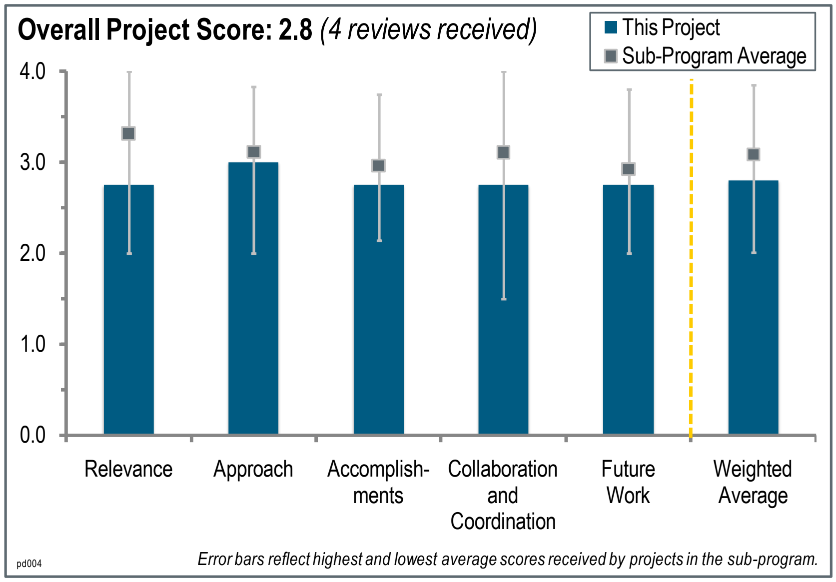
Recommendations for additions/deletions to project scope:

- This project should include testing on actual bio-oil (or at least mixtures of the 10 components) to ensure that there are not unforeseen interactions. The metrics could also be further improved. Right now, the only goal is to achieve near 100% selectivity or conversion; there needs to be other, more specific metrics against which to judge progress.
- More detailed economic analysis needs to be carried out to quantify effects of catalyst life and capital costs (for example, it is unclear how materials required for handling corrosive liquids affect the capital expenditures for reactors).
- As indicated above, a parallel effort on system engineering (reactor design, process integration, and optimization) would be beneficial.
- Given the fact that bio-oils will never be stored in the forecourt, DOE should consider termination of this project.

Project # PD-004: 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 the process definition of automated distributed reforming; and (2) demonstrate the technical feasibility of the process. The objectives for fiscal year 2011 are to: (1) select a commercial catalyst for autothermal reforming of bio-oil, (2) construct an integrated system for producing hydrogen from bio-oil, and (3) demonstrate operation of the integrated autothermal system for producing hydrogen from bio-oil at 100 liters per hour (l/h).

Question 1: Relevance to overall U.S. Department of Energy objectives

This project was rated **2.8** for its relevance to U.S. Department of Energy (DOE) objectives.

- Bio-oil is made from renewable feedstock and merits attention.
- Hydrogen production from domestic renewable sources supports a sustainable and secure hydrogen infrastructure.
- Bio-oil reforming is an important area that needs both applied and fundamental research. This project focuses more on the application.
- Distributed reforming of bio-oils is a non-starter due to liability issues surrounding storage of toxic or potentially toxic water-soluble oxygenates at forecourts (consumer fueling stations). As a result of the legal issues arising from methyl tertiary butyl ether, no energy company will consider storing toxic oxygenates at the forecourt, even methanol. Ethanol is an exception because it is non-toxic and is rapidly metabolized by soil organisms.

Question 2: Approach to performing the work

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

- This project has a straightforward approach. There is not much complexity, just a focus on optimizing each unit process. Researchers selected a commercial catalyst (produced by BASF), but there are not many, if any, comparisons. This reviewer asks if optimization is taking place, and if they just tested one catalyst.
- The project focuses on the process development for reforming bio-oil for hydrogen production. The work to date has been performed using a commercial catalyst. The principal investigator indicated that there is a collaboration effort with the University of Minnesota for catalyst development, but it is not clear what that collaboration entails. Catalysts will be a very central part of the process, so a more clearly defined collaboration on catalyst development would be beneficial.
- The platinum catalyst has to last a very long time. The economic impact of low catalyst life is compounded by the high cost of replacement at this small scale. Therefore, catalyst lifetime tests are imperative, especially on the weeks or months scale. Economic analysis needs to be performed to assess the impact of catalyst lifetime on hydrogen costs. Analysis should also include the sensitivity to biomass price (dollar amount/dry ton). It is not

obvious whether the atomization process is essential to this project. The Program's other bio-oil project appears to use a traditional trickle bed reactor to achieve high conversions. Construction of an integrated system is a good extension of the work, but hydrogen separation should not be a part of the system. This is off-the-shelf technology and not a critical component of the system. The use of a non-standard separation system makes its incorporation even more questionable.

Question 3: Accomplishments and progress towards overall project and DOE goals

This project was rated **2.8** for its accomplishments and progress.

- The hydrogen yields reported are impressive. Catalyst durability is also promising; however, use of a platinum catalyst should be re-evaluated.
- The increase in conversion is a good accomplishment, but it was not obvious how it was achieved. It was not obvious how the fiscal year 2011 funding received to date was spent.
- Higher hydrogen yield appears to have been achieved at a relatively low space velocity (higher capital cost).
- This project demonstrated performance at multiple space velocities for a commercial catalyst and achieved 10% weight conversion. Costs are high and do not seem to show a pathway to cost reduction. The researchers have not charted key cost drivers, nor have they established component or specific goals that are necessary to achieve the target cost.

Question 4: Collaboration and coordination with other institutions

This project was rated **2.8** for its collaboration and coordination.

- The Colorado School of Mines (CSM) process modeling is a good addition. It would have been good to see how the results of this work are being applied to improve this project. If heat and material balances were performed, they should be used as inputs to the project's Hydrogen Analysis (H2A) production cost modeling to improve results.
- The progress made by collaborators in the past year is not clear.
- The collaboration efforts should be better defined. For example, the oxidative cracking work is attributed to CSM, but it is not clear what the collaborators have contributed so far.

Question 5: Proposed future work

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

- The proposed future work is reasonable and is based on past progress.
- The project's future work consists exclusively of system scale-up. Further component or process optimization would be ideal.
- Longer runs are needed to validate the viability of the system.
- Given the fact that bio-oil reforming will never occur at the forecourt, DOE should consider abandoning this project.

Project strengths:

- This project addressed oil stability issues by adding methanol and achieved 73% energy conversion efficiency (lower heating value). This is close to steam methane reformer efficiency.
- The process approach is very good. The results to date, including hydrogen yield and durability, are very impressive.
- This project has good experimental work.

Project weaknesses:

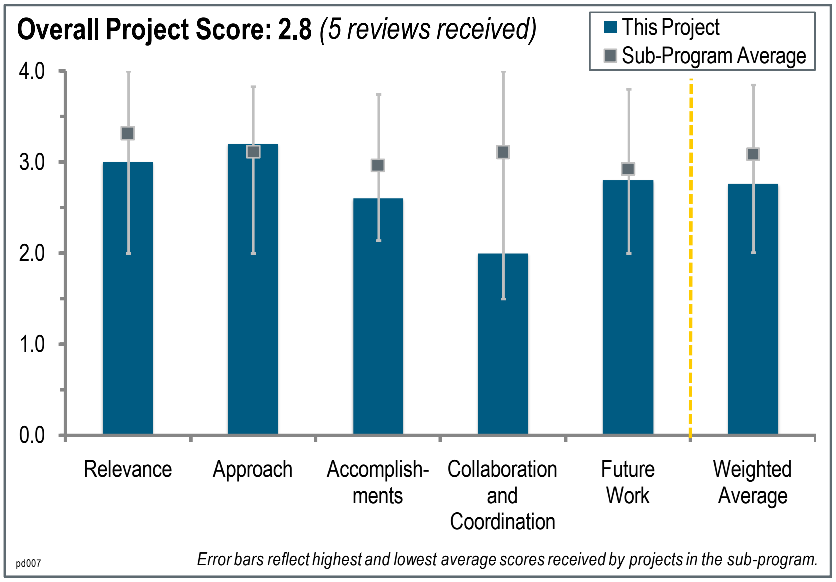
- This project does not include much catalyst optimization and no longevity data was reported. Low space velocity of the reaction will lead to high reactor costs. The use of catalytic partial oxidation forces the system to operate at relatively low pressures, thereby complicating linkage with pressure swing adsorption.
- The catalyst technology is rather vague. This reviewer wants to know if the work will continue with the commercial catalyst, or if there will be a catalyst development effort. This point needs to be addressed.
- The failure to include high-pressure processing adversely affects the overall cost of hydrogen.

Recommendations for additions/deletions to project scope:

- Researchers should examine other catalysts, conduct catalyst lifetime tests in microreactors, and discuss key cost drivers and ways to further reduce cost.
- Given the fact that bio-oil reforming will never occur at the forecourt, DOE should consider abandoning this project. The effect of steam ratio on conversion and yield should be investigated. H2A analysis should be expanded to incorporate increased capital expenditures due to the corrosion resistant materials required to handle bio-oil at the high temperatures used here. High-pressure experiments need to be carried out to minimize compression costs downstream. Researchers should look for non-precious metal reforming catalysts, and screening efforts should be able to test a large number of catalysts.

Project # PD-007: Composite Palladium and Alloy Porous Stainless Steel Membranes for Hydrogen Production and Process Intensification

Yi Hua (Ed) Ma; Worcester Polytechnic Institute



Brief Summary of Project:

The objectives of this project are to: (1) synthesize composite palladium and palladium/alloy porous Inconel membranes for water-gas-shift (WGS) reactors with long-term thermal, chemical, and mechanical stability, with a special emphasis on the stability of hydrogen flux and selectivity; (2) demonstrate the effectiveness and long-term stability of the WGS membrane shift reactors for the production of fuel-cell quality hydrogen; (3) research and develop advanced gas cleanup technologies for sulfur removal to reduce the sulfur compounds to fewer than 2 parts per million (ppm); (4) develop a systematic framework for 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 and 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 U.S. Department of Energy objectives

This project was rated **3.0** for its relevance to U.S. Department of Energy (DOE) objectives.

- The project is important to the Hydrogen from Coal research program and contributes to the fundamental understanding of alloy membranes for hydrogen separation. It is clearly focused on the DOE technical objective of developing a cost-effective, high-performance membrane process integrated within a coal gasification cycle to produce hydrogen for energy and carbon dioxide for capture and sequestration.
- The project is focused on making progress on the basic science that is limiting hydrogen separation technologies. Work on sulfur cleanup is particularly important, given its detrimental influence on palladium membrane performance.
- Stable and high-flux membrane development is relevant to hydrogen production. The membrane developed in this project does not tolerate even 2 ppm sulfur levels and needs an additional advanced cleaning unit. Mechanical durability is not established and there is no plan to study the mechanical property and embrittlement issues.
- This now-completed project pertained to the development of membranes that could meet DOE performance targets for hydrogen production and separation from coal gases. Improved performance levels and reduced costs are vital if large-scale production of hydrogen is to be achieved. However, the current project did not appear to thoroughly address issues with the removal of major impurities (e.g., sulfur compounds) and the robustness of systems during extended operation with compositions corresponding to production gases.
- This project has insufficient data and uses feed streams containing troublesome but likely impurities, including sulfur compounds and heavy metals.

Question 2: Approach to performing the work

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

- This project has a very good technical approach and results from the previous three years are very encouraging. Efforts planned for this year include testing membrane coatings from T3 Scientific. This coating may offer promise of enhanced membrane tolerance to feed-stream impurities.
- This project is a scientifically sound academic study of palladium/alloy membranes for hydrogen separation with an excellent focus on the fundamental understanding of the performance (flux) and stability of the membrane through both experimentation and mathematical modeling.
- Long-term testing is extremely important and has been lacking in many of the other membrane projects. It is good to see that Worcester Polytechnic Institute (WPI) is taking long-term testing seriously.
- The project focused on the fabrication and testing of palladium/alloy films deposited on Inconel porous tubing to determine optimal balance between permeation of hydrogen through the membranes that can provide sufficient separation and flux rates with minimal use of the highly expensive palladium. Modeling analyses of reaction dynamics and projections of costs for large-scale systems were also made. While acceptable levels were found for some configurations based upon laboratory-scale studies, permeation rates were generally too small or separations were insufficient using baseline components.
- The approach for this project is not clear. A number of membranes of the same composition (palladium) are fabricated and tested with the only difference being the membrane thickness. No attempt is made to develop sulfur and carbon monoxide (CO) tolerant membranes. Membranes developed in this project will work in an ideal gas mixture (i.e., hydrogen-helium mixture in the laboratory). There was no work done on more stable palladium/alloy membranes.

Question 3: Accomplishments and progress towards overall project and DOE goals

This project was rated **2.6** for its accomplishments and progress.

- Successful results include the demonstration of thin membranes supported in porous Inconel tubes. The membranes have achieved both an inherent lifetime of several thousand hours and high hydrogen flux. Some drawbacks are that lifetime has not been demonstrated with feed streams containing the sulfur compounds and heavy metals expected in coal gasifier streams. Recent data showing flux decline during a WGS experiment is also troubling.
- The principal investigator (PI) has made considerable progress using a systematic experimental plan and theoretical modeling to understand the process operational factors—such as temperature, pressure, support characteristics, alloy composition, and duration—that affect the flux and stability of the membranes for hydrogen separation. These progressive studies have been done with both hydrogen-helium and subsequently with mixed gas compositions analogous to average gasifier compositions. Researchers have also demonstrated target fluxes under simulated operational conditions likely to be encountered in the gasifier cycle. The PI has completed the work on pure palladium and palladium-silver composition and is beginning to investigate ternary alloys for improved performance. A new WGS composite membrane reactor test rig was designed to support the future work and advanced studies in the next phase of this project.
- This project has achieved DOE's 2015 flux target and identified an issue with support-limited mass transport. This target and lifetime were achieved with pure palladium, which will not likely meet DOE cost targets. As with other projects, this one should focus on reduced palladium loading membranes with long life and acceptable flux. The modeling effort in this project is good, but some quantification of how well the model fits experimental results is needed. The presentation showed that the fit is "good," which is vague.
- High flux (359 standard cubic feet per hour [SCFH]/square foot [ft2]) was obtained only in hydrogen-helium mixtures using a very thin membrane. Incidentally, this flux number was also reported in the 2010 Annual Merit Review. High-flux membranes show low selectivity even in ideal gas mixtures (hydrogen-helium selectivity of approximately 450 for a membrane with a flux of 359 SCFH/ft2). Flux under mixed gas conditions is only 44 SCFH/ft2, which is significantly below the DOE target. Membranes are not tolerant to even very low levels (2 ppm) of sulfur.
- Results reported that for thicker palladium membrane layers there was good separation of the hydrogen-helium test gas, but the hydrogen permeation fluxes were too low. On the other hand, for thinner palladium membrane

layers, hydrogen permeation fluxes met or just exceeded targets, but did not adequately separate the hydrogen from the helium. The researchers did not find a configuration that could simultaneously satisfy both the flux and separation criteria. Tasks planned for new (i.e., different) projects should have been examined sometime during the 4-year duration of the current project.

Question 4: Collaboration and coordination with other institutions

This project was rated **2.0** for its collaboration and coordination.

- The recent addition of T3 Scientific as a collaborator is positive and additional collaboration on economic modeling would be viewed favorably. There appears to be no plan for testing sample membranes in a coal gasifier slipstream; this would be a very important task component.
- All of the projects on palladium-membrane separation seem to have their own financial models. There should be some uniformity in the modeling methods so that models can be compared to one another, similar to the use of the Hydrogen Analysis model (H2A) in other parts of the DOE Hydrogen and Fuel Cells Program.
- Little collaboration existed in this project; this could be greatly improved. Collaboration with Adsorption Research, Inc. (ARI) does provide some technical breadth to the overall objective of the project. However, if this project is to go forward, partners need to be established to provide membrane fabrication and scale-up, gasifier testing, and industrial advisors for techno-economic process guidance or confirmation. Though absent from the slide presentation, the PI did mention orally that new partners are being brought in to the next phase of the project.
- The lone collaborator on this project, ARI, is only experienced in the area of sulfur cleanup and not membrane development. There was no gasifier partner involved in this project, and membrane work is all done in-house at WPI.
- From the material presented, it seems that the only significant collaboration was with the subcontractor, ARI, whose role in this project was only briefly identified in slide 22 and not clearly associated with the goals and objectives of this multi-year project.

Question 5: Proposed future work

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

- Future work on hydrogen sulfide (H2S) poisoning and palladium deposition techniques is important.
- The forward plan is solid and is focused on four important development areas to further improve selectivity, flux, and long-term stability: (1) applying advanced methods to prepare the alloy, (2) continuing materials development investigations on ternary alloys, (3) testing the T3 Scientific coating for H2S poisoning inhibition, and (4) beginning long-term stability tests in actual field studies using real coal gasifier slipstreams. The addition of collaborators is an important task for the future.
- This project ended in May 2011, meaning presented future plans on slide 25 pertain to a new task, which implied that these efforts are going to address issues that were not completed in the present effort.
- There are no plans to fabricate defect-free thin membranes. High-flux membranes exhibited poor selectivity even in ideal gas mixtures. Thicker membranes (approximately 20 micrometers thick) that showed better selectivity exhibited low flux. There are no quantitative measures for the planned future work; only qualitative measures, such as "continue to investigate," were given. There are no plans to develop sulfur- and CO-tolerant thinner membranes, or to study the mechanical property or embrittlement of the membranes. The project investigators did not respond to last year's reviewers' comments and the required mandatory "Reviewers Only" slides were not included.
- This reviewer asks why there are no plans to test the membranes in a coal gasifier slipstream. This is the target application and simulated feed streams cannot match the real challenges of an actual coal gasifier feed. The economic analysis needs to be refined, as porous Inconel tubes are very expensive. The reviewer also asks what the real costs are of making the membranes (yield must be accounted for, which likely is less than 100%). It is unclear what the real membrane lifetime and maintenance needs are. The reviewer also questions what the fundamental assumptions of cost (palladium market price, etc.) are, and how sensitive the overall economics are to key variables such as material cost, membrane lifetime, and manufacturing yield.

Project strengths:

- The long-term durability testing in this project is important and should continue.
- This project's strengths include the training of students and post-doctorates, a good number of publications, good fabrication and testing of palladium membranes by the team, and high flux under ideal gas mixtures (hydrogen-helium).
- A good many presentations and several papers were produced during this project. A high-quality gas testing station appears to have been fabricated at WPI, which should be useful for continued experiments.
- This project developed a proven basis for making thin, high-flux membranes on a porous Inconel support tube.
- The PI has focused his research on the most important aspects of the membrane and has conducted a thorough, detailed, and systematic and scientifically sound study to achieve a good understanding of the operational characteristics of the both the palladium and palladium/alloy membrane concept when applied to coal gas.

Project weaknesses:

- This project solely focuses on palladium and palladium-gold membranes and flux without looking at cost, which is critical to commercial success.
- The membrane is not tolerant to even 2 ppm sulfur and is easily poisoned by low levels of CO. This is expected of pure palladium. This team should look into palladium/alloy membranes; however, it does not have a partner in the membrane development area. There are also no gasifier partners involved in this project, which lacks the involvement of an end-user of this technology. There are no plans to make thin membranes with high selectivity and stability. High-flux membranes have low selectivity.
- There did not seem to be a clear pathway identified for optimizing the palladium/alloy composition with the configuration of the integrated manifold that could achieve the performance targets for enhanced production rates of hydrogen from coal gas.
- There is a lack of data showing promising lifetime in feed streams containing some troublesome contaminants expected in coal gas; there is also a lack of convincing economics.
- It is possible that collaboration with others could have improved the progress of the project. Other than that, there are no technical weaknesses apparent.

Recommendations for additions/deletions to project scope:

- DOE should continue to fund the project, but encourage the PI to focus more on testing membranes with simulated feed streams containing some of the sulfur compounds expected in coal gas, schedule slipstream tests on a coal gasifier, beef up the economic assessment, and include sensitivity analyses (cost as a function of key material market price, manufacturing yield, and lifetime).
- It is strongly advised that the research project be expanded to include fabricating larger scale membranes and that module design studies be initiated (though not mentioned during the presentation, it is presumed that this is the role of Membrane Technology & Research Inc. [MTR] in the forward program) to fabricate, test, and provide verification of the performance and cost projections predicted in the modeling studies of phase one. It is also strongly advised that the relationships with projected collaborators be expanded (as was suggested in the presentation via T3 Scientific, MTR, Siemens, and a gasifier test site), and that membrane testing be done as soon as possible on real coal gas slipstreams at a gasifier test facility. It is also advised that experimental coupon testing of promising new developments in the forward program be tested early on the coal gasifier slipstreams before incorporating such new development into the membrane-scaled designs. Researchers should continue the investigation of ternary compounds in future materials development, as other investigators are showing promising results in this area. There should also be focus on reducing the cost of the membrane and using the cost models that have been developed to verify the impact on cost.
- Reduced palladium membranes should be added to the project.
- Slide 2 shows that this project is 100% complete and that it is scheduled to end on May 6, 2011. Future plans are not defined well; therefore, this project should be terminated when its performance period ends. This team should bring on a partner to assist with commercialization and, for any future work, a strategy should be established to fabricate thin membranes with high selectivity.

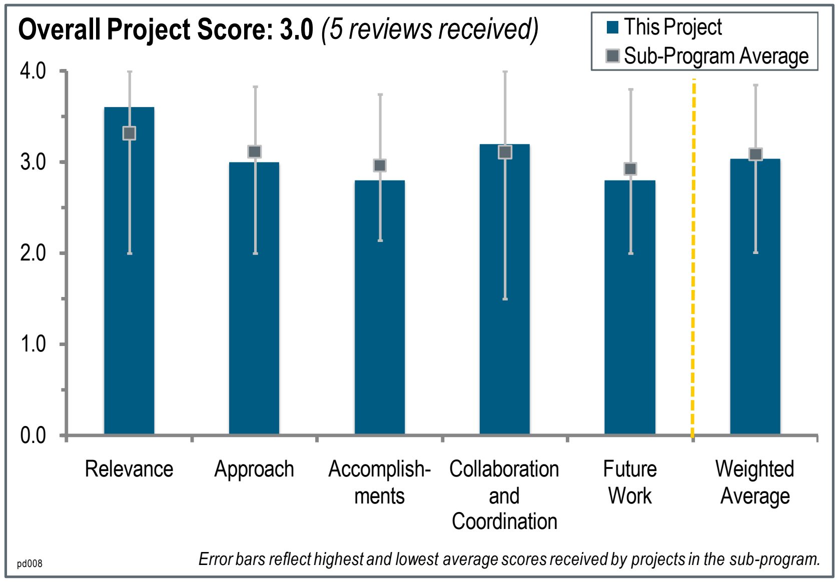
- There are no recommendations, as this project is completed as of May 2011. Following the project's end, WPI should attempt to focus on developing and evaluating composition membranes using its recently constructed test facilities.

Project # PD-008: 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 to develop robust hydrogen separation membranes for integration into coal conversion processes, including integrated water-gas-shift 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 U.S. Department of Energy objectives

This project was rated **3.6** for its relevance to U.S. Department of Energy (DOE) objectives.

- This project is contributing important fundamental understanding of alloy membranes to the Hydrogen from Coal research program, and is focused on DOE's technical objectives to develop a cost-effective, high-performance membrane process integrated within a coal gasification cycle to produce hydrogen for energy and carbon dioxide for capture and sequestration.
- The overall objective of this project is to develop robust hydrogen separation membranes for integration into coal conversion processes. This project is relevant to the DOE Hydrogen and Fuel Cells Program. This project is focusing on barriers such as hydrogen embrittlement, thermal cycling, and a sulfur poisoning mechanism.
- The primary objective of this presumably one-year project is to discover and develop palladium alloys that provide fast permeation of hydrogen with a greater tolerance of sulfur impurities during hydrogen separation from coal gas. The goal is to reduce the total cost of components and operation, which are important targets for the Program.
- Extracting hydrogen from syngas will be critical to clean coal when carbon taxes are implemented.
- This work has been underway for several years and is a very methodical approach. However, it remains rather distant from DOE goals in the sense that there appears to be little progress toward solving the long-known challenges of sulfur poisoning and heavy metal poisoning of high-flux palladium-alloy membranes.

Question 2: Approach to performing the work

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

- The research on ternary alloy development is focused on the important technical barriers of improving the robustness of the membrane and sulfur tolerance while maintaining the high selectivity and flux of the palladium-based membrane. Selective coupon testing at the National Carbon Capture Center (NCCC) is this project's key discriminator for early identification of performance issues related to actual gasifier-stream testing, which is being integrated in the development plan. The project is incorporating a fundamental thermodynamic understanding of the mechanisms associated with the performance of the alloys, as well as an understanding of the surface phenomena associated with sulfur layer formation and interaction mechanisms. Material development

studies to improve the membrane and seek better new alloy compositions are being accelerated using a high-throughput screening approach that will save time and more quickly down-select key promising compositions that can provide optimal performance when tested at NCCC.
- This project is taking an approach of parallel experimental and analytical research, which should enable the researchers to understand anomalies that arise.
- The project's approach is fair, but there has also been exceptional computational and structural work done in prior years aimed at understanding sulfur reactivity with palladium and palladium-copper membranes. However, it is disappointing to see that the technical approach has now become Edisonian research; that is, rapid throughput screening of an infinite array of ternary alloy compositions. This reviewer asks why there is such a fundamental shift in the technical approach, and if the investment in fundamentals was misdirected.
- This project applies computational and experimental capabilities to develop an advanced membrane system for hydrogen separation. The research is focused on poisons and structural integrity testing. This reviewer asks why thermal cycling is not considered in this work.
- This project is focused on the synthesis and detailed characterization of ternary alloys based on palladium-copper that is predicted from in-house thermodynamics calculations to possess suitable phase composition and crystal structures in order to provide high permeation rates and resistance to corrosion and passivation by gaseous sulfur impurities. First principles methods are employed to identify the most promising chemical bonding to enhance the stability of these ternary alloys. A variety of conventional materials and laboratory techniques will provide phase identification, assess the stability of the alloys in the presence of impurities, and measure hydrogen permeation parameters. However, these screening assessments do not ensure that candidates with the desired combination of properties can be achieved as phase boundaries and are often quite sensitive to processing temperatures and other variables, and resistance to detrimental reactions with sulfur species can still occur.

Question 3: Accomplishments and progress towards overall project and DOE goals

This project was rated **2.8** for its accomplishments and progress.

- This project made a very good effort to understand the impact of sulfur and how to minimize it.
- The project has been conducting a very thorough, thermodynamically based understanding of palladium-alloy membrane performance mechanisms and has used these models of basic understanding to experimentally verify the predictions. This has been done primarily with binary alloys with a focus on flux stability as well as the surface catalytic effects of the sulfur layer, which is critical for the overall membrane performance. A series of actual coupon tests at NCCC using slipstreams of real gasifier gas has been done and the resulting coupons have been characterized micrographically and chemically to understand the effects. Identification of arsenic has initiated an investigation into other gasifier stream contaminants. The project has moved into a comprehensive study of ternary alloys and has thus far conducted thermodynamic and phase-equilibria models to predict important compositional criteria.
- Extensive computational analyses of phase formation and stability have been done on numerous ternary alloys based on palladium-copper composition as well as formation of sulfide phases. A number of compositions have been experimentally examined for phase compositions along with assessments of hydrogen interactions with the alloys and impact of sulfur on isotope exchange and permeation. Techniques for more rapid screening of broad variations in alloy compositions are being developed. The researchers are currently trying to identify possible candidates with desirable properties. No outstanding composition appears to have been identified.
- After going through the slides in advance of the meeting and listening to the presentation carefully, it is unclear what this team's real accomplishments are. The progress related to sulfur poisoning was earlier work. The permeability of the palladium sulfide membrane layer is about an order of magnitude lower than palladium. This team also reported that hydrogen sulfide causes incremental flux decline, which is not new information. It is good to see that the team has started to look into a broader range of membrane composition (slides 22–24).
- After four years of effort from a very substantial team, there is no reason to believe that a sulfur-tolerant, high-flux membrane will result from this work. In addition to sulfur tolerance, the challenge of heavy-metal poisoning must still be addressed. This is concerning, as this work has not yet begun. The pace seems slow and, combined with an apparent shift in the technical approach, makes this reviewer question if the team is on track to solving these very challenging problems.

Question 4: Collaboration and coordination with other institutions

This project was rated **3.2** for its collaboration and coordination.

- This project boasts exceptional breadth and qualifications of collaborating team members. This is a model that should be the goal of all principal investigators seeking to develop strong collaborations.
- This project has an impressive list of researchers. At some point, the team needs to consider atomic resolution microscopy to add an understanding of alloy migration.
- Across-the-board collaboration for developing the membrane is represented by NETL, Carnegie Mellon University, the University of Pittsburgh, and Virginia Tech, and the incorporation of NCCC in Wilsonville, Alabama, provides the necessary capability of field test validation. However, there is no commercial membrane fabricator with a defined role in this project.
- There appears to be extensive collaboration between the lead institution (i.e., NETL) and its partner organizations, with good coordination of efforts. However, it was not very clear from the presentation which groups or individuals are performing specific tasks and how information is being exchanged.
- The list of collaborators is impressive on first look; however, most or all of the collaborators are related to NETL, and the role of each partner is not explained. It is good to see that, based on 2010 Annual Merit Review (AMR), this team added NCCC to test its membrane coupons in actual gasifier streams. Tests on coupons exposed to gas streams at NCCC showed that the surface morphologies of some samples were different from the tests that used gas mixtures prepared by using industrial gas cylinders. This is a very important observation.

Question 5: Proposed future work

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

- This project's future direction will clearly build on past work. A systematic fundamental study of ternary alloys with identification, synthesis, and testing of the performance of these materials is planned and should provide valuable knowledge to the field. The project plans to fabricate and test the membrane system under gasifier conditions at NCCC, but it is not clear who will apply the fabrication expertise to the engineering of the membrane or module.
- The future work plan is based on a computational evaluation of palladium-copper ternary-alloy surfaces followed by fabrication and testing. This appears to be a good approach.
- High-throughput and scale-up demonstrations seem to be a long way into the future. Making the full schedule available would establish confidence that throughput and durability really will be adequately researched.
- The tasks proposed for the remainder of this project are all valid and important to reaching researchers' stated objectives. The future work is a combination of theoretical and experimental efforts. However, accomplishing all these tasks within the less than six months remaining in this project's timeframe is highly unlikely. There does not seem to be enough time left to prepare and characterize the many alloys that may be predicted as especially favorable. One example is the necessary development of unspecified test methods for assessing the composition spread of alloy films (see slide 27), which can only be developed and verified before measuring samples.
- As presented, the plan relies heavily on rapid throughput screening to identify promising ternary alloys with respect to hydrogen permeability and sulfur poisoning. This is a brute force method (albeit highly effective in many examples), and there does not appear to be effective roles for all team members going forward. Alloying with reactive group III, IV, and V metals should be approached with caution, as these metals are very oxophilic and literature and data show that yttrium and cerium will oxidize and be removed from palladium alloys over time. Researchers need to pay attention to phase diagrams and remember that in operation, dissolved hydrogen atoms are yet another metallic alloying element.

Project strengths:

- The team has a good understanding of computational principles and membrane technology and a good facility to fabricate and test membranes. The inclusion of NCCC into the team is an excellent addition. This is a good project that combines computational and experimental work.
- Overall, the investigators seemed to be clearly focused on the pertinent issues to design and develop improved palladium-based membrane alloys for separating hydrogen from coal gas. There is a good balance of theoretical efforts for predicting promising alloys and various laboratory methods to test performance and assess

contamination issues from the sulfur species as impurities. A rather diverse group of conventional experimental systems are available at the various organizations to perform the necessary measurements.
- Over time, a strong theoretical understanding of the dynamic interaction of reactive sulfur compounds with palladium and palladium-copper membranes has been developed.
- This is a strong fundamental-based research project aimed at improving understanding of palladium alloy performance and the effect of sulfur. Coupon testing on real gasifier streams has provided succinct and important information that has been used by the research team to further understand the mechanism and improve the membrane. The initiation of a detailed fundamental study on ternary alloys using thermodynamic and phase-equilibria theory and the use of high-throughput screening will both facilitate and accelerate the identification and optimization of ternary compositions, which show considerable promise.
- This project is developing a thorough understanding of sulfur tolerance.

Project weaknesses:

- The progress reported is inadequate. No new flux data was presented and some mandatory presentation slides were missing. It seems this project is trying to do too many things.
- There are a potentially large number of systems and materials to evaluate in the remaining few months for this project, which will strain resources and affect the preparation and characterization of a sufficient number of samples or membrane configurations. Also, the detailed theoretical analyses of alloys without the presence of hydrogen gas may generate misleading results and conclusions. For example, the computation of yttrium migration to the alloy surface mentioned in slide 26 does not account for the probable formation of highly stable yttrium hydrides when heated in hydrogen gas, which could substantially alter the formation of other phases and hydrogen permeation behavior. There also did not appear to be any plans to temperature cycle the membranes, which could easily impact compositions in regions of the phase boundaries.
- The team has not shown that the fundamental understanding applied to computational methods can be extended to other alloy systems to solve the problem. Plans to use reactive metals as alloying elements may be seriously flawed. After years of effort, this project still does not have convincing data to prove that long-membrane lifetime and high flux can be achieved using a multilayered membrane (slide 7).
- Though the focus of the program is to understand the performance mechanism, there was not information in the slides or presented orally suggesting that any attention is being directed to membrane cost or membrane fabrication.
- Based on the materials presented, throughput does not seem to be adequately addressed.

Recommendations for additions/deletions to project scope:

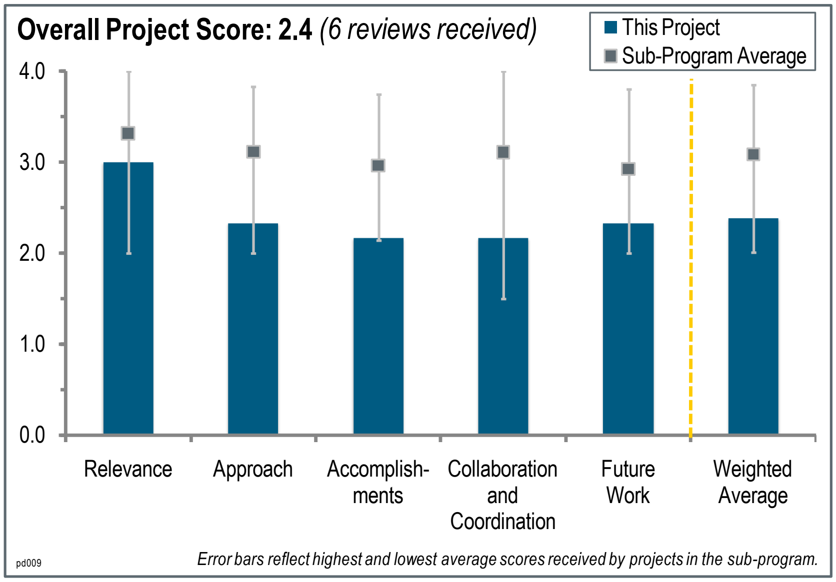
- DOE should continue funding this project, but direct the effort to become more efficient in its use of money and time. Specific suggestions include conducting a thorough review of literature on the lifetime of palladium-yttrium and palladium-cerium membranes in the presence of impurities, challenging assumptions of preferred phases for alloys by experimentally determining the phase of palladium-copper alloys in the presence of hydrogen, and seeking experimental validation that multi-layer coated membranes will yield long operational lifetimes. This reviewer wants to know if there is a role for computational modeling in the 2011 work plan.
- Process cost analysis and membrane manufacturing needs should be integrated into the project. Similar fundamental studies of arsenic poisoning and mercury or other syngas contaminants in coal gases needs to be studied at the same level of detail as was done for sulfur. If the project's goal is to proceed to phase two, additional participants need to be added to the development team to address the process analysis, design, fabrication, and manufacture of a membrane module suitable for testing in a later phase.
- This project should make throughput and scaling a higher priority.
- Researchers should continue the computational study and design of new membrane compositions and test the membranes under NETL test protocol conditions, and report flux data during the 2012 AMR. This team should also review the body of prior work, especially the palladium-ternary alloy work. This project should also include all mandatory slides.
- Computations of alloy thermodynamics and other properties should include the role of hydrogen interactions and concentration as soon as possible. The investigators should down-select only a limited number of the more promising alloys for detailed experimental characterizations during the remainder of this project, which may need to be extended to allow more time for further assessments.

Project # PD-009: Scale-Up of Hydrogen Transport Membranes for IGCC and FutureGen Plants

Carl Evenson; Eltron Research and Development Inc.

Brief Summary of Project:

The overall objective of this project is to create hydrogen transport membranes for integrated gasification combined cycle and FutureGen plants that: (1) achieve a cost effective hydrogen/carbon dioxide (CO_2) separation system; (2) retain CO_2 at gasifier pressures; (3) operate near water-gas-shift (WGS) conditions; and (4) tolerate reasonably achievable levels of coal impurities. Objectives for June 2010 to May 2011 include: (1) scale-up of membrane manufacturing; (2) construction, installation, and operation of a membrane reactor that produces 12 pounds (lb) of hydrogen per day; and (3) continued bench-scale testing.



Question 1: Relevance to overall U.S. Department of Energy objectives

This project was rated **3.0** for its relevance to U.S. Department of Energy (DOE) objectives.

- Metallic membranes are relevant to hydrogen purification. The objective of this project is to develop a hydrogen separation system that retains CO2 at high pressures, operates near WGS conditions, and tolerates reasonably achievable levels of contaminants. These objectives are very relevant to the DOE Hydrogen and Fuel Cells Program.
- This project supports the hydrogen production facet of DOE as well as attempts at CO2 sequestration programs within DOE.
- The project is critical to the Hydrogen from Coal research program's objective to find a cost-effective, high-performance membrane process integrated within a coal gasification cycle to produce hydrogen for energy and CO2 for capture and sequestration. This project clearly meets the objective and has progressed to the stage where actual field testing at a partner's gasifier facility will prove the concept as well as prepare for early scale-up and demonstration.
- The project supports the goals of the Hydrogen from Coal research program with the development of new membranes for hydrogen production.
- The barriers this project claims to address are reducing hydrogen cost, improving membrane durability, and conducting membrane testing and analysis.
- This project has been funded since October 2005 and there is still no convincing evidence that lifetime targets can be met under appropriate operating conditions. The principal investigator (PI) does not communicate an understanding of the need to meet this performance target.

Question 2: Approach to performing the work

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

- The approach for the 2010–2011 timeframe was to scale-up the Eltron alloy tubular membrane (no compositional data was publicly provided) developed in the previous work, test the membrane at Eastman Chemical Company

in a modular test rig designed to produce hydrogen at 12 lb/day using a slipstream from the Eastman coal gasifier, and use the test data to provide engineering data to refine the process' economic analysis and scale-up to the next phase of 250 lb/day.
- The membranes retain CO2 at high pressure, which is a plus for sequestration. Concerning the barriers claimed to be addressed, there is a lack of specific data on how exactly the project is addressing membrane durability and membrane testing. The membrane testing to date is lacking in test length and rigor. The characterization of decay and the mechanisms causing decay need to be addressed in much more detail.
- The technical results presented are primarily a scale-up of the membrane fabrication, module fabrication, limited durability data, and some mixed gas (simulated WGS gas stream) data. Without knowing the composition of the membrane and more information about the seals, it is difficult to assess this project's approaches. Knowing the composition of the membrane will help the reviewers judge if the approach taken is correct or needs changes.
- Eltron's approach to the project is well thought out; however, it is obvious that it is much larger than the development of a membrane technology. This appears to be a larger project focused on working up to a significant scale that would require significant funding from other sources.
- Membrane stability as well as adequate flux and testing versus contaminants have not been demonstrated before scale-up. This should have been done before moving to a full-scale reactor.
- The technical approach must be considered flawed unless the PI will supply clarifying information concerning the membrane composition and coatings. Lacking this information, but being told that a dense metal membrane is used that does not contain palladium, reviewers can only conclude that the membrane is based on a pure metal or alloy selected from the group III, IV, and V metals. These are poor choices for commercial applications, such as coal gasification. DOE and the National Science Foundation (NSF) have funded programs over the last 20 years that have extensively examined these metals as hydrogen permeation membranes. Furthermore, the application of coatings to group III, IV, and V metal membranes to impart the necessary chemical resistance to feed stream contaminants has also been proven to be a faulty approach (again, through the funding of numerous programs by DOE and NSF).

Question 3: Accomplishments and progress towards overall project and DOE goals

This project was rated **2.2** for its accomplishments and progress.

- Eltron should be complimented for building the entire system. Scale-up to any relatively sized piece of hardware is a big effort and big achievement. With that said, DOE should not have allowed this before stability and flux could be demonstrated.
- Eltron has made fair progress, but it was unable to share adequate information and was reluctant to answer simple questions about its system and the company that it is working with on the membrane construction.
- Five-foot (ft) long, half-inch membrane tubes were successfully scaled by two different substrate manufacturers, and a uniform alloy catalyst coating was successfully deposited on the inner and outer wall of the tubes. A hydrogen flux achieving the DOE target was demonstrated in the laboratory using a simulated WGS gas stream under a nitrogen sweep. A 12 lb/day hydrogen membrane reactor was completed and equipped with two 5 ft membranes mounted in a series with the modular rig installed at Eastman. Operation of the unit using a slipstream from the Eastman coal gasifier was successfully started up and is currently underway and scheduled for a minimum of 30 days of continuous operation.
- It would be helpful to see the status of the membrane flux relative to DOE targets, as well as some indication of how that flux will decay over time, as it is unclear in the techno-economic analysis whether flux decay was considered. Having the reactor run on actual coal syngas is a good test. In the techno-economic analysis it is unclear whether a carbon tax was assumed or not. The reviewer wants to know how the financials change in the presence or absence of a carbon tax.
- The flux degraded in 16-hour test. A flux of 28 standard cubic feet per hour (SCFH)/square foot (ft2) (slide 8) is much lower than the DOE target. Tubular membrane manufacturing was scaled-up to produce 5 ft and 10 ft sections. It is a little disappointing to see that the membrane module (total membrane tube length of 10 ft) designed to produce 12 lb of hydrogen/day produced only 2–5 lb/day. The reviewer asks whether this means if this membrane cannot be scaled-up. Without knowing the composition of the membrane, it is impossible to offer suggestions or recommendations. No hydrogen purity level was reported.
- Since October 2005, the project has not demonstrated anything close to an adequate operational lifetime under relevant operating conditions. Slide 8 is the only data presented to justify the adequate lifetime of the membrane

(which is planned to begin testing on 12 lb/day gasifier), and this data spans only 16 hours and shows conclusively a decline in flux from 27.5 to 26.2 SCFH/ft2. This is a 4% decline in performance over 16 hours. The initial flux was also much too low, which is not surprising for a dense metal membrane that is 500 microns thick. It should also be noted that this lifetime data was collected at an operating temperature of 340°C (too low for coal gasification applications) because, according to the PI, operation at higher temperatures leads to a more rapid decline in performance. These results are unacceptable.

Question 4: Collaboration and coordination with other institutions

This project was rated **2.2** for its collaboration and coordination.

- Eastman is a great collaborator. This team needs a collaborator in the area of membrane characterization to understand the decay mechanism.
- There is clear collaboration with Eastman; however, all of the other partners in the project are not clear. In fact, the speaker refused to name two of his key suppliers, which is inconsistent with the goals of collaboration. Awards of the size received by Eltron demand more transparency.
- Eastman is a key collaborator and is the critical partner to the success of the project. There are also important collaborations with membrane fabricators, which is a critical part of accomplishing scale-up and producing membranes. However, it is difficult to assess the quality or appropriateness of these fabricators because Eltron elected to not disclose their names publicly.
- Limited information was provided in the presentation about the project's collaborators other than Eastman. The researchers have collaborators that they would not identify.
- Collaboration is unclear because the efforts of Eastman seem to be limited to site supply, and the membrane manufacturers are not mentioned. Based upon membrane performance, this should have been a bigger effort.
- Eastman is the only named collaborator and it is not clear whether Eastman has contributed anything substantial to the project beyond its name. The slipstream testing is planned to take place at an Eastman facility, but, given the extremely poor performance of the membrane, these experiments are not expected to yield promising results. The PI mentioned that two membrane fabricators are now part of the team, but repeatedly refused to name these collaborators. Therefore, there is no basis to review their potential contribution to the team. DOE should not allow this degree of secrecy to pervade a merit review of projects largely funded with taxes. This project has received more than $7 million in funding from DOE and the PI has only contributed a little more than $1.7 million, meaning the contractor cost-share is only 20%.

Question 5: Proposed future work

This project was rated **2.3** for its proposed future work.

- Completion of the field tests with the 12 lb/day unit and analysis of the data is the most important next step to verify performance and prove that the membrane will remain stable in the presence of syngas contaminants under real gasifier operating conditions. The PI plans to continue with the 12 lb/day test run to evaluate the effects of real gasifier operating conditions on the performance of the membranes, including cycling and lifetime testing. If this all goes well, the PI has laid out a logical next-phase scale-up plan. One technical comment is the need to get the full-size commercial tubes (10 ft) into testing as soon as possible to avoid any late surprises. Evaluation of the data from the Eastman tests is important to update the techno-economics of the process and to initiate a preliminary design of the next scale. A go/no-go decision to proceed with the 250 lb/day unit has been strategically placed in the program after the 12 lb/day testing has been completed. Presuming the decision is to move forward, Eltron has received significant American Recovery and Reinvestment Act (ARRA) funds from DOE that will be used to accelerate the 250 lb/day unit and testing and to scale-up the technology further to achieve a 4–10 tons/day demonstration at a commercial gasifier facility.
- This reviewer wants to know what the go/no-go criteria are for future work.
- The aggressive future plan assumes success. The problem of gradual flux decline is not understood. The lack of an alternative research and development plan is a concern, should the performance of this project's current membrane not meet DOE targets. A flux of 28 SCFH/ft2 is well below the DOE target and the 70% recovery is not acceptable (slide 8). The project has no plans to study the mechanical properties of the membrane. This reviewer wants to know more about the creep rate. Without knowing the composition of the membrane, it is

impossible to judge if this membrane will survive in real-world applications. Plans for future work are all focused on the ARRA project. The current DOE project that the reviewers were asked to evaluate is scheduled to end in June 2012; however, no plans for work specifically for this project were reported.
- The test unit is only achieving one-sixth to one-half of the desired output, which is clearly due to not addressing flux issues earlier in the program. Researchers should try to rectify this.
- The proposed plan is to proceed with pilot-scale testing (12 lb/day of hydrogen) and then move into scale-up. This is fundamentally flawed because the PI has not presented a convincing case that membrane durability and hydrogen flux through the membrane are adequate in light of DOE targets. The only sensible part of the presented plan for fiscal year 2011 is the go/no-go decision in the fourth quarter. This project should not have proceeded to this stage without having a well tested membrane module that meets DOE performance targets. In this reviewer's opinion, the planned slipstream tests are unnecessary.
- This is difficult to judge, as the presenters announced that they are receiving a significant amount of funding from ARRA funds for future work. With the amount of funding this project has already received or will receive, it should not receive any additional baseline funding in the future.

Project strengths:

- Having an end user (Eastman) of the technology onboard is good. Eltron has good research staff and a well-equipped development facility.
- The project's true scale unit operating at a demonstration site is a major accomplishment.
- Eltron has successfully focused on scaling up its membrane processes and has achieved expected flux performance in the preliminary laboratory tests. Testing of the 12 lb/day of hydrogen production unit at Eastman will provide definitive tests that will prove the membrane and determine whether it is ready for scale-up to the next stage. The collaboration with Eastman is key to the success of this membrane project, as the integration with the Eastman commercial gasifier facility will provide unequivocal validation of the concept under real operating conditions.
- The project has a good connection with Eastman and its demonstration site. The researchers have a good approach for the overall system engineering, design, and integration for the demonstration.
- This project has no strengths. The PI has simply confirmed the results of several previous investigators, including a group with Oak Ridge National Laboratory that coated dense metal membranes (group III, IV, and V metals), which do not meet the target performance requirements published by DOE. These requirements serve as the overall guide for these membrane programs.

Project weaknesses:

- There is no data on mechanical property of the membranes. This reviewer wants to know if a 0.5 millimeter thick free-standing membrane tube can survive the real-world pressure and temperature conditions and achieve DOE's target lifetime. The decay of flux with time is of great concern, as is the unknown membrane composition. Flux decay suggests there is something going on either in the membrane itself or in the catalyst layers. This project is very secretive and the reviewer has to assume that the researchers are using palladium as the catalyst. Palladium is poisoned by sulfur and carbon monoxide, which could be the reason why the flux is decaying with time. The lack of relevant information regarding composition of the membrane makes it difficult to evaluate this project.
- Stability and flux are the "Achilles heels" of this project and need to be rectified before moving forward.
- There are many weakness in this project:
    - The dense metal membrane is too thick to meet flux targets (and cost targets).
    - The coating on the dense metal membrane is not stable under appropriate operating conditions, leading to a rapid decline (as in 4% over 16 hours) in flux.
    - The membrane tubes will be expensive to manufacture with a 500-micron wall thickness (half-inch diameter). The metal is most likely also expensive because it must be very pure and the native oxide coating needs to be removed to achieve optimal hydrogen permeability. It is very likely that the dense metal membrane is a group III, IV, or V metal, which are all extremely reactive.
    - Hydrogen embrittlement is also a major concern during process upsets.
    - The PI has not referenced prior work done with coated metal membranes based on group III, IV, and V metals, and has failed to recognize known drawbacks and deficiencies of this approach.

- Eltron's laboratory test unit used to test the performance of the 5-ft tube membrane was physically limited so that the lifetime data was only obtained for 16 hours. This was the sole evidence presented to validate that the scaled-up, 5 ft membrane met the performance target prior to building the 12 lb/day unit. Unfortunately, there was a slow but steady flux decline of approximately 8%, which, if extrapolated to 1,000 hours of testing, results in an unacceptable deterioration in performance. Eltron was questioned about this during the review and explained the limits of the laboratory unit, but said that it was currently studying the possible reasons why this decline occurred and that more extension lifetime testing will be done at Eastman. Not revealing the membrane manufacturers or the comparative processes used to scale the substrate and manufacture the tubes was a weakness in the presentation of the collaborators. Reviewers were unable to assess the quality of the collaborators despite the fact that Eltron identified that they were collaborating with membrane manufacturers as part of the project.
- This project is funded primarily by government funds; however, the presenter refused to answer a question regarding who the membrane manufacturer is. While there is no doubt that intellectual property issues may prevent the presenter from discussing the details of the membrane itself, the names of the manufacturers should not be held back. There was no way to address the overall collaboration beyond with Eastman and other partners. Also, the title of this presentation is all about membranes. To date, all the techno-economic analysis performed is based on models only. After six years of funding, that analysis should be based on real test data.

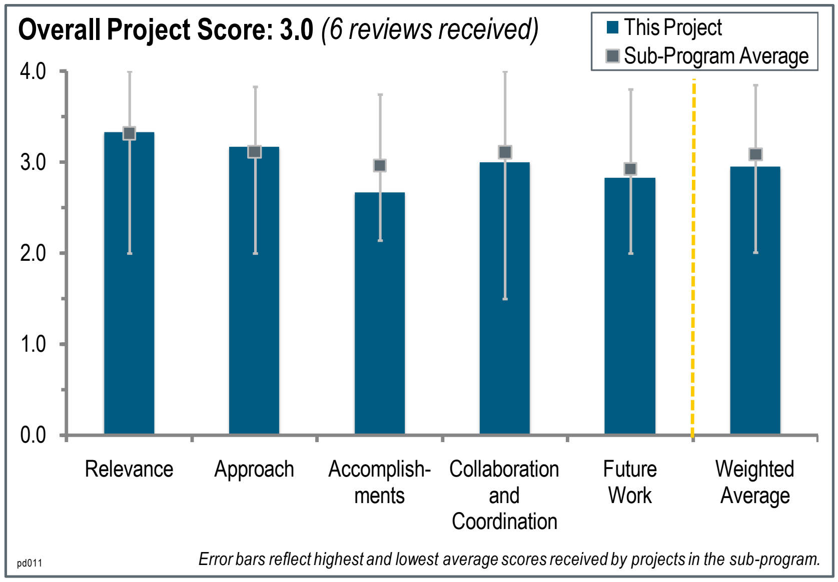
Recommendations for additions/deletions to project scope:

- This project should work to better understand the degradation in flux in laboratory studies and seek a material solution before going forward. Adding a collaborator to work in the area of membrane materials development is also recommended. It is impossible to evaluate this project's performance without knowing the composition of the membrane. If its composition cannot be disclosed, please do not schedule this project for review in 2012.
- Flux and stability should be proven at extended times before DOE allows any funds to be spent on a scale-up. With the present performance, no economic systems can be built.
- Based on previously reported results, Eltron has studied membrane tolerance toward sulfur and the results of the Eastman testing will, presumably, verify the sulfur tolerance. Future studies should also address other contaminants, such as arsenic, which others have shown could be of issue with the alloy membranes. It is recommended that this aspect of contamination studies be considered in the post-evaluation of the membranes used in the Eastman tests. Assuming the 250 lb/day unit goes forward, it is recommended that the actual commercial-scale membrane tubes (of about10 ft length) be utilized in the testing during that phase so that there are no surprises when and if the technology proceeds to the 4–10 tons/day scale. It is recommended that Eltron incorporate a project partner or the DOE analysis group at the National Energy Technology Laboratory for independent verification of the techno-economics of the process before proceeding to the larger-scale expenditures.
- The presenter indicated that the researchers recently received significant ARRA funding to scale-up this project for a demonstration. The reviewers appreciate the information, and it is important to disclose that. Based on the focus of the ARRA funding, this reviewer recommends that the fiscal year 2012 funding be re-directed, as the real focus of this work is going to be on the full-scale system.
- This project should be stopped; if not immediately then certainly at the go/no-go decision point in the fourth quarter of 2011. It is unclear why DOE would choose to award an additional $73.7 million in funding to scale up this membrane for a 250 lb/day pilot test (slide 16), given the lack of durability data, performance data limited to unacceptably low operating temperatures, unacceptably low flux, lack of transparency on key partners, and lack of any previous slipstream test data.

Project # PD-011: Advanced Palladium Membrane Scale-Up for Hydrogen Separation

Sean Emerson; United Technologies Research Center

Brief Summary of Project:



The objectives of this project are to: (1) construct, test, and demonstrate a palladium-copper metallic tubular membrane micro-channel separator capable of producing 2 pounds (lb) per day of hydrogen at greater than 95% recovery when operating downstream of an actual coal gasifier; (2) quantify the impact of simulated gas composition and temperature on separator performance; (3) compare the performance and durability of a surface modified, higher-hydrogen flux palladium-copper membrane with the baseline palladium-copper tubular membrane; (4) evaluate various materials of construction for the separator structural parts to ensure durability under harsh gasifier conditions; (5) perform an engineering analysis using the National Energy Technology Laboratory (NETL) guidelines for the separator design, based on gasifier test performance, for the co-production of electric power and clean fuels; and (6) select a gasification facility partner for phase three.

Question 1: Relevance to overall U.S. Department of Energy objectives

This project was rated **3.3** for its relevance to U.S. Department of Energy (DOE) objectives.

- The primary objective of this project is to construct, test, and demonstrate a palladium-copper separator capable of producing 2 lb/day of hydrogen operating downstream of a coal gasifier. The membrane will be tested at the Energy and Environmental Research Center (EERC) at the University of North Dakota in a coal gasifier slipstream. Development of hydrogen separation membranes for the central production of hydrogen is critical to the DOE Hydrogen and Fuel Cells Program; therefore, this project fully supports DOE research and development objectives.
- This project is examining the performance of prototype palladium-copper membranes to separate hydrogen from coal gas on a moderate scale (i.e., nominal 2 lb/day level). The objectives are to determine whether several key DOE targets for hydrogen production can be met and to look at the impact of sulfur impurities. This information will be useful when assessing whether coal gas can be a viable and cost-effective source of hydrogen to support fuel cell technology in various applications.
- The project supports the goals of the Hydrogen from Coal research program and is clearly focused on the DOE technical objective of developing a cost-effective, high-performance membrane process integrated within a coal gasification cycle to produce hydrogen for energy and carbon dioxide for capture and sequestration.
- Extracting hydrogen from syngas will be critical to clean coal when carbon taxes are implemented.
- The focus of the presented work was on identifying suitable steel alloys for constructing the membrane module and deliver acceptable resistance to sulfur corrosion under operating conditions. Although this is important, a more important question is identifying a suitable membrane composition with adequate flux and chemical resistance to sulfur and heavy metals. This project is scheduled for completion on December 31, 2011, yet the work addressing the membrane composition is not given sufficient priority.

Question 2: Approach to performing the work

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

- The approach seems to be good. Based on coupon testing under DOE and NETL test protocol, this team plans to down-select the best material for separator construction. Down-selected composition will be used to construct a laboratory-scale (less than 2 lb/day of hydrogen) separator. The impact of gas species on performance will be evaluated before proceeding to the construction of the 2 lb/day of hydrogen module for further testing at EERC.
- The project is leveraging Power+Energy, Inc's (P+E) commercially established process, module fabrication, and assembly experience in hydrogen purifiers. The scaled modular concept illustrated in the presentation is a unique approach to demonstration testing of up to 100 lb/day of hydrogen production; however, costs could be an issue. The main approach is to quantify gas composition impact on the durability and performance of 2 lb/day of dense metallic palladium-copper hydrogen separators operating downstream of a coal gasifier. The project is focusing on contaminants with an emphasis on the corrosion resistance of materials of construction. Hydrogen flux and permeability improvements are being approached by using a proprietary membrane surface modification process.
- The sequencing of separator test size occurs in three steps to have the best shot at success in this phase of the project. They include: (1) laboratory-scale simulated gas, (2) 2 lb/day of simulated gas, and (3) 2 lb/day of gasifier off-gas test. The methods of risk mitigation, including the earned value management system, are well addressed.
- Sulfur and corrosion testing are being performed in parallel with scaling research. The approach to durability testing, which will enable the team to understand individual component impacts, seem especially promising.
- This is phase one of a demonstration effort of hydrogen production and separation from coal gas. It involves construction, laboratory testing, and initial operation with data analyses of palladium-copper membranes prior to designing larger-scale demonstration facilities. Emphasis will be on evaluating the performance of modified commercial hydrogen purifiers while using gas compositions to simulate species produced during coal gasification. The durability of membranes with operating conditions and impurities will be determined for comparison with modeling predictions and current approaches. These results will be used to design and fabricate larger-scale units for field tests during phases two and three, if funded.
- The technical approach seems sound, but there is little data to support it. To increase flux to an acceptable value and achieve tolerance to sulfur by an appropriate choice of palladium-copper alloy, modification of palladium-copper tubular (i.e., thick walled) membranes is needed. In the presence of sulfur, palladium-copper alloys are not known to have a high permeability to hydrogen, so this approach is not likely to show high flux in the presence of sulfur. Even if some form of surface modification does increase the flux in the presence of sulfur, the reviewer wonders what will happen when heavy metals are present (as will be the case with coal gas).

Question 3: Accomplishments and progress towards overall project and DOE goals

This project was rated **2.7** for its accomplishments and progress.

- The laboratory-scale results of hydrogen sulfide (H2S) and carbon monoxide (CO) effects at 400°C, 450°C, and 500°C are promising with respect to this project's objectives. It was unclear whether the description of hydrogen flux with and without surface modification was a single measurement, or if all the subsequent data in the presentation were with the surface modified membranes.
- This project has established a good understanding of impurity impacts. Researchers are slightly behind schedule on the separator, but the revisions required to compensate for materials issues are justified.
- This project was able to demonstrate in the laboratory hydrogen flux and permeability improvement using the proprietary membrane surface modification. This project also demonstrated the negligible impact of H2S on hydrogen flux performance at temperatures greater than 400°C over a range of pressures and in long-term testing. Researchers conducted coupon testing for a section of corrosion resistant materials constructed for use in membrane assembly devices.
- As this project is scheduled for a little over 1 year, the research team needs to move fast. Actual achievements to date are limited and little basis was presented to evaluate progress with the membrane development.
- The maximum flux (40 standard cubic feet per hour [SCFH]/square foot [ft2]) is low (slide 14). The surface modification (by P+E) is not clear. Some plots show the hydrogen flux in a DOE unit (i.e., a SCFH/ft2 system), and others show permeability. It will be helpful for comparison if the SCFH/ft2 system is used throughout the

presentation. The modularization effort (by P+E) is not new. The permeability of new separators (slide 13) is less than the original one tested in 2010. There is discrepancy in the data presented on slides 14–16, which show a flux around 40 SCFH/ft2, whereas slide 20 lists the current status as 125 SCFH/ft2.
- During the first half of this 15-month project, the two main activities appear to have been (1) defining and organizing the initial laboratory and prototype separation and analysis testing facilities, and (2) conducting screening experiments in the laboratory on permeation parameters of palladium-copper membranes, including assessing the impact of sulfur and CO impurities on performance. However, there do not seem to be any strong candidates that can meet the DOE flux rate and durability targets. It appears that the cost projections have yet to be done.

Question 4: Collaboration and coordination with other institutions

This project was rated **3.0** for its collaboration and coordination.

- P+E is a qualified supplier of membranes and EERC is a capable partner for slipstream tests.
- This project has a good, well-rounded team with the complete technical package—P+E for membrane fabrication and EERC for membrane testing on actual coal gasifier streams.
- The project partner has experience with moderate sized separators. The researchers also mentioned working with Oak Ridge National Laboratory, but it is not on the list of collaborators.
- The team is collaborating with P+E to fabricate a membrane module. EERC is the partner to test the separator module in a coal gasifier stream.
- There appear to be very good interactions within the various United Technologies Research Center (UTRC) groups as well as the EERC and P+E organizations on initial testing and preparing for future work with the coal gasifier. However, the involvement of any other organizations regarding palladium-copper membrane development or formulating for the larger-scale demonstrations was not really evident.

Question 5: Proposed future work

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

- Plans for immediate phase one tasks seem completely adequate; however, the scope of the effort needed for phases two and three are vague. This looks like a quick resolution on which membrane configuration and palladium-copper alloys are necessary to allow testing prior to selecting one for prototype and demonstration.
- The work plan makes sense (with the exception that the alloy chosen to make the membrane is not likely to yield success), but the team must move quickly without any wasted time or effort. There is no room in the timeline to accommodate technical setbacks, so the plan must be based on first-time success, which is risky.
- UTRC will use current laboratory test results to modify commercial membrane and assembly designs to build a 2 lb/day unit that will be tested using slipstreams from the EERC coal gasifier. To validate performance, testing is planned using the coal gasifier slipstream at one of EERC's gasifiers. Testing will include a variation in temperature, thermal cycling, and post-run separator characterization. Coating applications will be improved for next-generation separators.
- Phases II and III have scale-up elements and will most likely have a good mix of general performance results with gasifier gas and specific material choice and contaminant studies. It is not clear how the team will address the gaps, particularly in hydrogen flux and pressure difference capability compared to the DOE 2015 targets. The reviewer asks whether there is a plan to show analytically or empirically how these targets can be achieved.
- The schedule will likely be tight, but the researchers have a reasonably good probability of completing the project by December 11, 2011.
- There are no plans to improve the flux of the membrane. There are plans to test the pilot-scale separator unit in a gasifier stream at EERC by September 2011. With the reported flux value, the DOE target will not be reached in phase one. There was also no explanation for the reduced flux value.

Project strengths:

- The team has demonstrated the ability to test membranes and has good team members, as well as a facility to test the membrane module in a real gasifier stream. Identifying all performance targets (although it is questionable if all targets are attainable) is also a strength.
- This project has a diverse and experienced research team on hydrogen purification and membrane development. The approach of adapting existing commercial systems for this effort will greatly expedite the process of getting a prototype and field-test units operational.
- The collaboration partners are the primary strength in this project.
- UTRC is collaborating with EERC to conduct gasifier testing and is leveraging the commercial fabrication and module assembly experience of a commercial vendor.
- The modular concept is highly scalable and will facilitate large-scale testing if and when the project moves forward into phases two and three.
- This project has an emphasis on the materials of construction and corrosion issues, which is a unique approach not addressed in other studies.
- The research team is carefully isolating impurity impacts.

Project weaknesses:

- The backgrounds of UTRC and other team members seem appropriate; however, it is unclear whether sufficient laboratory tests can be done to choose and verify the best membrane materials for the prototype designs. Even if the test facilities and components are available, the observed performance may be inadequate, especially regarding robustness and durability in syngas.
- The flux level is not high enough in this project and there is a need for sweep gas to obtain 95% hydrogen recovery. There is also an increased footprint area for the membrane in order to obtain pure hydrogen.
- The technical approach of this project is risky. Palladium-copper alloys are not known for high permeability in the presence of sulfur, and the surface modification that is proposed to solve this drawback was not presented with sufficient detail to evaluate its potential for success. If one assumes success, what good is a sulfur-tolerant hydrogen separation membrane to coal gasification if it also is not tolerant to other real-world contaminants, the reviewer asks. The PI did not present a plan to deal with this issue.
- No attention has been paid to other coal syngas contaminants, such as arsenic and mercury, which could deteriorate membrane performance in long-term operation. No cost analysis plan was presented to verify economic feasibility of modular assembly approach.
- Simply adding separator modules to achieve scale-up may not be the most economical approach.

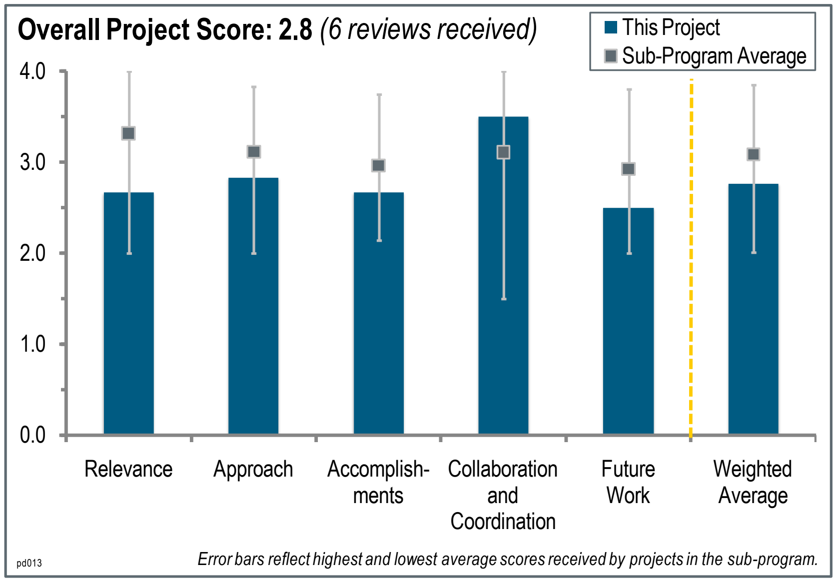
Recommendations for additions/deletions to project scope:

- It is recommended that the project focus on improving the flux and manufacturability of membranes that will achieve DOE targets.
- Researchers should determine how the project will address gaps in performance with respect to DOE 2015 targets.
- The researchers should look at the cost trade-offs of adding modules versus scaling-up modules to get to 4 tons/day throughput.
- The team should settle on only a few membrane and alloy configurations as quickly as possible in order to allow more in-depth characterizations prior to developing the larger-scale systems.
- If the team can remain on schedule, DOE should continue to fund through the slipstream test at EERC. If the tests on coal gasifier slipstream do not provide convincing data for tolerance to impurities (i.e., high flux is retained) then the project should be terminated.
- This project should include systematic studies of other syngas contaminants, such as techno-economic analysis, to verify the cost potential of proposed concepts.

Project # PD-013: Membrane/Electrolyzer Development in the Cu-Cl Thermochemical Cycle

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 U.S. Department of Energy (DOE) cost and efficiency targets using the copper-chlorine thermochemical cycle. The features of the copper-chlorine (Cu-Cl) thermochemical cycle that promote meeting targets and overcoming barriers are: (1) the 550º C maximum temperature, which allows coupling with the solar power tower and is near commercialization; (2) the conceptual design, which uses commercially practiced processes; (3) the high yields in thermal reactions, which require no catalysts; and (4) the preliminary ASPEN (modeling software, computer code for process analysis) flowsheet, which indicates it is possible to meet the efficiency and cost targets. Key challenges are to: (1) inhibit copper crossover and achievement of stable cell performance in the electrolyzer, (2) identify and cost-out materials of construction, and (3) reduce steam demand for the hydrolyser.

Question 1: Relevance to overall U.S. Department of Energy objectives

This project was rated **2.7** for its relevance to DOE objectives.

- Thermochemical cycles such as this represent the best mid-term technology for the production of hydrogen from water splitting. This project is aligned well with the needs of the DOE Hydrogen and Fuel Cells Program.
- As a process for the generation of hydrogen potentially from a solar-thermal and (solar-derived) electricity source, it fits well with the Hydrogen Production and Delivery sub-program. The major advantage of the process is the exceptionally low maximum temperature (550°C).
- DOE remains committed to solar hydrogen (high-temperature heat), which is clearly an advanced topic. During the last decade, technical work repeatedly demonstrated the challenges with this energy approach. Argonne National Laboratory's (ANL's) work continues on that track—fairly simple concepts that develop into difficult and technically challenging engineering.
- The cost targets do not seem to be at the right level yet. The point of going with the more complex, high-temperature redox cycles was to take advantage of the lower potentials needed, which would reduce the overall cost of hydrogen through the lower electricity costs. If there is not a pathway to do that, there should be more rationale given for why this technology is more attractive than low-temperature water electrolysis.
- With what is currently known about economics, this technology will be hard pressed to support the Program objectives. The technology faces daunting technical obstacles, the resolution of which will undoubtedly increase costs. The economics of this project are much further from target than the principal investigator indicates, as the target includes compression storage delivery. Also, the Hydrogen Analysis (H2A) modeling results, while good for comparisons, ignore the total erected cost multiplier on capital, which will potentially multiply cost three times and may dramatically increase the cost of implementing these processes, which are essentially all capital.

Question 2: Approach to performing the work

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

- From a science perspective, this approach had a key focus on well defined critical issues, a good discussion of fundamental needs, an understanding of membrane requirements and copper species, and screening protocols for membranes. This project's experiments are providing good information and advancements were made based on the knowledge gained. The technical approach was described very well.
- The project's approach is well designed to focus resources on the technical hurdles, such as copper crossover. The subcontractors are well aligned with the goals of the project.
- The team's approach this year—addressing the membrane showstopper—was described as being recommended by last year's reviewers. While perhaps necessary, that approach did not substantially address the barriers of cost and efficiency. The question, as posed, does not give researchers credit for the work that was done.
- The project is operating at a relatively low temperature for thermochemical cycles. The electrolyzer step is a critical part and the researchers are focusing on the key problems of inhibiting copper crossover. However, even though the electrolyzer is a critical path, researchers should not completely neglect the other parts of the system.
- The process comprises two chemical steps and one electrolysis step. The chemical conversion steps seem to have been fairly well established (though by no means optimized), and the effort over the past year has been reasonably focused on improving the hydrogen generating electrolysis for which a crossover of copper ions has been a major concern.
- The fact that copper-chlorine thermochemical cycles could be useful is a given for this project. However, the program was redirected to focus on just one technical concern: the electrolysis step during which the cathodic reduction of protons is prompted by a chemically promoted electrolysis reaction (technically anode depolarization). This process is conducted by ANL using a planar electrolysis reactor of rather standard design (commercial). This design is a polymer electrolyte membrane (PEM) electrolysis unit with a zero-gap electrode design. This project has been complicated because copper metal is being reduced within the membrane, fouling that component. Consequently, the program effort focused on developing an alternative membrane that can operate without the copper depositing concerns. In that way, this activity mirrors membrane development in other parts of the Program portfolio in which considerable effort has been spent on "alternative membranes."

Question 3: Accomplishments and progress towards overall project and DOE goals

This project was rated **2.7** for its accomplishments and progress.

- The team is very focused on critical barriers and has made many advancements in the membrane area for the electrolysis cycle. These advancements help to demonstrate the overall feasibility of this approach, which was in serious question without a membrane that could prevent copper crossover while maintaining acceptable proton conductivity.
- Progress has been good, but there is still no answer to the issue of copper crossover. Even the best membranes showed unacceptable levels of copper deposition for long-term operation, and conductivity is an issue with the membranes that show low crossover. However, the project seems to have good ideas for how to move forward.
- The team has made excellent progress at addressing the objective of the membrane showstopper. That progress notwithstanding, the side trip resulted in a year spent improving feasibility, but did not substantially address the barriers of cost and efficiency. If anything, switching from a well established Nafion 117 to an experimental membrane will raise costs in the short term.
- There has been good progress toward finding membranes that display a good combination of proton conductivity with high selectivity for protons over copper ions. The Pennsylvania State University's (PSU's) CM2 membrane system appears to have the best combination of properties; unfortunately, it appears that some of the experimental data was not reproducible.
    - Suggestion: Sometimes losses in selectivity may be due to pinhole defects in a membrane. This could be easily mitigated by layering two membranes or by putting a high-permeability, low-selectivity "cure" coating on the operative membrane (see M. Tripodi, Monsanto Gas Separation Patents, http://patent.ipexl.com/inventor/Tripodi_Mary_K_1.html).
- This project has made some progress on decreasing copper crossover, but the tests need to be run for longer periods of time. Fifty-hour tests are not sufficient for a system that is to run for 40,000 or more hours at a

minimum. Tests need to operate for a minimum of 1,000 hours to be meaningful. The theoretical power is 0.4 volts (V), so the efficiency is at 0.8 V and operation is at 50%. This is substantially lower than that of low-temperature (69%–74%) and high-temperature electrolysis. Now that the crossover issue seems to be mitigated, the project needs to lower the operating voltage in order to make the process viable. The potential to reduce the amount of excess steam is interesting. Should less steam be required, it would result in lower cost and higher efficiency.
- The project was first funded in October 2006 and still seems far from completion. There is certainly a focus on the single-current show stopper. Several alternative membranes were tested and did not prove satisfactory. Some rather preliminary results from one of the team partners show promise; however, none of the required performance and durability results have been achieved.

Question 4: Collaboration and coordination with other institutions

This project was rated **3.5** for its collaboration and coordination.

- This project has very good collaboration with project subcontractors and collaborators outside of the project.
- There are clear handoffs of samples between institutions for different measurements and plenty of collaboration between team members to provide input in various areas of expertise.
- There appears to be an outstanding level of cooperation with outside partners, particularly with PSU and Canadian investigators.
- The researchers have improved the collaboration with the Canadian group, and it seems to be working.
- The Canadian government has an interest in this program and has provided some valuable supporting technology, which appears useful. The ANL fuel cell team has considerable Nafion experience and is obviously a valuable contributor, although there was no specific mention of that.
- This project might have too much collaboration. It seems like everything that was done was done somewhere else. This is not necessarily bad, but research by committee does not always work best.

Question 5: Proposed future work

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

- This project is on the right path technically and should result in important information that will be valuable to this application and the membrane field in general. There is a need to understand what the key advantages of these high-temperature processes are in relation to other technologies, and which niche markets they may serve.
- The key to the future work seems to be finding an appropriate membrane and set of electrolysis conditions that minimize the copper crossover.
- This technology needs dramatic improvement if it is to reach the threshold value of $2–$4 per kilogram hydrogen, including the cost of compression, storage, and delivery. There is little in the future work that has the potential to create such a breakthrough.
- The future work is focused on the electrolyzer. Researchers need to do their H2A analysis to show that their process is economically viable. Although the electrolyzer development is critical to the success of the project, researchers should not forget the other areas of development that need to be done, including reactor development and system demonstration.
- While the electrolysis step remains the process of most concern, both of the chemical steps still require attention. The ability to generate oxygen at as low a temperature as 550°C is quite remarkable and has been confirmed by the Canadian partners. The purity of the generated oxygen needs to be established. Even low levels of potential hydrogen chloride or chlorine impurities, while readily scrubbable, could alter the stoichiometry of the process when conducted at a large scale.
- Membrane engineering is difficult and time consuming. Going from membrane organic synthesis to working that new chemical formulation into a stable and useful membrane is a large step. Totally "new" (university derived) membrane samples were entering the program for testing, which could have amazing potential. However, it is likely that these casual materials will not prove useful. It is not apparent whether the pathway forward is totally dependent upon demonstrating the useful proton transport materials.

Project strengths:

- This project has excellent team collaboration with partners who are experts in the key critical areas of focus.
- This project has good collaborations with strong institutions and good scientific understanding of the technical challenges. The very low temperature of this thermochemical cycle versus other competing cycles is a strength. This cycle is relatively uncomplicated compared to other cycles.
- There are a diverse team of contributors on this project.
- This is a strong team, especially with the additions of the Gas Technology Institute and PSU. The process operates at low enough temperatures to enable thermal storage for constant operation.
- The remarkably low temperature (550°C) for the most thermodynamically difficult step in water splitting, the generation of oxygen, is an amazing strength
- This project has a clear, well defined target and goal.

Project weaknesses:

- There are well established, excellent companies that supply electrosynthesis membranes, such as DuPont, which sell rugged, reliable membranes for the production of chlorine. Chlorine production membranes include a protective surface layer that has proven highly effective as a fence that keeps out unwanted anions ions. This commercial membrane could be useful for this project as well as partners who are well versed in this area. The chloralkali membranes are reinforced materials and have proven very durable, with a typically 10-year operation life. The membrane team for this project could use some additional expertise, as membrane engineering is complex.
- This group needs to better outline the relevance of this project.
- The thermochemical cycle under consideration requires an electrolysis step that may result in unfavorable economics versus all-thermal cycles. There may be a technical showstopper with the copper crossover in the electrolysis step.
- The economics of this project's concept is a weakness.
- The electrolyzer step efficiency needs to be considered, it seems to be around 50%. Low-temperature electrolysis is at 70%–74% efficiency lower heating value. Researchers need to achieve similar efficiencies, or demonstrate that their electrolytic process is less expensive than the low-temperature PEM processes.
- Imagining this project as a continuous process is difficult unless an off-sun storage of one of the more energetic materials of the cycle (e.g., copper oxychloride) is used. This would not be a problem if nuclear energy was the energy source. Cost penalties for the inherently non-continuous nature of this process need to be well addressed.

Recommendations for additions/deletions to project scope:

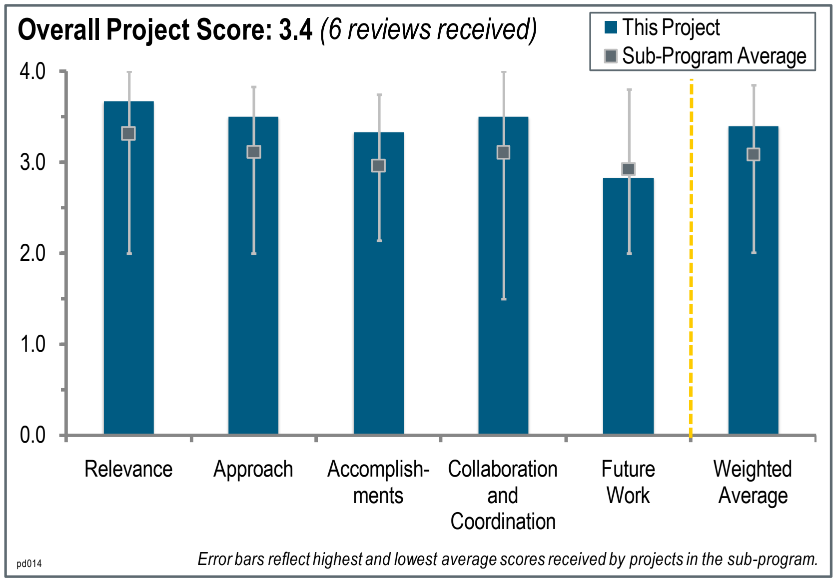
- The electrolyzer crossover challenges are very similar to what occurs with flow batteries. Researchers should look at the redox flow battery work to deal with the crossover problems. Researchers also need to do the H2A analysis, which should separate out the heliostat costs from the rest of the system so the impact of the research on the costs can be clearly seen.
- This project should consider extending the operation of the process beyond sunlight hours.
- The anode compartment needs to utilize the copper +1/copper +2 ion couple. However, the anode electrolyte (anolyte), using the existing electrolyzer design, is necessarily in direct contact with the membrane and experiences the change in potential through that membrane. Some of the copper solution invades the membrane, and hydrogen produced on the cathode membrane face reduces those ions to copper metal. (Hydrogen does transport through thin Nafion materials at appreciable rates, especially when the hydrogen is under pressure.) Conductivity is lost. The emphasis to date has been on membrane improvements. The other possible approach is with an electrochemical reactor design. It is possible that a solution will be found; however, if a new membrane is developed successfully, that advance alone will probably not be sufficient. Cations (e.g., copper +2) are strongly adsorbed on Nafion sites. Fouling is often minimized by flushing with a high proton flux. However, in the ANL design the fluxes of both protons and copper +2 are concurrent. (One can think of ways of driving a proton flux counter current.) Zero-gap electrodes are necessary when high-current density is required. However, "small-gap electrodes" where the ion exchange membrane would be a separate element and the cathode would be at some distance away could also be considered. If product hydrogen is removed promptly, the chemical reduction might be reduced. There will be iR losses, but if current is modest, iR could be modest too. A new reactor design might be far more successful than a new membrane design. The need to greatly reduce copper plating is apparent.

Project # PD-014: 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) assist in program planning to investigate potential delivery pathways to achieve cost goals and help define future funding priorities; and (3) develop new tools that build off existing U.S. Department of Energy (DOE)-sponsored tools (e.g., the Hydrogen Analysis [H2A] production model; the Fuel Cell Power Model; and the Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation [GREET] Model).



Question 1: Relevance to overall U.S. Department of Energy objectives

This project was rated **3.7** for its relevance to DOE objectives.

- This project has good relevance toward determining the feasibility of the different technologies. The codes produced appear to be a good compendium of available information on delivery systems.
- This project fits well with the goals of the DOE Hydrogen and Fuel Cells Program. Delivery is a salient topic in the transition to hydrogen.
- This is an extremely important tool for planning and decision making. Understanding process costs and their origins is critical in designing a program to minimize delivery pathway costs.
- The Argonne National Laboratory (ANL) hydrogen model work is critical to the Program's selection of the right technical hurdles to investigate. It enables reviewers to cost out the most expensive barriers and to work on those with a priority basis.
- Program direction, especially during periods of budget constraints, relies on accurate cost analyses to direct scarce funds toward the highest pay-off technology pathways and their sub-systems and components. This project and the Hydrogen Delivery Scenario Analysis Model (HDSAM) offer such a capability. The update of the HDSAM cost database maintained the accuracy of the tool.
- With the early rollout of smaller stations and the development of refueling station costs for 100 and 200 kilograms (kg) per day deployment, it is critical to understanding the delivered hydrogen cost. Continual updating of the costs of other aspects of potential hydrogen delivery is important to ensure that DOE focuses on the necessary gaps and prioritizes research efforts.

Question 2: Approach to performing the work

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

- This project's approach toward the model's relevance and applicability to current issues with hydrogen delivery is a strength.
- This project offers rational and thorough modeling of delivery systems.

- Overall the spreadsheet's approach makes the results and processes less of a "black box" and more accessible to potential users. This project's integration with other delivery projects could be improved, but this may depend on external factors that may be beyond the scope of the project.
- The authors have done an excellent job of considering all of the hard and known factors that can influence the cost of pipelines. Given the range of delivery pathway possibilities, the progress obtained on this project is quite an accomplishment. The "soft" factors, such as the perception of safety and security and the uncertainties associated with previously unknown failure mechanisms for new materials that have little or no service record, are very difficult to quantify in a numeric cost model of this type. However, these factors frequently determine the final decision and some means of probability analysis should be incorporated to account for these.
- This project addresses Hydrogen Delivery Barrier "A" (Lack of Hydrogen/Carrier and Infrastructure Options Analysis) of the Multi-Year Program Plan. The incorporation of recent data from the Oil & Gas Journal and Chemical Engineering Plant Index improves the accuracy of the project's cost database and provides the ability to communicate and compare analyses and results with resources outside of the Program. Additionally, the Oil & Gas Journal data provides insight into regional cost differences that Barrier A seeks to understand and overcome.
- Comparison of the first plant technology and cost to that of the "nth" plant is critical in understanding the path to full deployment and the gaps to be addressed.

Question 3: Accomplishments and progress towards overall project and DOE goals

This project was rated **3.3** for its accomplishments and progress.

- The researchers have made continued progress by incorporating further model details for pipelines, refueling stations, and refueling modes.
- The focus on the near-term 200 kg/day stations is good. This makes the results more relevant to near-term objectives. The pipeline cost study was a sorely needed addition to the model. This reviewer has not had a chance to look at the results in depth, but a review of 30 years of pipeline data should be a decent starting point for analysis. The investigation into new pipeline materials is also a good direction to start, due to a potential reduction in costs.
- Progress on updating pipeline cost functions, cost and price indexes, service station analysis, and delivery cost target analyses were well defined and significant. Adoption of Oil & Gas Journal's pipeline costs provided credibility and the ability to communicate and compare with resources outside of the Program. Updating the equipment cost index has corrected the unusually high cost escalation experienced in the 2006–2008 timeframe, and returned it to rates more in line with historic long-term trends. The station analysis provides sensitivities that can guide DOE funding decisions, while confirming the feasibility of achieving technical cost targets.
- This project has made excellent progress, but the work is a little like trying to hit a moving target. Better estimates of future trends may reduce the impact of these changes.
- Reviewing items on an individual basis is important to understanding their effects. An analysis on the effect of a combination of factors through simulation would be useful. While the range of station sizes analyzed may not be commercially similar, it is important to understand at what point a change in delivery method and cost impacts will occur. For example, it is unclear if the delivery method at 100 kg/day will scale to 1,000 kg/day, and what the cut-off points are and why.

Question 4: Collaboration and coordination with other institutions

This project was rated **3.5** for its collaboration and coordination.

- The authors appear to be well coordinated with the Program and gathered data for their cost models from a range of organizations and institutions.
- ANL, the National Renewable Energy Laboratory (NREL), and others all work well to maintain and upgrade the models.
- The range of review and collaboration is appropriate for this task.
- The Pacific Northwest National Laboratory (PNNL), NREL, and ANL are collaborators. Information exchanges are made with other institutions as well.
- A number of national laboratories are involved in the work, along with DOE.

- The presentation's relevance, approach, and summary slides state that the project has “Active partnership among ANL, PNNL, and NREL, plus regular interaction with Fuel Pathways and Delivery Tech Teams, DOE researchers and industry analysts.” The breadth of the team is commendable; however, these partnerships and types of interactions and contributions were not always evident within the body of the presentation.

Question 5: Proposed future work

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

- The future work looks good and appears to be focused on expanded station configurations.
- The proposed future work appears to be well designed to advance and complement prior work. While understanding the cost of geologic storage may be an important consideration in program planning, the main limitation may be performance.
- This project has a good plan for future work on the model.
- Alignment and continual feedback are appropriately addressed in the future work, and are essential to ensuring continued value from this activity.
- It seems viable to continue with the same approach and add geological storage.
- The milestones for 2011 are clear and significant; however, the 2012 milestone “Examine technology and pathway options to reduce refueling station cost” is vague.

Project strengths:

- This project is good at collecting information and adding it into the code to project the costs associated with future capabilities.
- This project’s spreadsheet-accessible results and good basic research on pipeline costs are its strengths, along with a focus on 200 kg/day for near-term stations.
- This project provides a thorough detailed analysis of every input factor in the model and uses good margins to make the estimates.
- This project’s models enable DOE and U.S. DRIVE to target needed cost reduction breakthroughs.
- This project focuses on areas of current interest and relevance; has detailed, thoughtful analysis, and is accepting feedback on an approach

Project weaknesses:

- Little work beyond gathering models and cost data was done on this project. It would be nice to see more detailed discussions on how the results will impact future hydrogen vehicles in terms of storage, dispensing, etc.
- The presentation of how to add together refueling station, delivery, and feedstock costs was confusing. This reviewer asks what exactly is separated and what is together in the numbers presented. Seeing this information all on one slide with the categories clearly delineated would help with understanding the numbers and the focus area of the research. Also, this will help describe what a kilogram of hydrogen may cost and where the sensitivities lie.
- An uncertainty analysis would be helpful. That is, the authors did not include uncertainties in their presentation estimates. A good uncertainty estimate can be more important than the estimate itself. For example, if approach “A” is estimated to cost 3% less than “B,” that is significant if the uncertainty estimate is 1%, but it is not significant if the uncertainty estimate is 10%. An uncertainty analysis is needed to identify the decision point.
- Unfortunately this project is unable to validate the model’s predictions, as no commercial facilities are installed to verify costs. The researchers are currently attempting to use the validation projects to gather costs, so that is some help.

Recommendations for additions/deletions to project scope:

- It would be helpful if these results were integrated with the vehicle modeling results (also from ANL) to obtain a more integrated view of how infrastructure and vehicle storage options affect future vehicle technologies.
- This data might be available in the pipeline cost study, but this reviewer would like to get a sense of the variability in cost data for urban pipelines. The reviewer wants to know if merely laying pipeline is enough, and

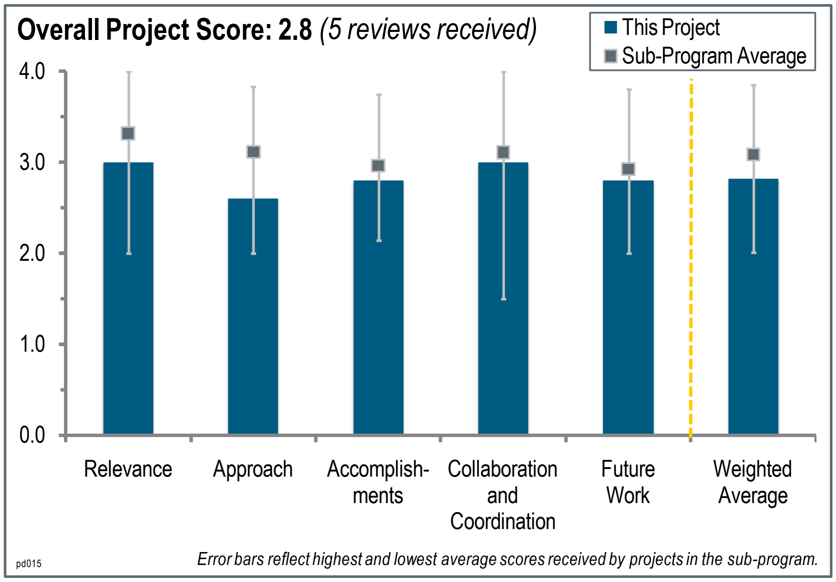
if there are any costly upgrades to guard against "backhoe Joe." In short, the reviewer wants to know if urban pipeline construction could start with these cost estimates, and what additional costs might be incurred in an urban setting.
- A good uncertainty analysis can take as much time as the original estimations, but in a way it is more important because it quantifies the variability and uncertainty in the cost factors and determines decision points. Including the uncertainties in the presentation can be difficult, but it helps the reviewer follow and understand the important points uncovered by the study.
- This project should show comparisons versus other analyses, and benchmarking versus early deployment systems. Identifying boundary issues for delivery pathways (i.e., what is in or out of scope) and ensuring that they are captured within production (if not in delivery) should also occur. This reviewer wants to know what happens with modular systems and how they can be appropriately characterized in terms of station capacity.

Project # PD-015: Hydrogen Delivery Analysis

Olga Sozinova; National Renewable Energy Laboratory

Brief Summary of Project:

The objectives of this project are to: (1) update and maintain the Hydrogen Analysis (H2A) Delivery Components Model; (2) provide cost analysis on hydrogen delivery infrastructure; (3) support other models and analysis that include delivery costs; (4) expand the H2A Components Model by designing new components; and (5) develop new delivery scenarios.



Question 1: Relevance to overall U.S. Department of Energy objectives

This project was rated **3.0** for its relevance to U.S. Department of Energy (DOE) objectives.

- This work is valuable to the DOE Hydrogen and Fuel Cells Program goal of significantly reducing the cost of hydrogen production and delivery. A comprehensive analysis with consistent assumptions and a common basis for comparison of different options addressed in this project is necessary and useful.
- Work on the components of the H2A delivery model is important when evaluating future hydrogen scenarios and the costs and emissions related to the delivery portion of the pathway. However, the relevance of this project and the viability of hydrogen delivery via existing natural gas pipelines, especially in light of the expanding U.S. natural gas resources and its use in power generation, are not clear. This reviewer asks if there are not other areas that should be of higher priority for analysis.
- This project has relevance to the Program in that it evaluates different delivery alternatives. However, the value of rail delivery and hydrogen transport in existing natural gas pipelines relative to other modeling and analysis needs should be questioned.
- There have been two prior comprehensive studies funded by the Hydrogen Production and Delivery sub-program on delivering hydrogen via the natural gas pipeline network. The work done on this issue within this project was less comprehensive and did not include a review of this prior work. It is not clear how much value the multi-node delivery model Scenario Evaluation, Regionalization, and Analysis (SERA) will have. The existing Hydrogen Delivery Scenario Analysis Model (HDSAM) appears to provide sufficient cost, energy efficiency, and greenhouse gas (GHG) analysis to guide hydrogen delivery research efforts. In terms of estimated hydrogen transport distances, use of railways is only cost efficient with very long distances. Thus, the analysis of the costs of this mode of transport is a low priority.

Question 2: Approach to performing the work

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

- The development of H2A and the enhancement of characteristics are useful for system evaluation. However, the collection of tasks seems scattered. The researchers should try to focus modeling on doing a very thorough job with just a few key technologies that seem the most promising for the future work.
- The approach is acceptable. However, using rail reports from 2007 is a bit out of date, especially with the recent problems shipping fuel grade denatured ethanol from the Midwest to the coasts. More recent experience and data should have been used to assess the capability of the U.S. rail system to "deliver." There was no explanation of

how the natural gas distribution system could be used for hydrogen transportation without sacrificing some capacity for needed natural gas distribution (the reviewer may have missed this point in presentation), and researchers need to make how this will work more apparent. Also, there needs to be more references and building on prior studies of this concept from previous hydrogen delivery technology team reports and European efforts.
- Within the scope of this project, a large part of the barriers are adequately addressed. However, there is a lack of one-to-one correspondence between barriers and the approach as described. For example, Barrier 3.2 F, as described, is not directly addressed in the approach.
- There are several areas of concern relative to the approaches used in this effort.
  - The work on rail transport includes transport distances up to 1,250 miles. It shows that rail is the most cost-effective only for distances in excess of 500 miles. It is very unlikely hydrogen will be transported more than 500 miles. It is very costly to transport it by any means. There are already a multitude of hydrogen production facilities that are well within 500 miles of almost all the major urban areas in the United States. The hydrogen produced is used predominantly for gasoline refining, but some of it could be diverted to transportation and other uses as additional hydrogen capacity is brought online. Hydrogen can be made using many production technologies. The renewable resources of off-shore wind and biomass are available close to the coasts. This is where the majority of people in the United States are located. There is every reason to believe hydrogen will be produced reasonably close to the market demands.
  - Most of the rail delivery work is focused on liquid hydrogen. Liquefaction is very costly and energy inefficient. The rail delivery analysis results do not include energy efficiency and GHG emissions.
  - The renewable hydrogen study utilizing wind-based electricity for hydrogen production assumes renewable hydrogen will need to be produced far from the hydrogen demand. This is based on looking at the high-wind areas in the West and Midwest. Off-shore wind may prove to be an excellent source of renewable energy and the vast majority of people in the United States live on the coasts. Use of offshore wind to produce hydrogen would greatly reduce the hydrogen transport distances and the energy needed to do so. Hydrogen can be produced from biomass via biomass gasification. Although the greatest potential for biomass growth is in the U.S. heartland, studies have shown that very significant biomass supply could be available to a very broad U.S. geographical area. The Southwest is perhaps the only area where biomass would be scarce. Solar-based hydrogen could serve this area. Also, in addition to strictly renewable-based hydrogen, hydrogen could be produced using coal gasification with carbon sequestration and nuclear energy. Both of these approaches would result in low GHG emissions. This would further broaden the geographical space that could have “green” hydrogen production in close proximity. All of this is ignored in the work on providing renewable hydrogen throughout the United States.
  - The basis for the cost analyses is not provided other than to say that it was based on the Delivery Components Model. For example, there is no information provided on how the capital costs and operating costs for hydrogen rail transport and tube trailer transport were derived. There are a number of different approaches being taken to develop high-pressure composite tubes for hydrogen storage and transport. The resulting costs can vary widely.
  - The study on the use of the natural gas pipeline infrastructure seems to ignore two prior very comprehensive studies done on this by Concurrent Technologies Corporation (CTC) and Nexant. Both were funded by the Hydrogen Production and Delivery sub-program. They raised legitimate concerns relative to hydrogen embrittlement of the pipelines and recommended no more than 10% hydrogen. This differs with the conclusions in this project. The researchers’ cost analyses showed that the separation of the hydrogen from the natural gas would likely be cost prohibitive. This work suggests that doing this separation at the pressure reduction facility could dramatically reduce this cost. The basis for the costs presented is not included. It is not clear why the cost reduction in this scenario would be so dramatic, as the hydrogen would still need to be recompressed.
  - It is not clear how much value the multi-node delivery model (SERA) will have. The existing HDSAM model appears to provide sufficient cost, energy efficiency, and GHG analysis to guide hydrogen delivery research efforts.
- There was no explanation for reaching milestone 12: achieving less than $1 per gasoline gallon equivalent for delivery by 2017. The volume delivery costs will need to be low at that point, as vehicles and infrastructure will still be small and evolving.

Question 3: Accomplishments and progress towards overall project and DOE goals

This project was rated **2.8** for its accomplishments and progress.

- The researchers have done good work on a multitude of tasks; however, they need to explain to the audience how all these models—including Biogas; HyPro; Scenario Evaluation, Regionalization, and Analysis (SERA [although SERA is covered later in the talk]); Macro-System Model (MSM); and Hydrogen Demand and Resource Analysis (HyDRA)—are used together. The reviewers and audience do not have working understanding of all these acronyms.
- This project provided a thorough analysis of liquid delivery by rail.
- Although a great deal of effort was expended on this project, there does not seem to be a significant amount of meaningful new knowledge derived from this work. The analysis of the railcar delivery of hydrogen is new, but it is a low-priority delivery option. The rest of the work presented has either been done before or has issues due to the approaches taken:
    - It is not clear how much value the multi-node delivery model (SERA) will have. The existing HDSAM model appears to provide sufficient cost, energy efficiency, and GHG analysis to guide hydrogen delivery research efforts.
    - The study on the use of the natural gas pipeline infrastructure seems to ignore two prior, very comprehensive studies done on this by CTC and Nexant. These make it clear that there may be technical issues relative to hydrogen embrittlement and that the cost of separating out the hydrogen is likely to be cost prohibitive. Furthermore, the natural gas pipeline infrastructure is already fully utilized. Adding hydrogen to it would likely require capacity expansion. It would likely be better and more cost-effective to simply develop hydrogen pipelines.
    - The renewable hydrogen study utilizing wind-based electricity for hydrogen production assumes that renewable hydrogen will need to be produced far from the hydrogen demand. The analysis done appears valid and somewhat useful, given this assumption. However, as discussed in the comments under question three, it seems like there are many alternative scenarios to provide renewable or "green" hydrogen to most or all of the United States without needing to transport it long distances.
    - It is not clear what the components model adds compared to the full HDSAM model. If individual component analysis is needed, it can be extracted from HDSAM. Trying to keep two delivery models up to date and in agreement is difficult, at best, with no clear added value.

Question 4: Collaboration and coordination with other institutions

This project was rated **3.0** for its collaboration and coordination.

- This project had broad collaboration with multiple institutions and is leveraging knowledge and experience from multiple collaborators. However, it is not clear which collaborations are current and which are from previous work.
- This reviewer would like to see review and detailed discussion with U.S. DRIVE's Fuel Pathways Integration Technical Team.
- Although there is an extensive list of organizations labeled as collaborators, there is no evidence of true collaboration. This list appears to be more of a list of sources of information. It appears the actual work done was done alone by the principal investigator (PI). It appears the PI got her own information on tube-trailer costs and did not collaborate with other program-funded delivery analysts who have researched these costs in the recent past.
- The fact that the PI is not aware of the previously funded projects on the use of the natural gas pipeline infrastructure for hydrogen delivery demonstrates a lack of collaborative effort.

Question 5: Proposed future work

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

- The future plans, as described, are adequate as far as work to be performed is concerned. One suggestion is to provide feedback to technology developers and reiterate the models based on technology program output. In the end, it would be more productive if technology developments and modeling efforts are more closely aligned.
- The researchers need to review rail delivery of ethanol to determine the potential for hydrogen delivery. There is also a need to review prior work on hydrogen delivery via natural gas pipelines and to address capacity issues for those pipelines.
- This project seems scattered and needs to focus on the most relevant technologies.
- It is not clear how the separate Delivery Components Model adds value beyond the HDSAM model. Work on updating both and keeping them in sync is duplicative. Continuing to develop wind-to-hydrogen scenarios for one or two specific urban areas is less valuable than perhaps analyzing how to supply renewable or "green" hydrogen to most of the U.S. market. There should be no more work done on the use of the natural gas pipelines for hydrogen delivery, as extensive and comprehensive work has already been done on this.

Project strengths:

- This project offers a good compilation of results.
- This is the first thorough analysis of hydrogen transport by rail.
- This project completes the study of hydrogen logistics in terms of pipelines, trucks, on-site generation, and now rail. The multi-node model allows for optimization of various transport options. However, there needs to be interpretation of what the results mean for various market scenarios and how this can guide DOE decision making, otherwise this is just a simulation exercise.
- This project has strong modeling capabilities and a good understanding of the barriers, underlying technologies, and desired outcomes to meet the overall DOE goal.

Project weaknesses:

- The researchers need to think in more detail about exactly what to model for maximum impact in making key decisions for the program.
- This project has duplicated earlier work on the use of the natural gas pipeline infrastructure for hydrogen transport and the prior work was more comprehensive. It is not clear how much value the multi-node delivery model (SERA) will have. The existing HDSAM model appears to provide sufficient cost, energy efficiency, and GHG analysis to guide hydrogen delivery research efforts. It is not clear how the separate Delivery Components Model adds value beyond the HDSAM model. Work on updating both and keeping them in sync is duplicative. There is little collaboration with other delivery analysts on this project.
- This project needs to update rail capability with comments from ethanol shippers, and should to address the capacity of natural gas pipelines to ship hydrogen by reviewing prior work.
- This project needs more coordination and a higher degree of engagement with delivery technology development players.
- The path to achieving the delivery target is unclear, along with the applicability of sub-areas to hydrogen deployment.

Recommendations for additions/deletions to project scope:

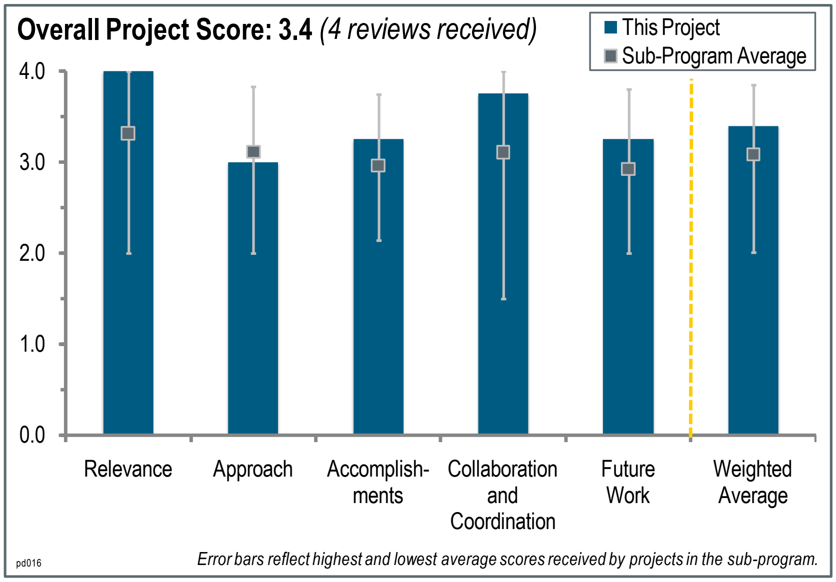
- The researchers are carrying out some work that should be continued.
- This project should extend modeling from "just" incorporating new capabilities in H2A to more result interpretation and predictions of future hydrogen technologies that minimize environmental impact and cost.
- The Hydrogen Production and Delivery sub-program should consider stopping this project, with the exception of possibly an effort to analyze how to supply renewable or "green" hydrogen to most of the U.S. market if it is of a high enough priority to the Program. It is not clear who should do this or how this should be done. Perhaps the SERA model could be of value in this effort. It should first be confirmed that there have not been similar analyses already done that could answer this question.

- This program should address the weaknesses mentioned above.
- This project should not spend any more time on hydrogen delivery in natural gas pipelines.

Project # PD-016: Oil-Free Centrifugal Hydrogen Compression Technology Demonstration

Hooshang Heshmat; Mohawk Innovative Technology, Inc.

Brief Summary of Project:



The current compression technology used for hydrogen is unreliable, resulting in the need for redundant compressors and thus higher costs. A centrifugal compressor was selected as the most reliable and efficient technology to meet the U.S. Department of Energy (DOE) 2012 and 2017 performance targets. The objective of this project is to design a reliable and cost-effective centrifugal compressor for hydrogen pipeline transport. Performance requirements of the compressor include: (1) flow of 240,000–500,000 kilograms (kg) per day; (2) pressure rise of 300–500 pounds per square inch gauge (psig) up to 1,200–1,500 psig; and (3) contaminant-free and oil-free hydrogen.

Question 1: Relevance to overall U.S. Department of Energy objectives

This project was rated **4.0** for its relevance to DOE objectives.

- Reducing hydrogen pipeline delivery costs is essential to meeting the DOE objectives and enabling hydrogen as a mainstream transportation fuel. This project is developing technology with the potential to reduce the costs and improve the reliability of pipeline compressors.
- Centrifugal compressors have the potential to impact multiple areas of hydrogen production and delivery.
- This is a very different approach to meeting compression requirements for the DOE Hydrogen and Fuel Cells Program. The project is 48% complete.
- The researchers claim to be developing a compressor that meets DOE's efficiency and capital targets. One issue that should be considered is the linkage to the pipeline, and potential dissimilar materials problems between the two that may arise.

Question 2: Approach to performing the work

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

- The project appears to be well designed—material limitations seem to be the primary barrier. The presenter suggested that a titanium alloy is desired. More details on the materials issues anticipated and the strategy for addressing them would allow a more accurate assessment of the project's likelihood of success. The project is adequately integrated with other efforts.
- Mohawk Innovative Technology (MITI) has made progress toward the barriers identified within the scope of the program and based on an advanced compressor design methodology.
- MITI continues to build on its expertise in a well planned and executed manner to meet DOE goals.
- The selection of foil bearings and foil seals is the crux of this project. This seems to be a good approach, along with the two parallel designs. The presentation contained a lot of information about why the MITI design is better. It would have been good to hear a rebuttal from Mitsubishi Heavy Industries (MHI).

Question 3: Accomplishments and progress towards overall project and DOE goals

This project was rated **3.3** for its accomplishments and progress.

- This project has made excellent progress towards meeting and possibly exceeding DOE goals and indicates that barriers will be overcome once project is completed.
- Designs from MHI and MITI have been completed, and the movement toward prototypes is a significant step.
- Designs are much further along than they were a year ago. The amount of work done to get to this point is impressive, and it is exciting to see the results of the proof testing. The researchers claim that the cost of $12.5 million is for only two units, and will go down with a full capacity. If that can be validated, those results will be very good compared to DOE targets.
- DOE goals appear to have been achieved and testing is planned to validate the technology. The excellent correlation between the MITI and MHI designs is promising.

Question 4: Collaboration and coordination with other institutions

This project was rated **3.8** for its collaboration and coordination.

- The partners are appropriately coordinated. Collaboration with additional materials experts and developers should be explored.
- Full partner collaboration exists and is well coordinated with DOE.
- The interaction with MHI is a very good step.
- The MITI-MHI pairing is excellent.

Question 5: Proposed future work

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

- Fabrication and testing and materials compatibility assessments are logical next steps.
- The operation of a prototype is critical for success of this project.
- More detail on the design activity and the test specifications would have been helpful. The durability of the equipment is especially concerning, and preliminary plans for testing should have been presented.

Project strengths:

- The project offers a unique approach to high-speed pipeline compressor technology and has made good progress toward the demonstration of a lower-cost hydrogen delivery solution.
- The technology feasibility was first demonstrated under the Small Business Innovation Research (SBIR) program. The technology is configured in a modular approach so it can be readily reconfigured to user requirements.
- Design and construction expertise and relationships with MHI are strengths of this project.
- The project is a good leverage of SBIR funding.

Project weaknesses:

- It is not clear whether testing in a hydrogen environment is planned and verification of the material's compatibility is needed.
- To validate the design, a demonstration test of the tool in a single stage needs to be built and tested to prove the high-speed machine design. In addition, testing in a hydrogen environment is needed to show hydrogen compatibility.
- Although not the fault of the project itself, the total potential hydrogen delivery costs savings that could be realized through the development of effective hydrogen centrifugal compression technology is not as large as the Hydrogen Delivery sub-program first anticipated, as a better understanding of hydrogen delivery has been realized over time. The projected capital cost presented for this compressor design for 240,000 kg/day of hydrogen is $4.8 million. This appears to be about twice as much as the capital cost for a current, equivalently

sized reciprocating compressor. This should be looked at carefully, although the typical high reliability of a centrifugal compressor might eliminate the redundancy common with reciprocating hydrogen compression operations due to their poor reliability.

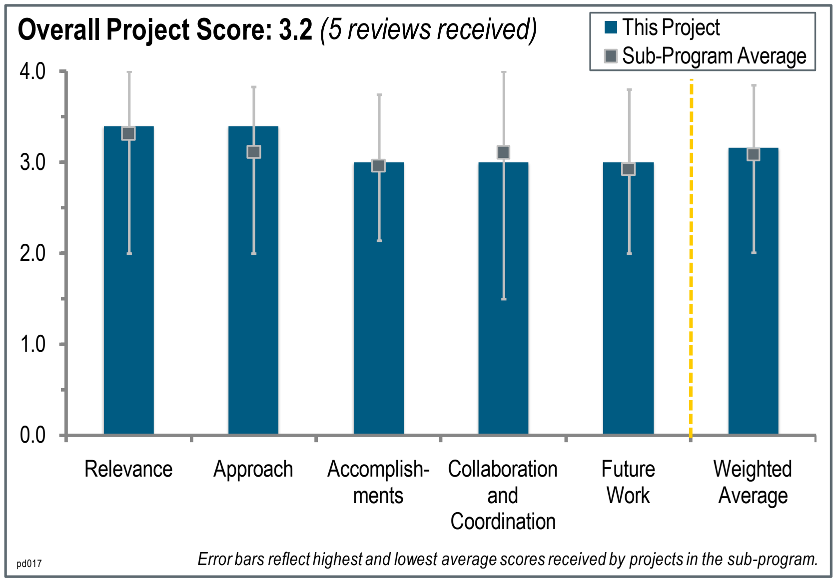
Recommendations for additions/deletions to project scope:

- Careful attention should be paid to the projected capital cost. Potential capital cost reductions should be identified and pursued.
- Once a single stage design is built and demonstrated, multistage systems need to be built and tested. Communication with others in the industry of high-speed machines to review and advise on the design and material selection could be beneficial. Possible collaborators include Boeing aircraft engine manufacturing, Rolls-Royce aircraft engines, Pratt and Whitney Space Propulsion, and Hypersonic (in West Palm Beach, Florida), with their work in scram jet engine designs for materials selection issues.

Project # PD-017: 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 the U.S. Department of Energy's (DOE's) Strategic Hydrogen Economy Infrastructure Plan. Objectives are to: (1) deliver 1,200+ pound-force per square inch gauge and 100,000–1,000,000 kilograms (kg) per day of pure hydrogen to the forecourt station at less than $1 per gasoline gallon equivalent; (2) reduce initial installed system equipment cost to less than $5.4 million uninstalled based on DOE's Hydrogen Delivery Scenario Analysis Model (HDSAM) 2.0 model; (3) reduce operating and maintenance costs via improved reliability; and (4) reduce system footprint.

Question 1: Relevance to overall U.S. Department of Energy objectives

This project was rated **3.4** for its relevance to DOE objectives.

- This project is very relevant to developing low-cost, high-throughput hydrogen compressors for plant application.
- Concepts NREC has done a great job over the years moving toward a technological success in compressing hydrogen with low-molecular-weight hydrogen.
- This project addresses the development of centrifugal compressor technology for the pipeline delivery of hydrogen—a critical issue for infrastructure scenarios that involve centralized production of hydrogen. Alternative routes such as distributed hydrogen production at the point of use will not require the type of compression systems developed in this project.
- Centrifugal compressors have the potential to impact multiple areas of hydrogen production and delivery.
- The pipeline transport of hydrogen is a viable approach for hydrogen delivery, especially in non-urban areas and when long distances are involved. Current compression technology for this service is limited to reciprocating compressors that have relatively poor reliability, resulting in the need for installed spares, relatively high capital costs, and oil lubricating, which results in hydrogen purity concerns. If a cost-effective centrifugal compressor could be developed that could operate effectively with hydrogen gas, all of these issues could be alleviated and the cost of compression for this service could be significantly reduced. The cost of compression for pipeline transport contributes only about $0.10–$0.20/kg of hydrogen using current technology, and is thus only a minor contributor to the overall cost of hydrogen delivery. If similar centrifugal technology could be applied to refueling at the vehicle refueling station, a much greater reduction in delivery cost could be achieved. The costs for compression at the refueling station ranges from $0.40–$1.40/kg of hydrogen.

Question 2: Approach to performing the work

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

- The project's approach is good because of the theoretical and computational fluid dynamics design of the compressor system and parts, and the development of components for testing
- The principal investigators (PIs) are taking a well thought-out approach to the issues surrounding this difficult task. The use of off-the-shelf components should keep costs low.
- The approach being taken to this project is excellent. It consists of a strong collaborative effort, and includes organizations that have excellent knowledge and capabilities for all of the relevant expertise needed. This includes expertise designing and building centrifugal compressors (Concepts NREC), operating hydrogen compression facilities (Praxair), material expertise (Texas A&M University), and motor and machining expertise. The project includes design, modeling, building, and testing components, and building and testing a prototype two-stage system under real-world conditions. Excellent science is evident throughout this effort.
- The approach has been methodic and steady. The ability to change gearbox vendors shows the PI will not accept the limitations of one vendor, but search for best solution, which is a great benefit to the project.
- The project approach starts from scratch with a clean sheet design of a complete centrifugal compressor system designed specifically for hydrogen. The compressor is designed to achieve DOE targets of 100,000–1,000,000 kg/day of hydrogen at a cost consistent with cost guidelines. During the second phase, the PI's completed detailed designs including subsystem modeling and detailed cost analysis. Phase three will involve completion of detailed designs and fabrication of a functional prototype system with testing at a Praxair facility scheduled for fiscal year 2012.

Question 3: Accomplishments and progress towards overall project and DOE goals

This project was rated **3.0** for its accomplishments and progress.

- The accomplishments and progress of this project are on schedule. The testing of individual subsystems would be useful in advance of the full-scale build.
- It is clear that a great deal of progress has been made on this project. The initial and detailed designs have been completed, critical components have been built and tested, and the two-stage prototype compressor materials are being tested. The project has come up with what appears to be excellent solutions to all of the very challenging aspects of this effort. The projected capital cost presented for this compressor design for 240,000 kg/day of hydrogen is $4.8 million. This appears to be about twice as much as the capital cost for a current, equivalently sized reciprocating compressor. This should be looked at carefully, although the typical high reliability of a centrifugal compressor might eliminate the common redundancies in reciprocating hydrogen compression operations due to their poor reliability.
- This project has made good progress for 2011. The results of a detailed analysis have led to important changes in the design. Construction and operation of the prototype is the critical next step.
- The researchers have moved to a new gearbox supplier and found a technical solution to compressor shaft deformation at high speed.

Question 4: Collaboration and coordination with other institutions

This project was rated **3.0** for its collaboration and coordination.

- It is very clear that this is a well coordinated and strong collaborative effort among the project team members and outside experts. This includes organizations that have excellent knowledge and capabilities for all of the relevant expertise needed.
- This project has great collaboration with other partners and is seeking new technical answers from resources.
- This project brings in critical team members, such as Praxair and HyGen, and materials research on tribology.
- This project needs to have strong industry partners who will pull this work strategically.
- The project would benefit from collaboration with a major centrifugal compressor manufacturer. This would establish a path to commercialization and provide a second set of eyes to vet Concepts NREC's work.

Question 5: Proposed future work

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

- The future work plan is excellent, and is following the original project plan to build the two-stage prototype compressor and test it under real-world hydrogen service.
- This project has a good plan to demonstrate technology by running a full-scale, two-stage compressor.
- Future activities include the fabrication of a full-scale system and completion of materials coating testing.
- It is critical to develop a compressor module that can be tested (even if it is only a single stage)
- Device construction and operation is the crucial step.

Project strengths:

- This is an excellent project plan that includes preliminary design, detailed design, and final fabrication and validation. The team involves appropriate members, including Praxair and HyGen.
- The approach being taken in this project is excellent. It is clear that a great deal of progress has been made. The initial and detailed designs have been completed, critical components have been built and tested, and the two-stage prototype compressor materials are being tested. The project has come up with what appears to be excellent solutions to all of the very challenging aspects of this effort. It is clear that this is truly a well coordinated, strong collaborative effort among the project team members with good consultation to outside experts as well. This includes organizations that have excellent knowledge and capabilities for all of the relevant expertise needed.
- The use of off-the-shelf components and lack of exotic materials are strengths of this project.
- This project has a methodic and disciplined approach to the compression problem.

Project weaknesses:

- The approach used by Texas A&M University has limited value in confirming the sensitivity of materials to hydrogen.
- Although not the fault of the project itself, the total potential hydrogen delivery costs savings that could be realized through the development of effective hydrogen centrifugal compression technology is not as large as the Hydrogen Delivery sub-program first anticipated, as a better understanding of hydrogen delivery has been realized over time. The projected capital cost presented for this compressor design for 240,000 kg/day of hydrogen is $4.8 million. This appears to be about twice as much as the capital cost for a current, equivalently sized reciprocating compressor. This should be looked at carefully, although the typical high reliability of a centrifugal compressor might eliminate the redundancy common with reciprocating hydrogen compression operations due to their poor reliability.
- This project assumes that fewer stages results in greater reliability, but there was no data shown to verify that claim.

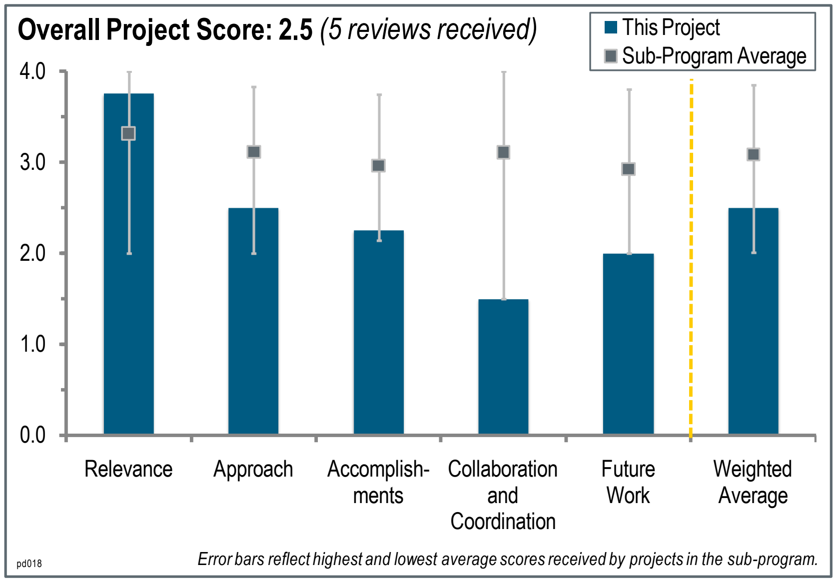
Recommendations for additions/deletions to project scope:

- Researchers should pursue subsystem testing validation of the components prior to construction of a full-scale system.
- Careful attention should be paid to the projected capital cost. Potential capital cost reductions should be identified and pursued.
- Researchers need to present data showing fewer compressor stages that will result in higher reliability.

Project # PD-018: 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 30–300 tons per day that meets or exceeds the U.S. Department of Energy's (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 an improved ortho-para conversion process; and (6) develop an optimized and new liquefaction process based on new equipment and a new ortho-para conversion process. Goals for phase two (process development) are to establish performance targets for process equipment and ortho-para conversion and develop a preliminary capital cost estimate.

Question 1: Relevance to overall U.S. Department of Energy objectives

This project was rated **3.8** for its relevance to DOE objectives.

- This project is strongly relevant to DOE Hydrogen and Fuel Cells Program objectives. This topic cross-cuts other DOE hydrogen areas including delivery, storage, and fuel pathways. The role of liquid hydrogen in the hydrogen economy is made clear with a detailed discussion of the critical barriers. The quantitative status of 2005 liquefaction technology to targets clearly highlights the remaining technical barriers.
- This project addresses barriers of liquefaction.
- High-efficiency liquefaction is a key enabling technology for many hydrogen delivery options.
- Liquefying hydrogen is a critical element of reducing the cost of hydrogen.
- Low-energy liquefaction is a key technology for future hydrogen-based transportation.

Question 2: Approach to performing the work

This project was rated **2.5** for its approach.

- The approach to overcoming the technical barriers was clearly stated and delineated by a research phase. The approach integrates detailed thermodynamic and broader process modeling with an understanding of each model's capabilities and limitations.
- The approach builds on Praxair's knowledge of liquefaction and on identifying and addressing the critical technologies (compression and ortho-para conversion).
- The approach was to search for breakthroughs, but apparently only incremental improvements were found.
- This project has a very broad focus on the overall process. Perhaps prioritizing the most promising options is necessary.
- The approach (or the little of it that the authors revealed) seems very incremental. Increasing the temperature of para-ortho catalysis does not seem like a revolutionary approach to liquefaction. This should be done with company money instead of DOE funding.

Question 3: Accomplishments and progress towards overall project and DOE goals

This project was rated **2.3** for its accomplishments and progress.

- It is good that both positive and negative results were shared. Both modeling and experimental testing were explored to evaluate the various concepts and their performance in relation to targets; however, it seems that a great deal of the progress data shared was repeated from last year's talk. It is difficult to assess the specific technical concepts because they were not revealed in any detail and likely will not be in the future based on the response to the reviewer's comments of confidentiality.
- This project's targets were not reached and the authors decided to cancel the project. This reviewer appreciates the company's honesty in not billing for the rest of the money once it decided that the approach had little potential, but progress seemed to be rather weak. Given the company's secrecy, it is unclear what was actually learned.
- Although the study showed that the targets could not be reached with conventional technologies, it does show what can be done and established the technical limits for improvements that can be expected with existing technologies. This should be captured in a DOE document.
- The accomplishments were incremental improvements to the hydrogen liquefaction process. It is difficult to assess the value of Praxair's proprietary technology when it is not shared with reviewers.

Question 4: Collaboration and coordination with other institutions

This project was rated **1.5** for its collaboration and coordination.

- There is no apparent collaboration with other institutions.
- No collaborations were shown. This reviewer wonders if external expertise could be helpful, regardless of Praxair's experience.
- There was little outside collaboration in the project.
- There was no evidence of collaboration except with a software model supplier (not mentioned) that installed ortho-para capabilities in the model.
- There were no examples of collaborations provided. While the principal investigators (PIs) suggested (in response to reviewers' comments) that no collaborations are needed, it is hard to imagine that it is beneficial to not collaborate. At a minimum, interaction with interfacing entities or industries (e.g., station providers and original equipment manufacturers) would prove to be useful.

Question 5: Proposed future work

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

- No next steps were shown. It is understood that budget is 100% spent, but there should be some recommendations for future work.
- While the project is 100% complete, the PIs could have provided a future outlook, lessons learned, or recommended next steps. Such information is very useful to future projects and researchers in the same or similar technical areas, and is a routine part of project ramp-down.

Project strengths:

- This is a very capable team with proven experience in the field of hydrogen liquefaction. The project is a highly relevant topic and the technology cross-cuts and impacts many hydrogen areas (e.g., storage, fuel pathways, and delivery).
- The company has a lot of expertise in liquefaction.
- The approach to the overall process was broad and could potentially address all DOE targets on liquefaction.

Project weaknesses:

- The project did not deliver the desired results and was canceled. It is disappointing to see that the researchers did not run an experiment, but instead cancelled the project based on modeling. The project unfortunately seems to have produced very little knowledge that the company was willing to share, considering the amount of project funds spent.
- There were no collaborations to gather external expertise.
- The details of the analysis were not given. This reviewer would like to have seen more information on how the analysis was done.
- This project only achieved incremental improvements and there was little collaboration by Praxair.
- The technical details are unavailable and duplicative with last year's. There was also poor illustration of collaborations.

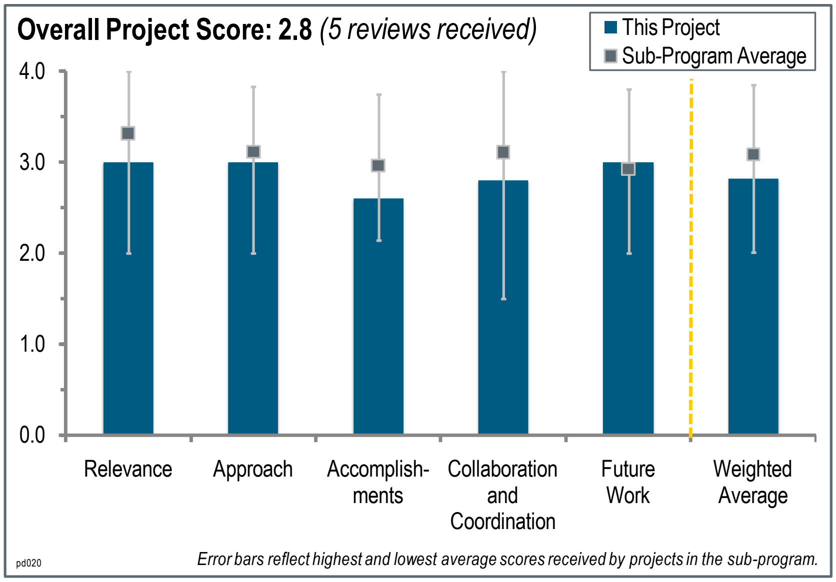
Recommendations for additions/deletions to project scope:

- Even though there is no more money available, recommendations for possible next steps should be requested.
- In the time remaining on this project, the investigators should work to develop an understanding of the "sweet spots" for the technology. When considering capital and operational expenditures for the process, this reviewer asks what the best option is for minimizing liquefaction costs and energy consumption for various plant sizes. Ensure that a comprehensive report on the work is published to guide future research.

Project # PD-020: 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 costs through synergy between low-temperature (140 Kelvin [K]) hydrogen densification and glass fiber strengthening. Benefits of glass fiber vessels include: (1) increased density by approximately 70% through colder temperatures (approximately 140 K) and small increases in theoretical storage energy requirements, which can be achieved at gas-terminal scale with liquefied natural gas refrigerators; (2) synergy with glass fibers through low temperatures; (3) minimized cost for high composite materials (approximately $6 per kilogram (kg) for glass versus approximately $23/kg for carbon fiber); (4) minimized hydrogen delivery costs through increased pressure (7,000 pounds per square inch [psi]), the same design can deliver up to 12,000 psi or build cascade; and (5) reduced vehicle vessel cost by approximately 25% using cold hydrogen and avoiding over-pressurization during fast fill.

Question 1: Relevance to overall U.S. Department of Energy objectives

This project was rated **3.0** for its relevance to U.S. Department of Energy (DOE) objectives.

- This is a good project to address storage capacity and capital cost targets.
- The project's goals and objectives are in line with DOE Hydrogen and Fuel Cell Program hydrogen delivery targets.
- Cold hydrogen delivery has the potential to lower delivery costs. Hazard analysis should be done for worst case scenarios where the tank sits on siding for days or weeks. It is unclear what happens with venting.
- The project is aligned with the key aspects of the Program, as the overall goal of the project is to reduce delivery costs by increasing storage capacity with lower-cost glass fiber.
- This project has the potential to address delivery costs as hydrogen needs scale-up. There is also the potential to reduce overall carbon fiber needs and implications for pathway cost reduction beyond delivery elements.

Question 2: Approach to performing the research and development

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

- Following manufacturing readiness level definitions was a good approach. The reviewer asks if the material research aspect is followed up sufficiently.
- This project's work looks at several different technical barriers while meeting delivery costs based on components of storage trailers along with the environment (temperature) in which the hydrogen is being delivered.
- The overall approach of the project appears to have an appropriate plan based on a progression of manufacturing readiness levels. However, the current work has a significant amount of trial and error failure-mode discovery.

The use of the fault tree to evaluate the root cause was good. The project should proactively consider the further use of these types of failure-mode assessment tools.
- This project has a well structured program and plan, including assessment points.
- The reviewer is not convinced that experiments with full-scale tanks are justified at this stage of development. It is not clear if issues with the effects of water or other environmental contaminants on glass fiber have been addressed.

Question 3: Accomplishments and progress towards overall project and DOE goals

This project was rated **2.6** for its accomplishments and progress.

- The project was successful in demonstrating a burst test of a full-scale, S-Glass fiber pressure vessel. This accomplishment demonstrates significant progress from last year's failed attempts to achieve the burst criteria.
- The project is looking into the future for projected uses of hydrogen and what will be needed to meet the delivery cost.
- The scale-up process and testing will be critical to understand if the barriers, such as material selection, wall thickness, structural needs, and impact on overall cost, are to be addressed.
- This reviewer questions if it is fair to claim that the burst test is passed with an unknown failure mode.
- The 2011 slides were almost identical to 2010 slides. The presenter should focus on what has been done in 2011, not repeat the presentation from last year. The future work slide was identical to last year's; the only difference was the date on the bottom of the slide. Work may have been done on this project this year, but there is no evidence of it in the presentation.

Question 4: Collaboration and coordination with other institutions

This project was rated **2.8** for its collaboration and coordination.

- The project partners include a good mix of industry experts, including Spencer Composites, Worthington-SCI, and Quantum. The presentation showed that Spencer was actively involved; however, the involvement from SCI and Quantum was unclear.
- This project showed good lessons learned over the past year and has a good learning curve on trade-offs of manufacturing capability issues.
- The reviewer wants to know what the potential applications are, what the focus is, if there are enough industry partners onboard, and more about the refueling infrastructure questions.
- Several collaborations were mentioned, but no information was given to describe how collaboration is aiding the project.
- The researchers need to interact more with other analysis areas to ensure alignment.

Question 5: Proposed future work

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

- The general items indicated for future work seem appropriate, but further focus could be planned to assess and eliminate potential failure modes. It is recommended that further modeling and material research is conducted to understand the current failure modes prior to the full-scale pressure vessel test program.
- Important things are covered, including demonstrations and industrial partnerships.
- Interaction with Argonne National Laboratory on cost projections to ensure alignment for others when evaluating various pathways would be useful.
- The researchers need to map out the future test plans.
- The future plans are the same as last year's slide.

Project strengths:

- This project has the potential to achieve DOE targets.

- The project is well aligned to deliver cost reduction, which is an important element of DOE and industry goals for commercializing hydrogen infrastructure. The project is conducting a significant amount of empirical results and evaluations of cylinders.
- The cost projects of cooling and delivering hydrogen appear to be reasonable (and believable).
- This project has a phased approach.

Project weaknesses:

- There is a need for some fundamental research on understanding material issues. While this was done early on to some extent in the project, covering a technology research and development range that spans these issues up to those of manufacturing may be too broad; i.e., there is not adequate coverage of any one area.
- The researchers need to communicate with the Department of Transportation Pipeline and Hazardous Materials Safety Administration on regulations based on size of over-the-road tube trailers.
- The principal investigator (PI) needs to show clearly what has been done in 2011 and how it advances the technology from 2010.
- As indicated in the approach comments, the project should ensure that it is being proactive in evaluating failure modes rather than reactive. The modeling and material evaluations conducted in the earlier stages of the project should be utilized and compared in the later stages to enhance root-cause assessments and scaling effects in the cylinder design. In the cost predictions, it would be helpful to indicate updated assumptions based on the current cylinder design and testing (i.e., cylinder material adjustments based on testing).
- This project needs to interact more with other analysis areas to ensure alignment.

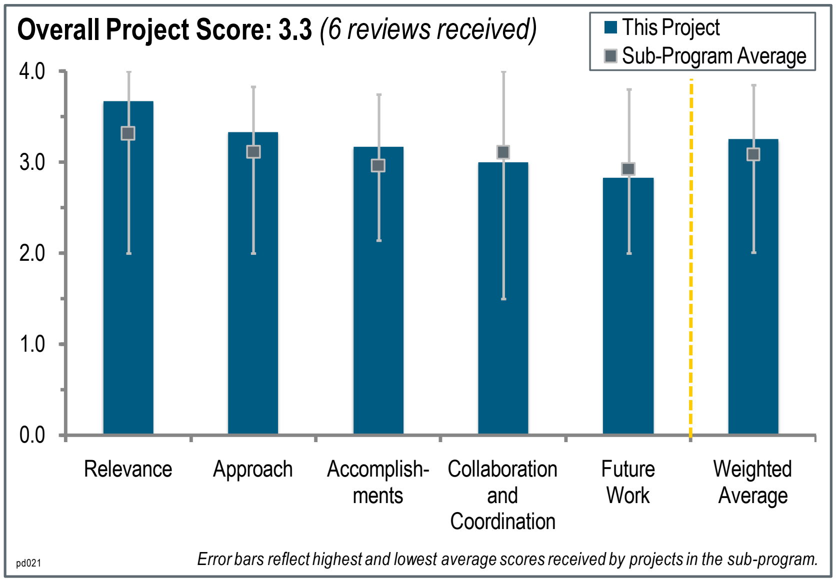
Recommendations for additions/deletions to project scope:

- Focusing on the application and understanding material fundamentals would be helpful.
- With large fabrication tanks, it appears that the project is at a stage where it should be moved to a tank fabricator with expertise in commercial development. If the technology is not at that stage, the PI needs to clearly identify outstanding issues and focus on them instead of tank fabrication.
- The project should confirm that the operating temperature selected is optimal when considering the complete infrastructure implementation chain. The key to this concept is the ability to maintain the cold temperature storage. It is apparent the insulation concept is not part of this project's scope; however, it should be further developed because the overall cost benefit and function depends on a developed insulated container unit. Extreme fail modes, such as bonfire and other transportation accidents, should also be considered.
- This project should evaluate the potential cost and greenhouse gas emission impact of this delivery mode on overall hydrogen pathways. This reviewer asks if station and vehicle synergies can be quantified.

Project # PD-021: 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 International Organization for Standardization (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 project (2009) was to design and qualify a 3,600 pound per square inch (psi) tank and ISO frame that holds 510,000 cubic inches, approximately 8,500 liters, of water volume. The objective for 2011 will be to perform trade studies for a 5,000 psi vessel and, based on the results, move forward on the design, manufacture, and the qualification of a 5,000 psi vessel/system.

Question 1: Relevance to overall U.S. Department of Energy objectives

This project was rated **3.7** for its relevance to U.S. Department of Energy (DOE) objectives.

- The project is well aligned with DOE Hydrogen and Fuel Cells Program objectives by focusing on the reduction of delivery cost through the optimization of the tube trailer design. The matrix of delivery targets in comparison to the current status and potential future opportunity is useful, but the cost status needed to be updated to match the summary slide.
- This project is critically needed to increase the tube trailer hydrogen storage capacity in order to reduce the cost of hydrogen transportation.
- This project is working to reduce the cost of transport. The main objective is to develop a cost-effective, over-the-road trailer configuration.
- High-pressure tanks will significantly enable a more cost-effective hydrogen delivery.
- Hydrogen delivery through a high-pressure tube trailer is a very attractive delivery method if the cost can be reduced. It could be used both initially, when hydrogen is being used in smaller volumes, as well as in the long term. The technology developed for tube trailers could also be used for lower-cost hydrogen stationary storage, which is also a significant cost in the hydrogen delivery infrastructure.
- The project has identified a necessary pressure of 8,300 psi; however, researchers are only going to work toward 5,000 psi. The reviewer agrees with the logic researchers used in making the choice to not attempt a higher pressure; however, DOE should revisit the possibility of compressed gas trucks meeting the objectives. The project may not be as relevant now as it was at its inception. This is not a criticism, but a realistic viewpoint of this option.

Question 2: Approach to performing the work

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

- The overall approach is excellent; however, the trade studies are too qualitative and should be utilizing an overall cost model and studying the trade-offs with it. The capital cost is only one of the trades to be considered (buyers need to balance capital against the capacity in their analysis).
- This project represents a good approach to deploying an existing natural gas composite trailer for hydrogen service. It has good analysis of the feasibility of storage pressure versus total available volume.
- This project looks at the strength and reliability of containers as critical barriers.
- The market pull of natural gas transport has allowed Lincoln Composites to move this technology to a commercial stage quickly. The team has identified parameters that will impact costs and capacity, and is carrying out appropriate analysis to target the best options for hydrogen transport.
- The approach being used in this project is to develop higher-pressure composite tubes for tube trailers so as to increase the carrying capacity. This lowers the cost of hydrogen delivery in two ways. Increasing the carrying capacity can reduce the capital cost on a cost-per-kilogram-(kg) of-hydrogen basis. It also significantly reduces the operation and maintenance (O&M) costs for the delivery itself because fewer tube trailers and labor are needed to deliver the same amount of hydrogen. The project is building actual full-sized tubes and tube trailers and doing all of the testing needed to get them fully approved. The more recent work in this project is also looking at lowering the temperature of the gas in tube trailers and storage vessels to further increase the hydrogen capacity. This is an excellent additional approach.
- The approach seems to have a narrow focus on the benefits of the tube trailer design rather than the entire infrastructure supply chain. The project trade studies would have benefited from an expanded focus. The approach could have been improved with further steps to combine task 5.0 (cost reduction) with task 3.0 (trade studies), as the next-generation trailer should be aligned with cost reduction opportunities. This is where collaboration with a gas company or a national laboratory infrastructure modeling team would be valuable.

Question 3: Accomplishments and progress towards overall project and DOE goals

This project was rated **3.2** for its accomplishments and progress.

- Excellent progress has been made on addressing the critical objectives, which have overcome the barriers. The researchers realize that increasing the diameter of the tube would increase the utilization of space; however, there are several other effects that off-set this advantage.
- Excellent progress has been made on this project. A 3,600 psi 8,500 liter composite tank has been fabricated and fully tested. The test results are very promising and work is ongoing with the U.S. Department of Transportation (DOT) for approval and use of hydrogen transport. This technology is now being utilized in other countries. A tube trailer with this design can hold 600 kg of hydrogen (versus about 300 kg for prior technology), and the money per kilogram of hydrogen has been reduced substantially (down to $500/kg of hydrogen). A thorough study has been completed, identifying that the best approach to further improve this technology for additional cost reduction is to increase the pressure to 5,000 psi and to also look at utilizing cold gas (about −40˚ Celsius).
- The level of qualification testing is impressive. The primary accomplishment in the past year has been the trade studies. This reviewer is surprised that the researchers did not complete more development. Trade studies are an important part of any design, but only qualitative results of the first two (cylinder size and packing) were presented. The reviewer would have liked to have seen how each option was scored against the others (e.g., actual cost estimates). Design, qualification, and manufacturing are the most important part of this project. This reviewer is concerned that DOE has spent $1.5 million of the $2.73 million cost share, and there has been insufficient progress in those activities.
- The project successfully created a 3,600 psi trailer that has been certified and utilized in the field.
- This project is at or close to the near-term DOE cost targets for storage. The researchers need to project what the achievable theoretical limit is in terms of cost and amount of hydrogen stored per trailer.
- The team appears to be on schedule to complete tasks, and the decision to go with mid-grade fibers is a good one.

Question 4: Collaboration and coordination with other institutions

This project was rated **3.0** for its collaboration and coordination.

- This research team is collaborating with industry and other state and federal agencies in regard to increasing the capacity of the trailer.
- An effort has been made to increase collaborative efforts by contacting and working with potential customers. The project continues to collaborate with the American Bureau of Shipping (ABS) and DOT.
- This project needs to have a proper industry partner on the delivery and infrastructure side—see comments above about having an expanded view of where this technology fits into the delivery infrastructure.
- More interactions may have provided additional options for materials and a better understanding of the role that compressors and refrigeration play in the overall costs.
- The project's collaborations seem limited to discussions with ABS and DOT for certification. The project would benefit from expanding and including the feedback from energy and gas companies as well as infrastructure cost analysis sources. Lincoln should include feedback from current customers regarding the current 3,600 psi trailers.

Question 5: Proposed future work

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

- The general proposal is good, but the reviewer would like more details regarding the next steps.
- This project's past progress has been sharply focused on overcoming barriers. Future work may look at the cost of fiber-reinforced composite materials and the strength of comparing them with other composites currently being used in tubes.
- Design and qualification is the logical next step for this project.
- The next step in this project will be to construct and test a 5,000 psi tube. Based on the study completed within this project, this design should make a significant further reduction in the cost of hydrogen delivery and storage.
- The future work to develop a 350 bar trailer builds on the previous learning and trade study results. The next-generation 350 bar will progress toward the longer-term DOE targets. The project would benefit from further assessment of the optimal pressure by including the entire infrastructure cost.

Project strengths:

- This project builds on a solid record of achievement in the natural gas field and logically extends its development to hydrogen applications.
- Hydrogen delivery by high-pressure tube trailer will be a very attractive delivery method if the cost can be reduced. It could be used both initially, when hydrogen is being used in smaller volumes, as well as in the long term. The technology developed could also be used for lower-cost hydrogen stationary storage. Excellent progress has been made on this project. A 3,600 psi 8,500 liter composite tank has been fabricated and fully tested. The test results are very promising and work is ongoing with DOT approval for use in hydrogen transport. This technology is already being utilized in other countries. A thorough study has been completed, identifying that the best approach to further improve this technology is to continue reducing costs. The next step in this project will be to construct and test a 5,000 psi tube. Based on the study completed within this project, this design should make a significant further reduction in the cost of hydrogen delivery and storage
- This is one of the few projects focusing on an important delivery option. The general plans are excellent.
- This project resulted in a commercial product for the 3,600 psi tube trailer. It is encouraging to see that DOE funding assisted the industry in a manner that resulted in commercial products.

Project weaknesses:

- Cost and storage targets may need to be revisited and revised. Steel end caps configuration may need to be re-evaluated to see if end caps can hold multiple tubes instead of a single tube.
- In addition to looking at just the capital cost of the tube trailer and storage tubes on a cost-per-kilogram-of-hydrogen-stored basis, the project should look at the overall tube trailer delivery cost (cost per kilogram of

hydrogen delivered). This can be done by utilizing the Program's Hydrogen Delivery Scenario Analysis Model (HDSAM). Increasing the capacity of the tube trailer can not only reduce the capital cost on a money-per-kilogram-of-hydrogen basis, but also significantly reduce the O&M costs of hydrogen delivery.
- This reviewer expected the past year's efforts to be further along (i.e., more design and manufacturing evaluation instead of just trade studies).
- The project could have included lessons learned, customer feedback from the 3,600 psi trailer development, and a broader trade study assessment.

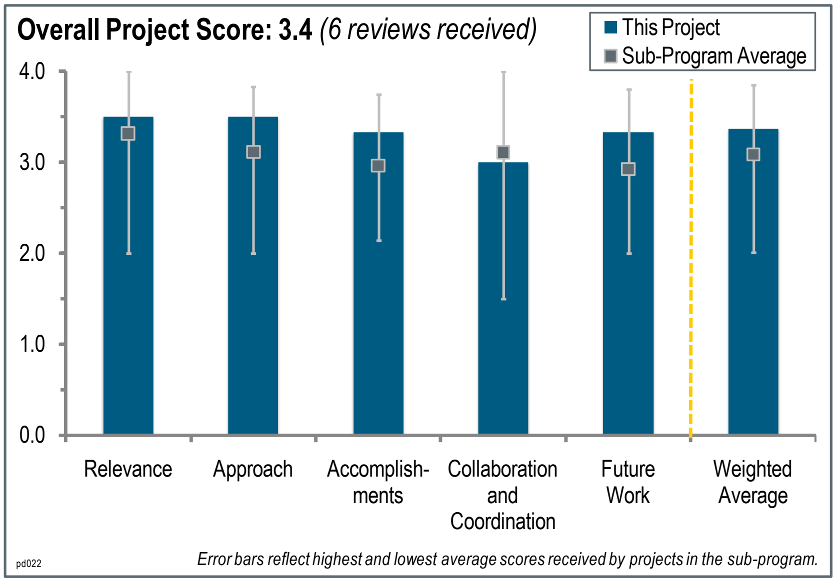
Recommendations for additions/deletions to project scope:

- The scope is good, but the reviewer is concerned that researchers will not meet the project's goal (or get close enough) at the current funding level. The reviewer cannot see what could be cut so that the project can be completed on time and within the funding level, but hopes that the researchers are moving into the next steps soon.
- The investigators should publish their results to ensure that the Program utilizes the full benefits of the work.
- In addition to looking at just the capital cost of the tube trailer and storage tubes on a cost-per-kilogram-of-hydrogen-stored basis, the project should look at the overall hydrogen delivery cost (cost per kilogram of hydrogen delivered). This can be done by utilizing the Program's HDSAM. Increasing the capacity of the tube trailer can not only reduce the capital cost on a cost-per-kilogram-of-hydrogen basis, but also significantly reduce the O&M costs of hydrogen delivery. The project should take a closer look at the concept of using cold hydrogen gas. This should be done on a well-to-vehicle basis for cost, energy efficiency, and greenhouse gas emissions. This could be done in collaboration with the Program's analysis efforts using HDSAM.
- The project should include a complete infrastructure assessment of optimal pressure and sizing for the tube trailer.

Project # PD-022: 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 polymer (FRP) composite piping for hydrogen service applications; assessment of the structural integrity of the FRP pipeline materials, including environmental effects, flaw tolerance testing, and joint integrity; and development of a life-management methodology. Challenges include: (1) reducing installation costs for FRP that offers the potential to meet the long-range (2017) cost targets for installed hydrogen delivery pipeline; (2) developing a suite of standardized tests for assessment of the hydrogen compatibility of FRP; and (3) developing a structural integrity and life-management methodology similar to the American Society of Mechanical Engineers (ASME) B31.8S.

Question 1: Relevance to overall U.S. Department of Energy objectives

This project was rated **3.5** for its relevance to U.S. Department of Energy (DOE) objectives.

- This project is a good way to address the goal of reducing the cost of pipelines.
- The long-term viability of hydrogen transport is critically important. This project is evaluating the use of composite pipelines as a means to reduce the cost. This is relevant and essential for the success of this DOE goal.
- Assuming that FRP is a viable candidate for the construction of pipelines, this project is absolutely necessary to enable the selection of this material and for the setting of codes and standards for its use.
- Reducing delivery costs in built-out hydrogen scenarios is important also with addressing current pipeline costs and potential technical issues (embrittlement).
- Some of the barriers in this project are associated with high capital cost, while other issues are related to the codes required for the composite construction of pipelines to transport hydrogen. This work is in support of the critical hydrogen gaps and challenges that are identified by DOE targets and appear to be addressed once completed.
- The Program elements' primary goal is to reduce the cost of hydrogen delivery. The use of FRP pipelines in place of steel pipelines has the potential to significantly reduce the cost of hydrogen pipeline delivery. Having said that, the pipeline transport of hydrogen will require significant investment in infrastructure and may not ever be used in urban areas due to excessive capital costs and safety concerns.

Question 2: Approach to performing the work

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

- This project is taking a sound approach to develop the tests and data needed to qualify FRP pipe for hydrogen delivery service. This is being done in conjunction with ASME, which would issue the codes and standards for FRP in this service. The tests being developed and performed focus on the key issues of FRP in hydrogen delivery service, including third-party damages, chemical resistance, and hydrogen leakage. The testing does not appear to include looking for delamination in a blow down or cyclic fatigue testing. These are also other

important parameters to test for. This project has not fully collaborated with the Oak Ridge National Laboratory (ORNL) FRP project, ASME, or other stakeholders to scope out and develop all of the testing and performance requirements that might be appropriate to issue codes and standards and qualify FRP for hydrogen delivery service. It was mentioned that there was a meeting being planned to address this; however, this should have been done near the start of this project. There was no discussion of the results of the hydrogen leakage tests relative to the leakage rate significance and the use of FRP for hydrogen service.

- The approach seems good, but it is not shown explicitly in the presentation (e.g., timeline, milestones).
- The scope of work is focused on addressing the critical barriers identified. Successful work on these will make a significant impact.
- The key barriers related to cost and material compatibility and durability are well addressed by the use of composite materials based on known properties. The work is focused on achieving the targets.
- The approach has vastly improved from the early projects in this area. However, the authors still need to keep in mind that it is not the reviewers' responsibility to identify potential failure mechanisms for them to test. It is their responsibility to prove to the reviewers that they have considered every possibility and have evaluated every one through either experimental work or literature data. Developers are not resisting FRP because they are committed to steel, rather they are committed to safety and reliability and they want researchers to convince them that they have given this material the same level of scrutiny as they expect from the steel community. This is not meant as a criticism, instead this is what this project is doing that makes it so useful, as so many in the FRP community want to claim immunity rather than prove it. In the end, the investigators should be able to present a matrix of possibilities against an evaluation showing that every conceivable time-dependent or hydrogen-induced degradation mechanism has been detected or quantified in one of their experiments or from literature data. This project is becoming sharply focused on the critical barriers, and this reviewer is happy with its progress. In addition, FRP materials and chemistry are frequently proprietary, making evaluation complex and product specific.
- This project focuses on leakage potential and potential in-service failure mechanisms, and how to address them through experimental designs.

Question 3: Accomplishments and progress towards overall project and DOE goals

This project was rated **3.3** for its accomplishments and progress.

- This project has made excellent progress toward the stated goals, objectives, and future plans.
- The work to date shows very good progress toward meeting all of the project's objectives while exceeding its barrier requirements.
- A meaningful amount of testing has been done on FRP for hydrogen delivery service over the past 12 months to address important performance questions and issues.
- This project shows very promising cost reduction potential. However, the priority should still shift to destructive tests and environmental impacts to overcome the acceptance barrier.
- While some further progress is evident, it is not clear what significant new data was obtained compared to last year with respect to burst pressure tests. Leak testing results look encouraging, but the economic analysis presented on slide eight is confusing. At the top of the chart it states that "Multi-Wrap Installed Cost 80% of Steel," while at the bottom of the slide it says, "Approximately 20%–60% Cost Reduction for FRP vs Welded Steel Construction." The range of 20%–60% is very broad and does not indicate if the target can be met. From the chart it appears there is a trade-off between material and installation costs for steel versus FRP. Bullets provide cost data for single-wrap, while the chart is shown for multi-wrap in percentage and not in actual costs. It is not clear what the exact comparison is, which is critical because cost reduction is the main goal and should be better explained.
- Field deployment and monitoring in a range of climates will be critical to understanding in-service degradation and performance relative to other, more costly alternatives.

Question 4: Collaboration and coordination with other institutions

This project was rated **3.0** for its collaboration and coordination.

- Collaboration with other institutions and partners looks to be excellent, as they are sharing data and results.

- There appears to be a very good collaboration with FRP manufacturers and ASME. There is neither mention nor evidence of collaboration with ORNL, which is also funded by the Hydrogen Delivery sub-program element, to work on FRP for hydrogen service. Collaboration with the Program's Pipeline Working Group is also not mentioned.
- This project has the appropriate involvement for the current phase of project.
- All industry players seem to be involved. This reviewer wants to know about the possibility of collaborating with other codes and standards authorities besides ASME.
- This project is actively participating in the Pipeline Working Group with other laboratories and standards setting organizations, and the presentation were very convincing in this aspect. While there is good coordination between existing partners, some additional collaboration would be helpful specifically in two areas: (1) a pipeline operator to get operational experience and (2) an entity that can strengthen cost modeling.

Question 5: Proposed future work

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

- This project has an excellent plan that builds on past work and accomplishments. The plan identifies the key barriers to adopting this material and the path toward its safe application. However, the investigators seem to be shifting the focus toward appeasing the needs of the standards committees as opposed to anticipating them and making sure every potential barrier is evaluated systematically. The reviewer had to think about the presentation elements for a while before deciding that they were, in fact, "sharply focused on barriers."
- This project has a good plan for performance testing. A suggestion would be to include cost analysis and firm up the cost benefits of FRP pipelines in order to confirm whether targets can be met and how. The future work is appropriate given the funding level.
- The next steps are good. There is a focus on codes and standards, demonstration projects, and analyzing public acceptance of the technology.
- This project has clear plans to validate case studies and complete performance testing with ASME and industry in order to get a good handle on the required testing and what is needed to get the composite pipe configuration in use. If researchers plan on conducting in-field demonstrations of the composite pipe configuration, they should work with the regional office of U.S. Department of Transportation Pipeline and Hazardous Materials Safety Administration Pipeline Safety for special permits for future plans.
- The future plan appears very good in relation to getting the additional data needed to qualify FRP for hydrogen delivery service. However, it should also include cyclic fatigue and blowdown testing. The proposed collaboration with ASME on performance qualifications for ASME B31.12 and on ASME B31.8S is excellent.

Project strengths:

- This project is well thought-out and has excellent data to support the program.
- This project is taking a sound approach to developing the tests and data needed to qualify FRP pipe for hydrogen delivery service. It is being done in conjunction with ASME, which would issue the codes and standards for FRP in this service. The tests being developed and performed focus on key issues for FRP in hydrogen delivery service, including third-party damage, chemical resistance, and hydrogen leakage. The future plan appears very good relative to getting additional data needed to qualify FRP for hydrogen delivery service.
- This project has done an excellent job of getting past the "polymers are immune to degradation so why bother testing them" philosophy to running any test deemed important. It is good to see FRP projects such as this one are starting to systematically address the critical potential barriers and quantifying effects rather than dismissing them off-hand as irrelevant and testing as unnecessary. Real data is very important and the pipeline community traditionally makes decisions on the basis of lots of real data.
- This project has high cost-reduction potential, and the product is commercially available.
- This project has a good understanding of material properties and testing capabilities.
- This project is testing and evaluating pipe failure mechanisms.

Project weaknesses:

- While this project has done a great job of identifying critically needed data and fulfilling this need, the researchers still seem to be less proactive than is appropriate for this situation. The next step is for the principal investigators to become proactive and to systematically identify all potential degradation mechanisms, then evaluate them through experiments or relevant literature data. The pipeline community is accustomed to seeing large quantities of data on every aspect of the performance of the materials it uses, and it should not be surprising to find that it expects similar thoroughness from a prospective alternative material. To get the industry to switch from a material that is working perfectly well, and for which it has lots of performance data but are still asking for more, lots of data on the new material must be provided.
- The focus on regulatory codes and standards requires public acceptance. This reviewer asks why there has not been a demonstration project yet.
- The projection of leakage due to joint design may need additional work in support of leakage, as well as codes and standards. This reviewer wants to know if the multi-wrap design will affect the diameter of the reel used in transporting the pipeline to the construction site.
- This project has not collaborated with ASME and other stakeholders to scope out and develop all of the testing and performance criteria that may be appropriate to qualify FRP for hydrogen delivery service. There is no mention or evidence of collaboration with ORNL, which is also funded by the Hydrogen Delivery sub-program element to work on FRP for hydrogen service. Collaboration with the Program's Pipeline Working Group is also not mentioned.
- The economic assessment needs to be further strengthened.
- Researchers should include South Carolina in their interaction. The reviewer believes California should be considered, given its likely early deployment of hydrogen fuel cell electric vehicles and extensive regulatory impact.

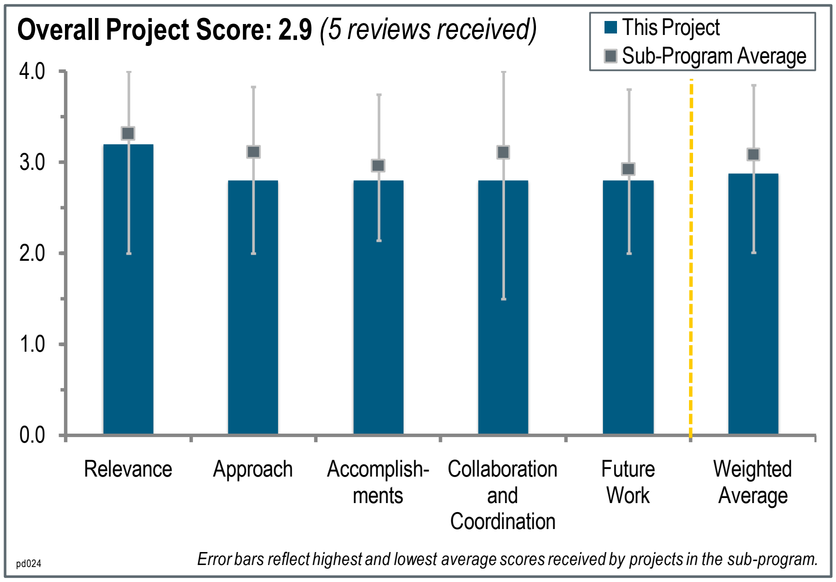
Recommendations for additions/deletions to project scope:

- This project should conduct a perform analysis on public acceptance.
- This project needs to collaborate in a robust way with the FRP work at ORNL and with the Pipeline Working Group. A rigorous review of the work being done in this project and in the ORNL FRP project needs to be completed with ASME, FRP manufacturers, and the companies that would build and operate FRP hydrogen pipelines. A comprehensive list of all of the testing and performance requirements needs to be put together with ASME and other stakeholders. A plan to conduct any missing testing needs to be established and assigned to Savannah River National Laboratory and ORNL appropriately.
- The investigators need to generate more data sharply focused on the potential barriers. This project has made great progress so far and the reviewer would like to see it continue. To get the industry to switch from a material that is working perfectly well, and for which it has large amounts of data, to one it is less familiar with will require thorough evaluations and real data. This should not be surprising. Full-scale testing as proposed in the FRP pipeline demonstration facility seems appropriate, but a thorough analysis of all real and imagined degradation mechanisms with a summary of experimental data from the literature, results of tests in the project, and future work would be helpful.
- This project should continue to monitor the progress of joining FRP and include an evaluation of potential new approaches.

Project # PD-024: 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 fiber-reinforced polymers (FRPs) and engineered plastics in high-pressure hydrogen environments; (2) define research and development issues in adapting the technology for hydrogen use; and (3) develop a path to commercialization for the technology. A key remaining milestone is to complete pressurization-depressurization cycle fatigue testing of FRP pipelines to determine the integrity of a pipeline material that will achieve the 2012 U.S. Department of Energy (DOE) hydrogen transmission target of less than $0.90 per gasoline gallon equivalent of hydrogen.

Question 1: Relevance to overall U.S. Department of Energy objectives

This project was rated **3.2** for its relevance to DOE objectives.

- FRP pipes are a promising technology for reducing pipeline labor cost.
- The Hydrogen Production and Delivery sub-program's primary delivery goal is to reduce the cost of delivering hydrogen. The use of FRP pipelines in place of steel pipelines has the potential to significantly reduce the cost of hydrogen pipeline delivery. However, the hydrogen pipeline transport of hydrogen will require significant investment in infrastructure and may not ever be used in urban areas due to excessive capital costs and safety concerns.
- In order to meet future cost projections, the use of compost materials technology for pipeline construction will be critical. The project objectives and tasks support the necessary milestones to meet the gaps identified by the DOE Hydrogen and Fuel Cells Program.
- Reducing the costs of installing hydrogen pipelines is an important objective in hydrogen delivery scenarios.
- This project addresses the delivery target.

Question 2: Approach to performing the work

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

- The project's barriers are well defined and a plan is in place to address those barriers and technology and cost gaps.
- The team has identified the critical issues relating to FRP performance and is addressing them systematically.
- The approach is not obvious and seems to focus on specific testing protocols.
- The leak testing reported last year and the improved test method for measuring hydrogen diffusivity and permeation are based on sound science. These are difficult measurement to make correctly. Hydrogen leakage is an important issue for FRP pipelines and the blowdown testing being done is important to qualify this type of FRP, especially in a hydrogen application. The accelerated aging tests on the glass fibers used in some FRP are also good science, and are important to FRP pipe qualification for hydrogen service. The planned cyclic fatigue testing is another important aspect for the qualification of FRP pipe for hydrogen service. There does not appear

to be a comprehensive plan agreed upon with the American Society of Mechanical Engineers (ASME) and other stakeholders as to what the full spectrum of testing and required performance is to qualify different types of FRP pipe for hydrogen delivery service.
- This project's approach to the issue has been fair at best. There seems to be no objective for studying the joining of composite pipeline segments, which is critical for any pipeline.

Question 3: Accomplishments and progress towards overall project and DOE goals

This project was rated **2.8** for its accomplishments and progress.

- This project has had promising results in hydrogen-compatible pipeline materials and pipeline leakage rates.
- The accomplishments and progress of this project are on path to meet the cost targets and Program objectives if funding levels remain in place.
- The team has made solid progress in implementing and executing relevant test protocols for FRP.
- For the amount of funding provided in fiscal years 2010–2011, a reasonable amount of progress has been made.
- If the project has been running since 2005 and current results presented in the poster are all of the accomplishments so far, then the small amount of progress made over the past seven years is very disappointing. If more results are available, then they should be presented.

Question 4: Collaboration and coordination with other institutions

This project was rated **2.8** for its collaboration and coordination.

- This project has excellent collaboration with the industry and other federal agencies on this critical technology.
- Many of the major players in FRP are involved in the project.
- There appears to be good collaboration with FRP manufacturers. It is glaring that there is no mention or evidence of collaboration with the Savannah River National Laboratory (SRNL), which is also funded by the Hydrogen Delivery sub-program element to work on FRP for hydrogen service. Collaboration with the Program's Pipeline Working Group is mentioned.
- This project has good collaboration with the industry. This reviewer asks how this project is coordinated with PD-022. The reviewer also wants to know more about codes and standards.
- There was a big list of collaborators, but there was no mention in the poster or the presentation of how they have contributed.

Question 5: Proposed future work

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

- The planned testing for cyclic fatigue and measurement of diffusion and permeability are good. The project appears to be jumping the gun on proposing a demonstration FRP pipeline project. A more comprehensive list of all of the testing and performance requirements needs to be put together with ASME and other stakeholders first. A plan to conduct this testing on the smallest, least-costly scale needs to be established. If some of the testing could only be done at a demonstration scale, then a demonstration project might need to be considered.
- The future work addresses the regulatory codes and standards and demonstration; however, it is very unspecific.
- The proposed future work is critical to overcoming the technical barriers while meeting cost targets.
- A prototype pipeline is a logical extension of this work and engaging the codes and standards community is well timed and appropriate.
- This project needs to address the joining of composite pipe and update the total costs and comparisons to the new steel pipeline installed costs.

Project strengths:

- There is a lot of expertise on hydrogen compatibility and leakage rates in this project.
- Collaboration with industry has aided the progress of this project, and sharing technical data with standards development organizations will strengthen the transfer to a commercial product.

- The leak testing reported last year and the improved test method for measuring hydrogen diffusivity and permeation are based on sound science. These are difficult measurements to make correctly. Hydrogen leakage is an important issue for FRP pipe. The planned cyclic fatigue testing is a very important aspect of qualifying FRP pipe for hydrogen service.
- This project offers an alternative to expensive steel pipelines.

Project weaknesses:

- Real-world demonstrations are required for this project. The standardization of test protocols is unclear.
- This project needs more communication with other state and federal regulatory offices as this technology is demonstrated in the field.
- There does not appear to be a comprehensive plan agreed upon with ASME and other stakeholders as to what the full spectrum of testing and required performance is to qualify different types of FRP pipe for hydrogen delivery service. The project appears to be jumping the gun on proposing a demonstration FRP pipeline project. A more comprehensive list of all of the testing and performance requirements needs to be put together with ASME and other stakeholders first. There is neither mention nor evidence of collaboration with SRNL, which is also funded by the Hydrogen Production and Delivery sub-program to work on FRP for hydrogen service.
- This project has a poor rate of progress since 2005.

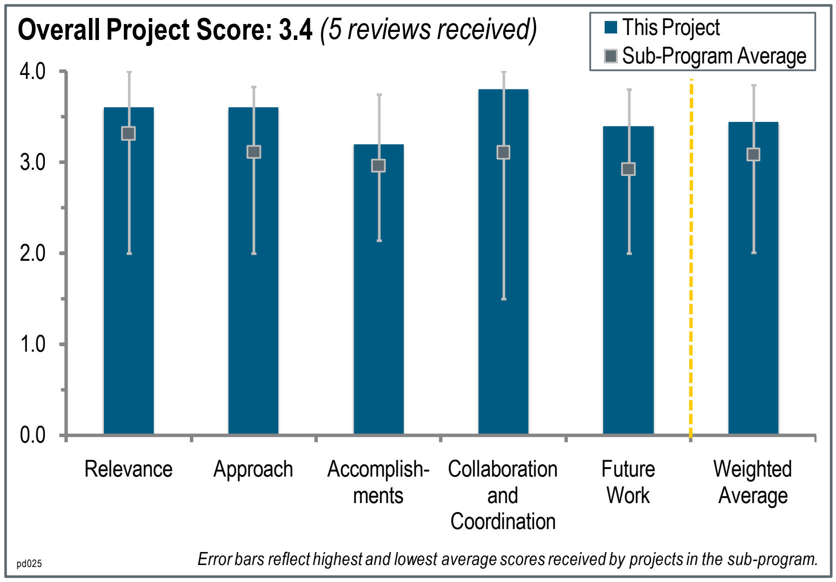
Recommendations for additions/deletions to project scope:

- Researchers need to specify their future work.
- There needs to be more communication with regulators.
- The team may want to include the effects of water in this work. The investigators may want to analyze a pipe that has been in service in other uses for several years to look at real-world aging effects associated with temperature, water, and other factors.
- This project needs to collaborate in a robust way with the FRP work at SRNL and with the Pipeline Working Group, ASME, and other stakeholders. A rigorous review of the work being done in this project and in the SRNL FRP project needs to be completed with ASME, FRP manufacturers, and the companies that would build and operate FRP hydrogen pipelines. The project needs to put together a comprehensive list of all of the testing and performance requirements with ASME and other stakeholders. A plan to conduct any missing testing needs to be established and assigned to SRNL and Oak Ridge National Laboratory appropriately.
- The researchers need to address the joining of composite pipes and update the total costs and comparisons to new steel pipeline installation costs.

Project # PD-025: Hydrogen Embrittlement of Structural Steels

Brian Somerday; Sandia National Laboratories

Brief Summary of Project:



The objectives of this project are to: (1) demonstrate the 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 the hydrogen pipeline design code issued by the American Society of Mechanical Engineers (ASME B31.12). During fiscal year 2010–2011, emphasis is on measuring fracture thresholds and fatigue crack growth laws for X-52 steel in hydrogen gas. Reasons for steel hydrogen pipelines include the already established safety of steel pipelines (e.g., third-party damage tolerance) and that hydrogen pipelines are already safely operated under static pressure.

Question 1: Relevance to overall U.S. Department of Energy objectives

This project was rated **3.6** for its relevance to U.S. Department of Energy (DOE) objectives.

- This project addresses the impact of hydrogen degradation on steel, which will be critical to the implementation of a hydrogen pipeline infrastructure. Information from this project will also be applicable to the design of forecourt delivery systems.
- Studying the effects of hydrogen embitterment on steel structures is presented as a critical knowledge gap for structural steels. The project objective appears to be in line with the goals and objectives of the DOE Hydrogen and Fuel Cells Program.
- This project is directly helping to answer the remaining critical technical questions relative to the safe use of steel pipelines for the transport of hydrogen. However, transporting hydrogen through steel pipelines is relatively costly and may not be able to meet the Program cost targets for hydrogen delivery. It is also unlikely that a significant hydrogen pipeline infrastructure will be needed for hydrogen delivery in the near term. Furthermore, it is very unlikely that hydrogen will be distributed in urban areas by pipeline due to the very high cost and potential safety concerns of such an infrastructure. Having said all this, transporting hydrogen through steel pipelines is utilized today for industrial use. Steel pipelines are a good fallback option for the transmission of hydrogen between urban areas and support the greater use of hydrogen as an energy carrier in the future.
- If one considers hydrogen to be just another alloying element that influences properties like any other alloying element, then for any material that can absorb hydrogen during service it is the properties of this alloying element that matter in the design of devices expected to operate in a safe, reliable manner. For historical reasons, any effect of hydrogen on the ambient temperature properties of materials has become known as hydrogen embrittlement. Hydrogen embrittlement does not make materials unusable, it just changes their properties, and it does so to varying degrees in different materials depending on the solubility, diffusivity, and chemical reactivity of hydrogen with the host lattice and other alloying elements. Understanding the hydrogen modified properties of materials exposed to hydrogen fuel is critically important to protecting public safety, delivering cost-effective hydrogen fuel, and designing reliable vehicles. It is good to see high-quality work in at least one area as represented by this project.

- Although pipelines are not absolutely essential to the Program, pipeline integrity is critical to hydrogen transport. If hydrogen is going to be used in a manner similar to natural gas, which seems to be a lower-cost method of distribution, pipelines will be ubiquitous. A better understanding of pipeline crack growth fully supports that aspect of the Program.

Question 2: Approach to performing the work

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

- This project is taking an excellent fundamental, science-based approach to the study of the safety of utilizing steel pipelines for hydrogen delivery. The key fundamental properties of fracture threshold and fatigue crack growth are being measured directly in hydrogen under relevant pressure, temperature, and frequencies. These properties can be directly related to the ASME B31.12 Hydrogen Pipeline Code. The principal investigator (PI) is looking carefully at the impact of the key testing variables (magnitude of ΔK, frequency, etc.) to establish the best testing conditions.
- The barriers are well defined and appear to be focused on the most critical challenges. Researchers may want to consider looking into the effects of traps within the material structure that hold the resolved hydrogen.
- This is a well designed and thought-out program. There is some evidence that inconsistent and uncertain funding has hindered its productivity, but these investigators seem to have overcome these issues. It seems that the best way to improve this program would be to provide it with good, solid, consistent funding.
- Although the approach is excellent, some questions remain. This is not necessarily due to project issues, but indicates that additional investigative methods may be required. The scanning electron microscopy work is very interesting and is a strength of the project. The additional work to understand the inter-granular failure will be important to follow.
- The approach taken by the PI utilizes unique, high-pressure Instron equipment to evaluate the fracture and crack growth data for X-52 steel, which is commonly used in current pipelines.

Question 3: Accomplishments and progress towards overall project and DOE goals

This project was rated **3.2** for its accomplishments and progress.

- This project has achieved excellent progress and accomplishments and will almost certainly have an impact on the competitive growth of hydrogen fuel in the marketplace and public safety.
- Good progress has been made on the evaluation of the crack growth properties of X-52 steel in pressurized hydrogen environments. The results show significant differences in the behavior of steel when exposed to hydrogen as compared to air. It would be interesting to compare the results with those of a natural gas environment to determine if significant variations exist for X-52.
- This project is working toward providing data and measurements to assist with the codes and standards development (ASME B31.12), as well as understanding load cycle frequency effects.
- Considering the limited testing facilities available for metal fatigue testing in-situ in hydrogen under relevant pressure and frequencies, this project has made good progress. It would be better if additional facilities, such as the National Institute of Standards and Technology, could be used or developed so more data on these critical properties could be measured quicker and on additional types of steel.
- Dealing with continual DOE funding issues is likely to affect the work of this project. It would be much better to have a plan that would be complete at a known date, rather than when funding runs out.

Question 4: Collaboration and coordination with other institutions

This project was rated **3.8** for its collaboration and coordination.

- There is excellent collaboration across national laboratories, a university, and the private sector within the Pipeline Working Group. It includes the relevant industrial gas companies, energy companies, and codes and standards (through ASME).
- There is excellent evidence of interactions within and outside of DOE through the Pipeline Working Group and standards developing organizations.

- This project has had good collaboration with other research institutes and experts on the degradation of steels from hydrogen. However, there is a lack of interactions with gas suppliers such as Praxair and Air Liquide.
- The researchers are working well with other national laboratories and agencies working on this issue.
- Collaboration with pipeline companies is a strength of the project.

Question 5: Proposed future work

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

- This project plans to complete the studies on X-52 steel and the impact of oxygen on inhibiting hydrogen accelerated crack growth.
- The researchers will continue their efforts on higher-strength steels (e.g., X-80), which are commonly used today when constructing new pipelines.
- The future work on X-52 steel should provide a complete set of data to quantify the suitability of this steel for use in the safe transport of hydrogen through pipelines. The work includes obtaining data on welds and in the presence of small amounts of oxygen, which is believed to be a potential inhibitor of hydrogen embrittlement. It would be better if other potential steels, such as X-70, X-80, and X-100, could be evaluated as well. This would not only determine their suitability for hydrogen pipeline delivery, but also might help elucidate why some of these may be more or less susceptible to hydrogen embrittlement.
- This project's findings need additional investigation. The plans to investigate these findings are good and need to be pursued.

Project strengths:

- This project has an excellent approach and facilities for examining the impact of hydrogen on crack growth. It also has a good team that includes collaboration with world leaders in hydrogen degradation.
- This project's approach and testing process are well thought-out.
- This project is relevant to establishing a firm, comprehensive knowledge on the use of steel pipelines for the safe transport of hydrogen as a fallback means to deliver hydrogen for use as an energy carrier. This is an excellent science-based approach to measuring the key properties of steels in-situ in hydrogen at relevant pressures and fatigue test frequencies.
- It is clear that the PIs of this program have an outstanding understanding of the critical issues they need to address and the experimental techniques required to overcome these issues. It appears that the project just needs the funding and time to do the work.
- There has been collaboration with pipeline companies and follow-up on significant findings.

Project weaknesses:

- This is an excellent project addressing what could be a show-stopping issue for hydrogen fuel. Even if the industry ends up using fiber-reinforced polymer (FRP) for all hydrogen pipelines, the scientific understanding of the impact of hydrogen on the properties of metals and alloys could be crucial to enabling hydrogen vehicle technologies. More than 50% of the projected cost of FRP hydrogen storage tanks is expected to be for special "hydrogen-resistant" metals and alloys used in valves, meters, and other elements. Similar issues will resound in every component exposed to hydrogen that needs to use metals but not "expensive hydrogen-resistant alloys" or higher-strength alloys to improve performance (e.g., compressors, valves, stacks, and storage systems). The only weakness is that the project is too small when considering the importance of the data it will produce.
- This project has a limited focus on X-52 steel. This reviewer asks if there are new alloys being proposed for use with hydrogen that should also be included in this study.
- Transporting hydrogen through steel pipelines may be too costly, never used in urban areas due to excessive costs and safety concerns, and not needed for several decades. It would be better to test several types of steels rather than just X-52. It would also be better if more testing setups for this work were available to generate more data in a timely manner.
- It seems that additional resources could be applied to this important topic, resulting in increased benefits in the short term. The PIs may need to do a better job helping the DOE sort out what has been done in understanding interactions between hydrogen and various materials of construction (i.e., what is known), what gaps remain (i.e.,

what is unknown), and what the potential impact can be. This may a particularly valuable step to take in an environment of declining budgets and requests to more carefully prioritize research and development investments.

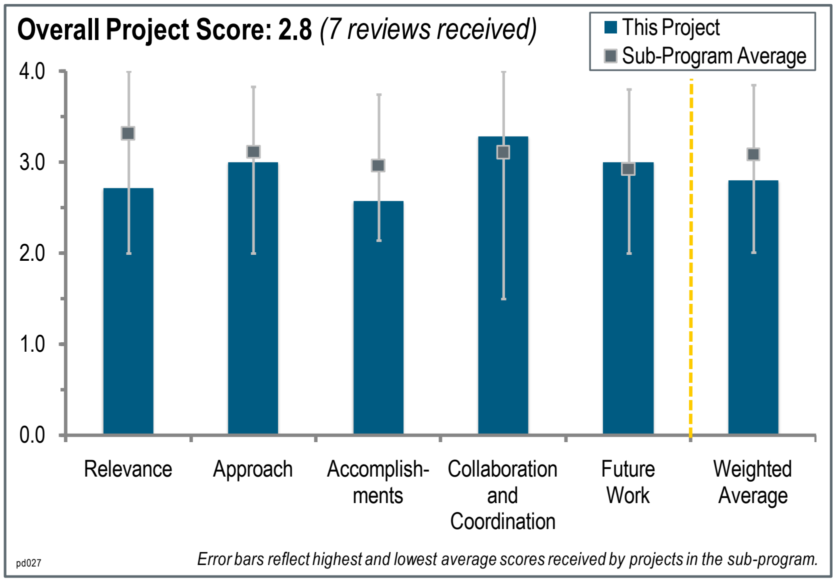
Recommendations for additions/deletions to project scope:

- It is suggested that the PIs indicate how the data will impact the design of hydrogen pipelines. The reviewer also wants to know where the information the researchers generate will be used in the design of pipelines; what computer codes and simulations are used by pipeline companies and whether this is the type of information required; if hydrogen can be transported in existing natural gas pipelines, as suggested by European studies, or if new steels and pipeline materials will be required; and if the issues studied here (cyclic behavior in hydrogen) are also important for forecourt hydrogen systems, such as small hydrogen compressor systems that operate at 5,000 pounds per square inch and above. It is recommended that the PIs also look at these issues.
- The future work of this project will depend on the findings and results of the current scope of work. It is suggested that an industry or government entity reviews the results and the researchers use those recommendations to plan future work.
- It would be better to test several types of steels rather than just X-52. The appropriate calculations in the ASME codes should be done even on the preliminary fatigue data to see sooner rather than later if there are any serious concerns about X-52 fatigue properties in hydrogen. This project should be supported in a manner that enables the researchers to accomplish their objectives in less time and encourages them to expand their scope. When there is success in one area, it is basic human behavior and economics to try to improve again and achieve lower costs. This will mean pushing the limits of the technology. This is the main project determining those limits for steel pipelines that will almost certainly be used for the first generation of transmission lines. Even if FRP pipe is used, similar alloys will be required in pumps, joints, valves, compressors, meters, and other elements.
- Additional resources should be applied to this important area to help bring results as quickly as possible—see the comment above (under "Weaknesses") on what steps Sandia National Laboratories should take to enable this.

Project # PD-027: Solar High-Temperature Water Splitting Cycle with Quantum Boost

Robin Taylor; Science Applications International Corporation

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, [S-A]) for large-scale hydrogen production using solar energy. Project goals are to: (1) evaluate S-A water-splitting cycles that employ photocatalytic or electrolytic hydrogen evolution steps and perform laboratory testing to demonstrate feasibility of the chemistry; (2) perform economic analyses of S-A cycles as they evolve; (3) select a cycle that has high potential for meeting the U.S. Department of Energy (DOE) 2017 cost target of $3 per kilogram (kg) of hydrogen and an efficiency goal of more than 35%; (4) demonstrate technical feasibility of the selected S-A cycle in bench-scale, closed-loop tests; and (5) demonstrate pre-commercial feasibility by testing and evaluating a fully integrated pilot-scale, closed-cycle solar hydrogen production.

Question 1: Relevance to overall U.S. Department of Energy objectives

This project was rated **2.7** for its relevance to DOE objectives.

- This is a good technology feasibility demonstration for the central production of hydrogen through a renewable means.
- Developing a process for producing hydrogen using sunlight as the thermal energy source aligns well with the DOE Hydrogen and Fuel Cells Program's research and development (R&D) objectives.
- Using solar cycles to generate hydrogen is very relevant to DOE's mission. This work is a new cycle rather than just an improvement of an existing concept.
- Thermochemical cycles in general are an important approach to consider over other technologies in order to get the best cost per kilogram of hydrogen. However, it is not really clear what the pathway is for making this competitive with the other technologies being evaluated (e.g., other cycles, electrolysis, reforming). Efficiency is not any better in thermochemical cycles, the cost is higher and the system is complex. The reviewer understands that this is an ongoing project and background research has probably already been reviewed, but the presentation did not really explain why the system needs three reactors—it is hard to see how this will be cost-effective.
- Thermochemical cycles represent one of the best mid-term technologies for producing hydrogen from water. The project aligns well with Program objectives of low-cost renewable hydrogen production.
- With what is currently known about economics, this technology will be hard-pressed to support the Program's objectives. The technology faces daunting technical obstacles, the resolution of which will undoubtedly increase cost. The economics of this project are much further from target than the researcher claims, as the target includes compression storage delivery. Also, the Hydrogen Analysis (H2A) project sponsored by DOE, while good for comparisons, ignores the total erected cost multiplier on capital. This can potentially multiply the cost-effect three times and may dramatically increase the cost of implementing these processes, which are essentially all capital.

Question 2: Approach to performing the work

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

- The technical approach and experimental design works well for the key elements that needed to be addressed, such as the catalyst efficiency for the electrolytic process. Good analysis of the discharge products ensured that the expected reactions are taking place.
- The focus of the project appears to be on clearing the most difficult technical hurdles such as the electrolytic oxidation process. It is also good to see that researchers are addressing the challenges of modeling constant operation with the molten salt heat storage.
- The approach and objectives are a mix of (a) work that helps understand where the barriers and feasibility issues might be (e.g., modeling and design work), and (b) work that actually addresses the barriers (such as cell voltage reductions). This was an appropriate mix for the past year.
- The high voltage of the electrolytic cycle (0.8 volts [V]) is very close to that of high-temperature electrolysis. A high-temperature electrolyzer process would be much simpler and probably less expensive.
- This thermochemical cycle requires about five chemical reactions, while typical thermochemical cycles have only three or fewer. This seems very complicated and the high number of reactions will mean a large number of separation steps and other unit operations. The increased complexity would most likely lead to more expensive processes. It is not clear whether the researchers will be able to store the thermal energy for the high-temperature reaction; yet they are claiming constant operation. The researchers need to demonstrate that they can effectively store the thermal energy needed for the high-temperature reaction.
- This is a very complex cycle. The principal investigator has broken down the work into discrete reactions and reactors, but the presentation was not completely clear on the approach or progress of each step.
- The energy for the process appears to be mostly derived from the electrolysis portion of the cycle, and the solar-thermal input appears to be minimal. Researchers need to report the efficiency explicitly for the entire process. If the electrolysis is operating constantly, this reviewer wants to know where the renewable electricity comes from. The reviewer also wants to know if solar or wind power is being stored in batteries. The researchers should indicate clearly what energy is being used and how much. Steam cycle electricity production looks like a good idea; however, given the overall demand for electricity, it is surprising that excess electricity is expected to be provided on the grid.
- While this approach to water splitting uses thermochemical cycles, it still has many significant hurdles to overcome. The employment of (molten salt) thermal energy storage systems that potentially allow a continuous (day and night) operation of the process is outstanding.

Question 3: Accomplishments and progress towards overall project and DOE goals

This project was rated **2.6** for its accomplishments and progress.

- The project has made good progress in lowering the over-potential at the anode and operating at higher current densities. However, additional progress on the electrolytic process must be made in order to lower the hydrogen production cost. Even though the H2A model predicted rather high hydrogen costs, it is good that the project has continued to refine the costs using this model.
- The scientific progress of this project seems to be reasonable, but it is not clear how the actual barriers are being addressed. There have been significant improvements in efficiency with the stand-alone process; however, in comparison to other technologies, the efficiency is still very low. As other reviewers pointed out during the discussion, it would be helpful to compare the results with electricity credits even though H2A says it “doesn't count.” This comparison could make this technology look more reasonable.
- The team has been tackling the right unit operations for developing the overall process.
- Lots of work has been done, but progress toward the project’s goals is slow. Only the reduction in cell voltage represents a measurable movement toward overcoming the cost and efficiency barrier, even if other work lays the groundwork for doing so in the future. Slow progress is not unexpected for such technology, due to the complex process involving layers of transient heat management in a corrosive environment that creates many materials challenges. This is not an easy technology to develop, and industry experience would suggest that costs will go up as details of the requirements become better known.

- Some improvements were made in the electrolytic step, but this process is still inefficient (the reviewer's calculations indicate about 14% efficiency for the electrolyzer). This project is using a molten salt for thermal storage that typically operates around 600°C, which is not hot enough for the high-temperature reactions. Some H2A analysis was reported, but the researchers' assumptions were not clear, making it difficult to comment on the H2A projections. The main cost reductions seem to be in the heliostat improvements.
- The specific progress toward achieving project metrics has not been clearly evaluated. Specifying a percentage of completion of a task is not an appropriate measure of progress. The work with TIAX on ASPEN (modeling software, computer code for process analysis) models and H2A modeling is a key step. It is good that the researchers have worked the modeling to a cost estimate.
- The ammonium-sulfate/potassium-pyrosulfate chemistry that provides, with increasing temperatures, the ammonia and sulfur trioxide (SO_3) products respectively still seems to be poorly understood and defined. The reviewer wants to know why (as stated on slide 14) the extent of reaction is limited to the production of only one mole of SO_3. The reviewer wants to know if there is the possibility of producing mixtures of ammonia and SO_3 at intermediate temperatures, and to what extent the thermodynamics (Delta H and Delta G data) of the inherent reactions have been estimated. Very little was said on the SO_3 decomposition process. The reviewer asks if it is purely thermal (requiring extremely high temperatures) or catalyzed. Although the possibility of an electrolytic over-reduction of sulfur species was mentioned, no data was presented relating to a potential crossover of such species through the membrane.

Question 4: Collaboration and coordination with other institutions

This project was rated **3.3** for its collaboration and coordination.

- Collaborations appear to be both appropriate and well coordinated.
- The presentation clearly described the roles of other partners and it seems like the results are being incorporated into the overall project from the various partners.
- This project has well rounded input from partners, covering science to systems integration.
- There appears to be a very good level of collaboration with various partners.
- Little was said on the division of work; however, the team appears appropriate and coordinated.
- There is good collaboration with project subcontractors, but no other listed collaborations outside of the project team.
- This project has a team that can do different aspects of the work.

Question 5: Proposed future work

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

- The initiation of durability testing will be very important. The team is focused in the right area of electrolysis efficiency and reliability, but the project still needs more explanation of the advantages of this technology in relation to the other options.
- The proposed future work is reasonable, but there needs to be more emphasis on understanding and quantifying (in terms of both thermodynamics and kinetics) the basic chemistry of the process.
- The focus should be kept on the sub-cycles with the highest technical risk.
- With H2A in hand (and with a realistic interpretation of the same), it is apparent that significant breakthroughs are required for this to have even a remote chance of being relevant. The proposed future work is incremental and unlikely to provide such breakthroughs.
- The future work plans seem to address the key problems of thermal energy storage and reduction of electrolyzer over potential.
- The plans lack detail but are generally appropriate for achieving the project's goals.
- The team is going to resume work on the electrolysis and regeneration portions of the cycle. The researchers will also work on their process and economics analysis.

Project strengths:

- A good project team, good characterization tools, and access to modeling capabilities are all strengths of this project.
- This approach is complementary to the other thermochemical cycles within the Production and Delivery portfolio. Lower temperatures for the sub-cycles are beneficial for materials of construction and long operation lifetime versus the very high-temperature (more than 1,200°C) thermochemical cycles.
- This project has a good team with good knowledge.
- This project has a diverse team with appropriate skills for this work.
- The cycle has been demonstrated as technically viable and a cost analysis was conducted to quantify the costs per kilogram. Hydrogen costs of approximately $4–$8/kg are high but not outrageous.
- The use by design of (molten salt) thermal energy storage systems allows for a continuous operation of the process.

Project weaknesses:

- The system's complexity and number of reactor vessels is a weakness of this project.
- The thermochemical cycle under consideration involves electrolysis, which can result in higher overall hydrogen costs. This is apparent from the H2A-derived hydrogen cost estimate. The solar thermal driven sub-cycle seems complicated, which could translate into operational issues.
- The technology has significant technical and economical challenges.
- The electrolyzer is not an efficient step and the system requires five reactions, making it extremely complex. One of the steps operates at a higher temperature than what current (or projected) thermal energy storage technologies can provide. It is not clear if the researchers will be able to operate continuously as they claim.
- The system is very complex, which raises questions of ultimate operational viability.
- The researchers need to better understand and quantify the underlying chemistry. There are some concerns about the selectivity of the separation membrane in the electrolysis cell and the possibility of a crossover of sulfur species.

Recommendations for additions/deletions to project scope:

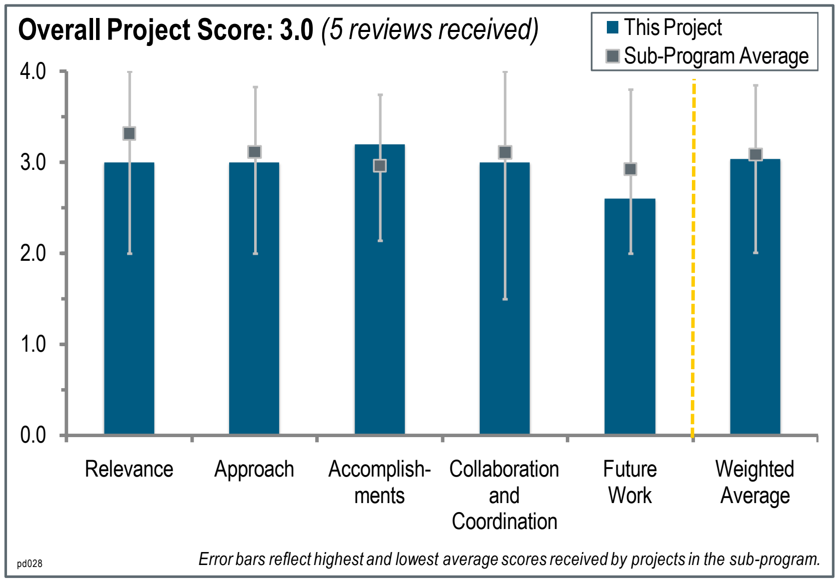
- Researchers need to clearly define in the H2A model what costs are from the heliostat and what costs are from their process. This would make it easier to understand which process improvements can reduce costs and then differentiate that cost reduction from the cost reduction in heliostats. This project's process is making electricity and then consuming it for an electrolyzer. The team should examine the cost of using that electricity for low-temperature (or high-temperature) electrolysis. The researchers should be able to use the analysis to determine the voltage (efficiency) at which they need to operate their electrolyzer so that it is superior to using the electricity for conventional water electrolysis.
- Hydrogen costs should include credit for the excess electricity generated. Although future systems will be optimized to eliminate excess electricity, the cost of an electricity credit is the best surrogate for that future optimized system. The project efficiency calculations should be clearer. The researchers cited 32% of second law, but the meaning of this is not completely clear. The team needs to diagram what energy is included. The electrolysis theoretical efficiency is stated as 0.11 V per cell, with an actual voltage of greater than 0.8 V. This suggests a very low efficiency rate. It is not clear how to reconcile the efficiency claims. To a certain extent, the efficiency of solar hydrogen generation is irrelevant if the cost per kilogram is low. However, reporting the efficiency is an important step in understanding loss mechanisms and in directing R&D efforts.

Project # PD-028: Solar-Thermal Atomic Layer Deposition Ferrite-Based Water Splitting Cycles

Al Weimer; University of Colorado

Brief Summary of Project:

The objective of this project is to develop and demonstrate robust materials for a two-step, thermochemical redox cycle that will integrate easily into a scalable solar-thermal reactor design and achieve the U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program cost targets for solar hydrogen of $3 per kilogram of hydrogen in 2017. The major project milestone is an on-sun demonstration of the hercynite cycle for a single reactor tube while monitoring product gases using mass spectrometry.



Question 1: Relevance to overall U.S. Department of Energy objectives

This project was rated **3.0** for its relevance to DOE objectives.

- Solar hydrogen production methods are very relevant to Program objectives.
- This project will develop and demonstrate robust materials for a two-step thermochemical redox cycle that will integrate easily into a scalable solar-thermal reactor design.
- In order for hydrogen to achieve its full potential as a basis for domestically sourced low greenhouse gas and other emission energy in the United States, solar energy needs to play a significant role in the production of hydrogen. New, cost-effective technology is needed for this to become possible.
- With what is currently known about economics, this technology will be hard-pressed to support Program objectives. The metal redox approaches appear to be the most attractive of the solar thermochemical hydrogen (STCH) alternatives; however, they still face the daunting obstacles that are discussed below. The economics are much further from target than the researcher claims, as the target includes compression storage delivery. Also, the Hydrogen Analysis (H2A) project sponsored by DOE, while good for comparisons, ignores the total erected cost multiplier on capital. This potentially multiplies the cost effect three times, which will dramatically increase the cost of implementing these processes, which are essentially all capital. Finally, if the cost of heliostat in all of STCH is 70%–90%, it is difficult to see how the researcher can achieve the three-fold cost improvement that is associated with the number of cycles per day.

Question 2: Approach to performing the work

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

- The comparison of experimental results for multiple active material depositions is a key approach.
- This project employs reversible, solar-thermal, water-splitting ferrite cycles.
- Over the past two years, this project has utilized and built on the knowledge gained from prior solar-based hydrogen production projects funded by DOE's Hydrogen Production and Delivery sub-program. The project is using the H2A production model to estimate the cost of hydrogen production based on the hercynite cycle being studied along with the proposed reactor and solar field design. This is providing a direction for research and has

shown that this project has the potential to achieve the DOE solar-based hydrogen costs targets. The project is currently and appropriately focused on material design for the atomic layer deposition (ALD) hercynite and substrate in order to achieve the reaction rates, temperatures, and material stability needed for the process to be economical. The project has been able to make an alumina "monolith" poor structure and use ALD to deposit hercynite on this structure. This eliminates any diffusion limitations, reduces the required reaction temperatures, and eliminates the aggregation problem with standard ferrites.
- So much of the approach has involved studying pristine advanced light source surfaces produced under unrealistic reduction conditions that it is hard be confident in the approach. There needs to be some approach that can look at materials under realistic temperatures and redox swings over thousands of cycles.
- Researchers are using a low-cost, non-toxic material, unlike the sulfur cycles in other projects. Testing operates at high temperatures, which will make thermal storage extremely difficult. The plan is to cycle every 2–12 minutes, which will result in hundreds of thousands of cycles per year. Researchers need to show that the materials can withstand the high number of cycles without degrading. The cycling tests need to replicate the rapid ramp rates. This system will not be able to constantly run, nor will it have thermal storage, causing the entire design to have to be heated up each day. The reviewer hopes the system will only need to be heated a few hundred degrees and not from room temperature. The heat-up time should be included in any calculations for production and efficiencies.

Question 3: Accomplishments and progress towards overall project and DOE goals

This project was rated **3.2** for its accomplishments and progress.

- This project has demonstrated fast kinetics for the material for a few cycles with ALD films showing higher productivity than bulk films. Adding the aluminum reduced the operating temperature and widened the window for operation. The tests ran on the materials had slow heat ramping rates. Researchers need to test the materials at the same ramping rates at which they plan on cycling. The tests resulted in highly porous alumina. The reviewer wants to know how many thermal cycles the material can withstand. This material will be packed in some reactor of some size. Researchers began to address the water issues for the system, which is excellent.
- A sound understanding of the formation of the hercynite and its stability at the temperatures of interest has been obtained. The use of the hercynite in place of standard ferrite eliminates the melting and aggregation problems with the ferrites in this proposed process. Kinetic studies have been done that show its advantages over ferrite and the other two-step metal redox hydrogen generation schemes with improved stability and sufficient reaction rates at lower temperatures. This project demonstrated the synthesis of a novel, high-surface area porous aluminum oxide (Al_2O_3) substrate, subsequent ferrite ALD coating, and hercynite thermochemical cycling to split water at 1,160°C. The H2A economic analysis is being used to guide the research and was reviewed and confirmed by an outside contractor (TIAX). The project will be testing on-sun this summer.
- The researchers are projecting a 20.8% overall conversion efficiency. There is one drawing of the scalable solar reactor, but it would be good to see supporting calculations that show the areas involved. It is not completely clear whether the window area is adequate for the target hydrogen production rate. The skeletal alumina support shows promise. Hercyanite cycle demonstrated below 1,200°C, which is encouraging as high temperatures are problematic.
- This project demonstrated the synthesis of skeletal Al_2O_3 substrate with subsequent ferrite ALD nanocoating and "hercynite" thermochemical cycling to split water at 1,160°C.
- The critical issues for this technology relate to the rapid and frequent cycling of materials and reactors in both temperature and oxidation states. Little progress has been made at addressing material or reactor suitability for these conditions. To date, the ALD redox analysis seems to suggest that the materials will decay significantly. Moving to a new material (i.e., hercynite) may be an improvement, but puts the program back at the beginning stages for materials. The reactor also has significant issues in its ability to swing in temperature. For example, it is unclear how the quenching of tubes during the water splitting step impacts the absorption of solar energy in the system. Radiative modeling may indicate that heat will shift to the cooler tubes. The reviewer wants to know how this quenching and tube cycling impacts tube durability.

Question 4: Collaboration and coordination with other institutions

This project was rated **3.0** for its collaboration and coordination.

- The partners are well integrated in the program and well recognized for the progress made.
- This project has a large team that has worked together for a long time, which enables them to make good progress.
- There is very good collaboration with experts at the National Renewable Energy Laboratory (NREL), Sandia National Laboratories, and ETH Zurich.

Question 5: Proposed future work

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

- The researchers are going to test the system on-sun, which will be a very interesting experiment. The key to achieving acceptable costs is the fast cycling of the material. The team needs to demonstrate that its materials (both active and reactor construction materials) can cycle at that rate and have acceptable durability.
- Increasing the number of redox cycles to thousands will help demonstrate the robustness of the approach and reveal weaknesses in the system.
- There needs to be a more realistic assessment of the economic prospects relative to the hydrogen threshold target. If continued, the project will need a bench-scale tool to evaluate the materials with a realistic simulation of the temperature and redox cycling over thousands of cycles.
- The only clear statement about the future work is that the project will next demonstrate the hercynite cycle in one reaction tube on-sun at the NREL High-Flux Solar Furnace (HFSF). This is very important, but it is not clear what other work is planned for this project.

Project strengths:

- This is probably the best of the STCH opportunities.
- This project has low-cost materials and a strong team that has been working together for a long time.
- This project has a much simpler cycle than proposed by others and a lower temperature (approximately 1,200°C) than other solar-to-hydrogen concepts.
- Over the past two years, this project has utilized and built on the knowledge gained in prior, solar-based hydrogen production projects funded by the Hydrogen Production and Delivery sub-program. The project is using DOE's H2A production model to estimate the cost of hydrogen production based on the hercynite cycle. This is providing the direction for the research and has shown that this project has the potential to achieve DOE solar-based hydrogen costs targets. A sound understanding of the formation of the hercynite and its stability at the temperatures of interest has been obtained. Kinetic studies have been done that show its advantages over ferrite and other two-step metal redox hydrogen generation schemes. This project has demonstrated the synthesis of a novel, high-surface Al_2O_3 substrate, subsequent ferrite ALD coating, and hercynite thermochemical cycling to split water at 1,160°C.

Project weaknesses:

- It would be helpful to include a Gantt chart with the milestones and timetable(s) for the various efforts undertaken and to measure progress. Without it, there is no indication or ability to assess how effective these efforts are and how long this project would last.
- This project's weaknesses are the economics and the absence of a realistic cyclical screening tool.
- The system is operating at very high temperatures and there is no technology currently available to store thermal energy at the desired temperatures. Therefore, there is no way to constantly operate. The system must cycle extremely fast, which will be more difficult at a large scale than what the researchers indicate.
- The cycle time is critical to the economics of this project. A compelling, clear assessment of the estimated cycle time has not been presented.

- The only clear statement about the future work is that the project will next demonstrate the hercynite cycle in one reaction tube on-sun at the NREL HFSF. This is very important, but it is not clear what other work is planned for this project.

Recommendations for additions/deletions to project scope:

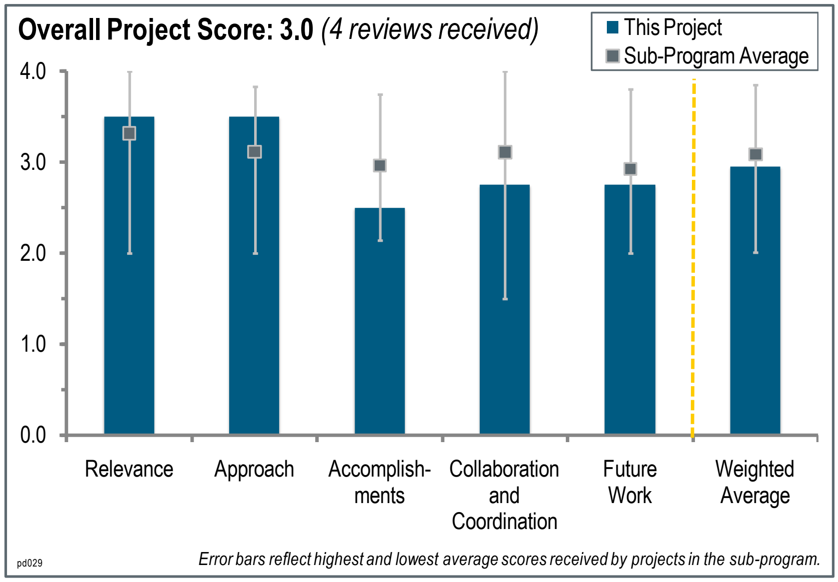
- This recommendation is for all STCH projects. The heliostats dominate the cost of hydrogen production. When presenting projected costs, researchers should separate out the heliostat costs from the other costs. This would enable an understanding of what cost reduction can be achieved by improving the materials and reactors, and what cost reduction is achieved by improving the heliostats.
- It would be good to see a more complete and clear translation of hydrogen production cycle time to total cycle time. Some of the graphs indicate a time of 60 seconds, yet the cost curves report cycle times of 2–12 minutes. A total breakdown of the cycle time would be helpful because there may be other pacing items. The reviewer would like to see a redox cycle to gauge durability and more details of the H2A analysis. The presenters only showed the results, so it would be good to see more details of the reactor modeling. It appears to be a basic concept without much or any supporting calculation.
- The future plans for this project need to be better defined.

Project # PD-029: High-Capacity, High-Pressure Electrolysis System with Renewable Power Sources

Paul Dunn; 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, which enables significant weight reduction; (3) build and test a 1/10th scale pilot plant; and (4) perform an economic assessment of a full-scale plant (300 kilograms [kg]/day, 750 kilowatts) that meets the U.S. Department of Energy's (DOE's) cost threshold.



Question 1: Relevance to overall U.S. Department of Energy objectives

This project was rated **3.5** for its relevance to DOE objectives.

- This project is highly relevant to DOE Hydrogen and Fuel Cells Program objectives.
- This project appears likely to meet the objectives of the Program in the near term.
- Reducing balance of plant energy requirements and costs contributes to the overall system performance and efficiency, including operation and maintenance costs for compressors. Taking the compressor out of the system also reduces site improvement costs and reduces the acoustic signature of the system. This is important if the systems are to be located in residential areas, as noise mitigation technology can be quite expensive.
- It is not clear if electrolysis can ever be more than a transitional technology, considering the costs of using electricity directly (e.g., in battery electric vehicles) versus converting to hydrogen and then back to electricity. However, this super-high-pressure approach is a good component of the overall portfolio.

Question 2: Approach to performing the work

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

- This project is well focused on critical barriers, of which a fair number have been identified.
- This project is well designed and sharply focused on the critical barriers.
- The researchers are very honest when identifying problems and developing solutions. High-pressure hydrogen systems present difficult technological challenges, particularly concerning the safety of the system. The focus on safety was good and the willingness to solve those issues no doubt has caused delays, but they have to be solved.
- This project is very sharply focused on the barriers being addressed. The researchers should move on from oxygen production as a value-added by-product, as that model will not work at fuel scale.

Question 3: Accomplishments and progress towards overall project and DOE goals

This project was rated **2.5** for its accomplishments and progress.

- Given the magnitude of the challenges, the researchers are making good progress in overcoming them in a careful and logical manner.
- A number of barriers have been identified and progress in addressing these has been steady but slow. Uncertainty still exists as to whether all of these barriers can be adequately addressed.
- The identification of the long dwell time due to small bubble formation was excellent. Issues related to scale-up and higher pressure operation are daunting, but it appears Avalence is making significant progress toward overcoming these barriers. There is no discussion of efficiency or the cost of hydrogen production. During the review, there was a question about the ability to reach efficiency targets. The rebuttal, "we believe we can easily achieve this efficiency," is insufficient. This reviewer recognizes that the efficiency will increase at higher temperatures (75°–80° C), but wonders by how much. The cost of hydrogen production at $3.70/kg cannot be completely offset by using a credit for research grade oxygen. In fact, large amounts of nearly pure oxygen represent a significant hazard.
- The presenter acknowledged the slow pace, which is mitigated by the very low spend rate. The value per DOE dollar is actually quite good. This is a very difficult undertaking and the progress has been significant and important. It is a little disappointing that the researchers are not running the circulating experiment at 6,500 pounds per square inch yet.

Question 4: Collaboration and coordination with other institutions

This project was rated **2.8** for its collaboration and coordination.

- The expertise found in other institutions was utilized well.
- It is obvious that there are collaborations because the cells are being sent out to be wrapped. This could be a high-functioning collaboration, but it is difficult to tell that from the presentation. Collaborations with "sister companies" are all but invisible.
- There are a limited number of partners, but coordination is good.
- The collaboration may be there, but it was not presented. It may also be that there are not many sources that can be accessed to provide that type of collaboration. Perhaps some of the high-pressure challenges could have been identified by consulting with others in advance, for example the masking of the electrodes by the effect of high pressure on the hydrogen bubbles. This reviewer asked if time has been lost in reinventing the wheel. Some of these issues and solutions could be proprietary and not readily available.

Question 5: Proposed future work

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

- The future plans build on past progress, but significant barriers remain and will be challenging to address adequately.
- A detailed project plan with timelines and milestones was not presented, so it is difficult to track the project's progress.
- The plans do not seem to take into consideration some of the concerns raised by the presenters about the impact of the circulation system on membrane support requirements or control of that circulation system pressure. These issues seem to raise development issues that should be considered in future plans.
- Avalence indicates that the nested cell remains to be fully proven—this reviewer wanted to know if there is a backup if not.

Project strengths:

- The researchers have good knowledge of the issues and logical solutions have been developed and implemented. There is an excellent emphasis on safety, and progress is being made. The world needs a high-pressure, non-compressor hydrogen production system.
- Avalence's alkaline electrolysis approach has the advantages of very dry product gases and a high-purity oxygen product.
- The technical expertise in this project is obvious.

Project weaknesses:

- It is not clear if the researchers are tapping into other sources of knowledge to solve problems.
- A number of challenging barriers still exist, and there are a limited number of partners.

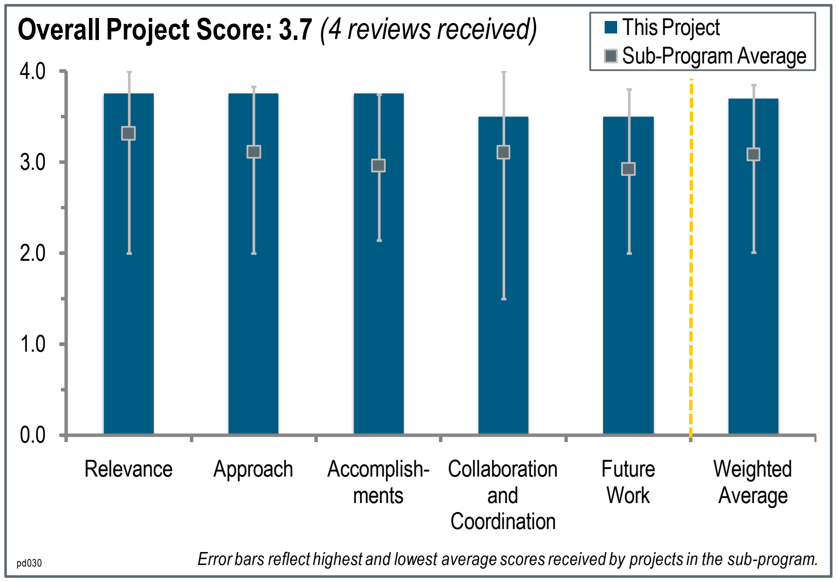
Recommendations for additions/deletions to project scope:

- This project should continue down the path as shown in slide 12 of the presentation.

Project # PD-030: PEM Electrolyzer Incorporating an Advanced Low Cost Membrane

Monjid Hamdan; Giner Electrochemical Systems, LLC

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 U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program targets for distributed electrolysis by: (1) developing a high-efficiency, low-cost membrane; (2) developing a long-life cell separator; (3) developing a low-cost prototype electrolyzer stack and system; and (4) demonstrating a prototype electrolyzer system at the National Renewable Energy Laboratory (NREL). Objectives for fiscal years (FY) 2010–2011 were to: fabricate scaled-up stack components (dimensionally stable membrane [DSM], cell-separators); assemble the electrolyzer stack/system; install the electrolyzer stack into the system and evaluate it; and deliver and demonstrate the prototype electrolyzer system at NREL.

Question 1: Relevance to overall U.S. Department of Energy objectives

This project was rated **3.8** for its relevance to DOE objectives.

- This project has exceeded Program goals for electrolyzer capital cost and efficiency.
- This project is very relevant to DOE's objectives with major efforts directed toward cost reduction and improved durability, which has the potential for major lifetime improvements and cost reductions. Progress in other areas is also good.
- This project is on target to meet DOE's objectives. The Giner Electrochemical Systems' (GES) electrolyzer efficiency is reported as 75% (lower heating value [LHV]), whereas DOE's 2017 target is 74% (LHV). The GES hydrogen production cost, based on the Hydrogen Analysis (H2A) model revision 2.1.1, was $4.66/kilogram (kg) in 2011 and $4.95/kg in 2010. GES identified changes in the membrane, separator, and stack and system components to obtain these cost reductions. The dome technology is a good approach to moderate pressure operation, but it may not be appropriate for large-scale operation.
- It is not clear whether electrolysis can ever be more than a transitional technology, considering the costs of using electricity directly (in battery electric vehicles) versus converting to hydrogen and then back to electricity.

Question 2: Approach to performing the work

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

- Designing for manufacturing by teaming with volume manufacturers is an excellent approach because they become part of the solution.
- This project has a very sharp focus on reducing cost and on the breadth of features needed to be addressed to do so.
- This project is very well designed with an appropriate focus on integrated tasks among appropriate team members.

- The identified barriers were addressed successfully, along with the quest for less costly and better performing materials. Improvements in the catalyst/membrane, separators, and stack components resulted in hydrogen production costs from $4.95/kg to $4.66/kg. These costs are higher than the $3.64/kg reported by Proton Energy Systems in 2010. If the comparison is legitimate, GES costs could be reduced further by implementing cost-reducing technology from Proton.

Question 3: Accomplishments and progress towards overall project and DOE goals

This project was rated **3.8** for its accomplishments and progress.

- This project has exceeded DOE's goals for efficiency and capital cost. Long-duration testing cannot be shortened when the goal is to determine the durability of the system components.
- The researchers gave an excellent and detailed talk that described how costs are being reduced. Progress seems to occur mostly in the cell structure area (e.g., part count). The "electrochemical" progress seems somewhat incremental as the project moves to chemically-etched dimensionally stable membrane (C-DSM), which may be a lot less costly, but does not seem to be quite as outstanding as the laser-drilled dimensionally stable membrane (L-DSM).
- The most significant progress has been accomplished with DSM cost reduction and separator durability.
- Sufficient details on the experimental work provided understanding and credibility to the preliminary conclusions of this project. The objectives for this project in 2010 were the development of high-efficiency, low-cost membranes; a long-life cell separator; and a lower-cost prototype electrolyzer stack and system. This work continued in 2011. The development of the safety manuals and failure modes and effects analysis probably took an inordinate amount of time. It is interesting that the dome design can accommodate a less-than-90 cell stack while satisfying codes pertinent to hydrogen refueling systems. The cost analysis indicates that a compressor is used to compress the hydrogen from 333 pound(s) per square inch gauge (psig) to 6,250 psig, which is the goal for centralized production. Distributed production requires more moderate pressures, so there is some confusion. The H2A model provides for economies of scale.

Question 4: Collaboration and coordination with other institutions

This project was rated **3.5** for its collaboration and coordination.

- There is excellent collaboration with the team, a good mix of industrial and academic partners, and eventual real-world testing.
- The expertise of the various collaborators is well utilized.
- There is a good mix of academic and business partners, which are very accomplished and credible, such as 3M, Parker, and Entegris.
- While the collaboration with 3M was identified, few other partnerships were highlighted in the talk, although the others were mentioned.

Question 5: Proposed future work

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

- It looks like the final system is progressing well and this reviewer is looking forward to seeing the results of the NREL test phase.
- This project is well focused on objectives.
- The future work is focused on eventual system testing under real-world conditions.
- The future plans address overcoming the technical barriers for small-scale, relatively low-pressure operation. However, there are no potential breakthroughs envisioned.

Project strengths:

- This project achieves cost-reductions by designing manufacturing with high-volume manufacturing industry partners and thorough durability testing to identify the best materials.
- There is an appropriate focus on cost reductions, durability improvements, and system fabrication and testing.
- Significant progress was made by building on the work done in 2010.

Project weaknesses:

- There were no project weaknesses detected.
- There are no significant project weaknesses.
- The coordination of activities at Proton and GES should lead to a shorter timeline, as they have complementary skills; however, this is unlikely to happen because they are competitors.

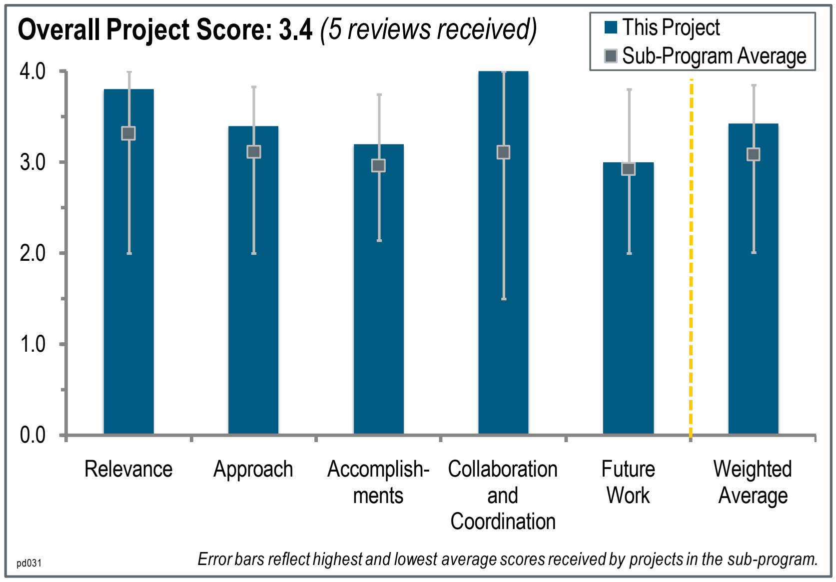
Recommendations for additions/deletions to project scope:

[No comments were made by any of the reviewers.]

Project # PD-031: 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 U.S. Department of Energy (DOE)-awarded projects; and (8) test electrolyzer stack and system response with typical renewable power profiles.

Question 1: Relevance to overall U.S. Department of Energy objectives

This project was rated **3.8** for its relevance to DOE objectives.

- This project is highly relevant to the goals and objectives of the DOE Hydrogen and Fuel Cells Program, as testing hardware under real-world conditions is a critical aspect of technology advancement.
- This project is very relevant to the Program objectives.
- The project aims to demonstrate the integration of renewable sources with electrolyzers for hydrogen production. It is very relevant to the objectives of the Program.
- Utilizing intermittent renewables, such as wind and solar, with electrolysis supports the increased capture of renewable energy sources, thus capturing primary power that would otherwise be wasted. This supports major reductions in the cost of hydrogen. This is important for "selling" hydrogen production to the electric utilities because it demonstrates the viable value propositions that they may not be aware of. Investigating the performance of electrolyzers coupled with real-world intermittent power generation is the final step in overall system validation and is very important. This project also identifies system interface issues.
- This project has good value in terms of exploring power electronics issues and generating public data on electrolyzer performance. It is less clear if the project's focus on direct coupling of a wind or solar resource with hydrogen electrolysis is an effective or valuable option.

Question 2: Approach to performing the work

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

- This project's approach is outstanding and addresses a good mix of issues, including capital cost, efficiency, and renewable energy source integration. This project sharply focused on all of these technology implementation barriers.
- The testing and engineering of renewable electrolyzer integrated system development, followed by industry participation in hardware and component input, is the right approach.

- This project has a good mix of model development coupled with actual hardware testing for validation. This is the correct way to develop and evaluate new hardware and control systems. Standardized test procedures are important for proper comparison of new systems against a common baseline. This is a good strategy for using National Renewable Energy Laboratory resources to conduct independent, third-party testing of DOE-funded electrolyzer development projects. The stack testing approach is providing valuable data on system operating strategies.
- The approach to reach the project's objectives is excellent, but this reviewer is skeptical that this project will be effective at addressing barriers.
- The approach consists of evaluating the field integration of renewable power sources with industrial electrolyzers and will provide valuable data to identify key parameters, improve systems, and give a realistic estimation of hydrogen cost.

Question 3: Accomplishments and progress towards overall project and DOE goals

This project was rated **3.2** for its accomplishments and progress.

- This project's progress has been significant, especially in the testing area. This testing is very valuable for technology advancement and will help guide future efforts.
- The results of the 2,000 hours of operation in stack decay testing are significant. In addition, the steady-state and the varying wind profiles work is important.
- The project has shown good progress in several areas—including long duration operation of polymer electrolyte membrane (PEM) and alkaline stacks, and comparison and understanding of the direct coupling of photovoltaic arrays versus power converters—that provide useful insights for future integrated system designs.
- The tests have yielded interesting results and may have identified areas for further technical investigation in improving durability. Research on direct versus inverter coupling is producing valuable insights leading to potential operational strategies and balance of system improvements. In reference to slides 16 and 17, it is unclear what the hydrogen fueling system adds to this project. This was highlighted last year and seems to have been ignored.
- This project's accomplishments are good, but progress toward overcoming barriers is only fair because this project is only weakly configured to address barriers. The most relevant discoveries were observations about where power converters have losses.

Question 4: Collaboration and coordination with other institutions

This project was rated **4.0** for its collaboration and coordination.

- The team has excellent collaboration at various levels (e.g., electrolyzer manufacturers, utilities, research centers, international agencies), which facilitates information sharing and accelerates the development of renewable electrolysis systems.
- This project has very closely integrated collaboration with electrolyzer developers and the utility industry. This is important for both providing relevant technical feedback to electrolyzer manufacturers by testing their devices under real-world operational conditions and exposing the utilities to the potential for hydrogen production from under-utilized resources.
- By nature, this is a very collaborative and well coordinated program. It would have been helpful to see comments from electrolyzer manufacturers about their expectations with respect to variable current results. It seems like there is a lot of data that was being reported with very few conclusions drawn.
- This project contains active and informal partnerships with industry, academia, and domestic and international researchers. These partnerships are well coordinated.
- Key players including wind-power utilities, electrolyzer vendors, and academia are represented. Industry involvement in the system integration and component development effort is very strong.

Question 5: Proposed future work

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

- This project's progress has been significant, especially in the testing area. This testing is invaluable for technology advancement and will help guide future efforts.
- The results of the 2,000 hours of operation of stack decay testing are significant. In addition, the steady-state and varying wind profile work is important.
- The various tasks of the future work are clear. They include a comparison of PEM and alkaline electrolyzers receiving current based on varying wind profiles. They will also provide interesting results on the management of the fluctuating power in order to increase the durability of electrolyzers. However, appropriate criteria have to be well defined to establish this comparison. The task of integrating a fuel cell is helpful if it clarifies the interest of such integrated energy systems in terms of system efficiency (e.g., power sold or not to the grid).
- Continued, independent third-party testing under real-world operating conditions provides important feedback to the Program and equipment developers.
- This is a good project with a good plan, but not a high likelihood of major progress on barriers.
- Progress has been significant, especially in the testing area. This testing is invaluable for technology advancement and will help guide future efforts.
- It sounds like the bulk of the project team's efforts are on the wind integration work, with less effort on the solar side.

Project strengths:

- Renewable hydrogen production is the key to boosting the hydrogen energy markets. The project, which has an overall system evaluation approach, will demonstrate the viability of an electrolyzer coupled with renewable sources.
- This project has excellent integration of real-world intermittent renewable resources with new electrolyzers. It identifies operating strategies and evaluates balance of system improvements. The modeling is very important for attracting utility interest in hydrogen production.
- This project has a great infrastructure and environment for the testing being performed.
- This project offers a good mix of addressing capital cost, efficiency, and renewable energy source integration. Test efforts are extremely valuable in guiding technology advancements in the industry.
- The experimental testing on fuel cell stacks is a strength of this project.

Project weaknesses:

- The reviewer did not identify any weaknesses in this project.
- The project does not mention the similar works underway in European countries. It will be interesting to have a benchmark.
- The distance from true barriers, which are in the hands of manufacturers, is a weakness of this project.
- The project team did not adequately address cost as one of the stated barriers.

Recommendations for additions/deletions to project scope:

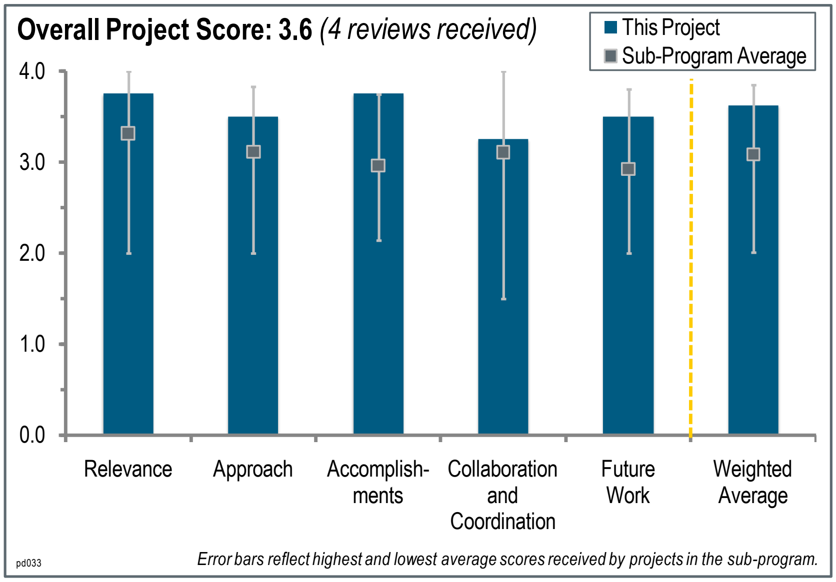
- This testing is important for the technology area, so the project has to be continued. It needs to focus on wind profile and long duration testing, and define appropriate criteria to have a realistic comparison of technologies. This integrated system evaluation should provide guidelines on key parameters to optimize electrolyzers, thus it is recommended to have a good understanding of performance losses. Based on the improvements, the project needs also to provide an updated hydrogen production cost.
- The Hydrogen Production and Delivery sub-program should be looking toward scaling up to multi-megawatt, utility-scale hydrogen production and should start working toward that now. This project should remove the hydrogen fueling component, as it is not relevant to this topic area. This aspect was identified last year and was not acted on.
- The project could be expanded even more to fund further tests, as these results provide such a significant value.
- It may be more efficient and productive for the project to narrow its scope to focus on wind-integrated electrolyzers only. The second and smaller effort on solar integrated work is not that unique and may be a distraction.

Project # PD-033: Nano-Architectures for Third-Generation PEC Devices: A Study of MoS_2, Fundamental Investigations, and Applied Research

Thomas Jaramillo; Stanford University/National Renewable Energy Laboratory

Brief Summary of Project:

The main objective of the project is to develop new photoelectrode materials systems based on quantum-confined molybdenum disulfide (MoS_2) nanocatalysts coupled to mesoporous conductive transparent support scaffolds that can potentially meet the U.S. Department of Energy's (DOE) Hydrogen and Fuel Cells Program 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 U.S. Department of Energy objectives

This project was rated **3.8** for its relevance to DOE objectives.

- This project has some potential technical benefits for DOE in the areas of hydrogen production and delivery. Photoelectrochemical (PEC) hydrogen production technology with nano-architectures could potential assist with DOE's technical milestones.
- This research is appropriately targeted to develop materials to meet DOE's guidelines for PEC production.
- This project has honestly and legitimately placed PEC hydrogen in the long-term section of the technological time scale.
- As a long-term technology, direct PEC fuel production is an important part of DOE's portfolio. However, to date, work has focused on electrochemical efficiency and not the overall system as it relates to gas drying, separation, and compression to a useable pressure. This is the first project that looks at the more practical aspects, such as how the balance of plant would be configured to enable a practical device. As this work begins, partnering these groups with companies that have already done this work would be much more cost effective than re-inventing the wheel.

Question 2: Approach to performing the work

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

- The research into the bandgap engineering of MoS2, with a particular focus on the catalytic behavior for hydrogen evolution, is an extremely viable approach for meeting DOE's metrics for PEC production. The proficiency for novel materials fabrication and evaluation was exceptional.
- This project is trying to exploit nanoparticle science to accrue benefits of surface area and catalytic activity.
- The technology barriers in this project are very challenging. They might be overcome over time by evaluating different materials, nanostructures, and techniques; however, the feasibility of a proposed technology to meet DOE's needs at a large scale was not identified.
- The scale of the analysis should be explicitly clarified in the analysis. The presenter was very clear that the model is for 1,000-kilogram-per-day (kg/day) production or greater, and that these reactor types only make sense at that scale. However, that was glossed over in the presentation. In addition, the costs claimed for water

electrolysis were incorrect and misleading. Commercial electrolysis units sold today produce hydrogen at approximately \$9/kg for total lifecycle costs (even at low commercial volumes), including electricity costs, maintenance, taxes, depreciation, and inflation. The initial capital cost for these units amortized over the life of the unit is less than \$1.50/kg, not the \$10/kg stated.

Question 3: Accomplishments and progress towards overall project and DOE goals

This project was rated **3.8** for its accomplishments and progress.

- This project has excellent materials science research with control over compounds and characterization of products. It includes novel research into different types of morphologies and how to make them. For both photovoltaic (PV) and PEC, these materials are the key to understanding the fundamentals of how to design the best structures for these applications.
- Very good results were presented on the MoS2 system. The facile nature of the hydrogen evolution reaction (HER) for this system is a very important criterion. It is a non-starter that must be able to receive charges across the semi-conductor/electrolyte interface from any PEC material with low losses. The presentation clearly showed that MoS2 was extremely viable as a catalyst for the HER reaction. The identification of the edge sites as the active site was very interesting; it would be good to see further treatment of the surface to enhance the density of active sites. This reviewer is curious to learn more about the molybdenum trioxide/MoS2/electrolyte interface and the band bending within.
- The hydrogen catalytic activity of nano-MoS2 is very impressive. Multi-deposited transparent conductive oxide substrate appears to be a clever, yet relatively easy, way to advance PEC hydrogen technology.

Question 4: Collaboration and coordination with other institutions

This project was rated **3.3** for its collaboration and coordination.

- The collaborative effort among the PEC Working Group is clear. However, at this point, it would be good to introduce an electrolyzer company and the industrial gas companies at least as technical advisors on the balance of system aspects. Researchers of hydrogen production should be working together to figure out what technology makes sense for what application (e.g., home fueling versus backup power versus grid/renewable buffering), rather than competing “against” each other.
- The primary collaboration cited enabled the combination of two materials classes. This reviewer would like to see more intensive collaborations with the characterization and modeling communities, as these will facilitate a more complete understanding of MoS2 as a PEC material.

Question 5: Proposed future work

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

- The proposed future work focuses on identifying advanced new materials with higher surface areas, lower charge-transport limitations, and unique nanostructures.
- The future work appears to be focused on combining the catalyst work with the support work, which is appropriate. If the MoS2 is showing better catalytic behavior than PEC conversion, it might be appropriate to look at these catalysts as purely electrochemical applications as well.
- This project has targeted ideas toward future experiments. Researchers should continue to focus on a photo-active catalyst for the HER.
- The project has achieved improvements in component materials and is looking forward.

Project strengths:

- The presented study shows a solid research program and evaluates different materials, nanostructures, and PEC substrates to meet the Program’s hydrogen production and delivery goals.

- This project has strong synthesis and characterization capabilities and knowledge of the critical parameters in solar energy conversion efficiency.
- The principal investigator (PI) has a very good understanding of how to synthesize these exotic materials. There appears to be a fairly good rate of progress from materials conceptualization to fabrication, characterization, and understanding.
- This project has breathed new life into the long-standing cadre of photocathode materials.

Project weaknesses:

- The questions that need to be asked and answered regarding PEC technology include how feasible the technology is, and whether it is scalable, especially in a large footprint (i.e., 10 tons per day, translated to 140 acres of PV fields, which requires 289,950 cells). The economic study proposed $450 per square meter for 20-year lifetime PEC cells, based on future material that has not yet been evaluated or developed.
- This project does not have a good understanding of the state of other hydrogen generation technologies.
- This reviewer believes there needs to be validation that these nanostructures are effective in sweeping and extracting carriers. For example, a nanoparticle sitting on an indium tin oxide scaffold would probably cause the majority carrier to diffuse to the center of the particle where the carrier density would build and then drive the process toward recombination.
- This project looked at all kinds of microstructures and fabrication methods. The reviewer suggests that an industrial partner monitor the project and advise the researchers on the cost aspects of the various approaches.

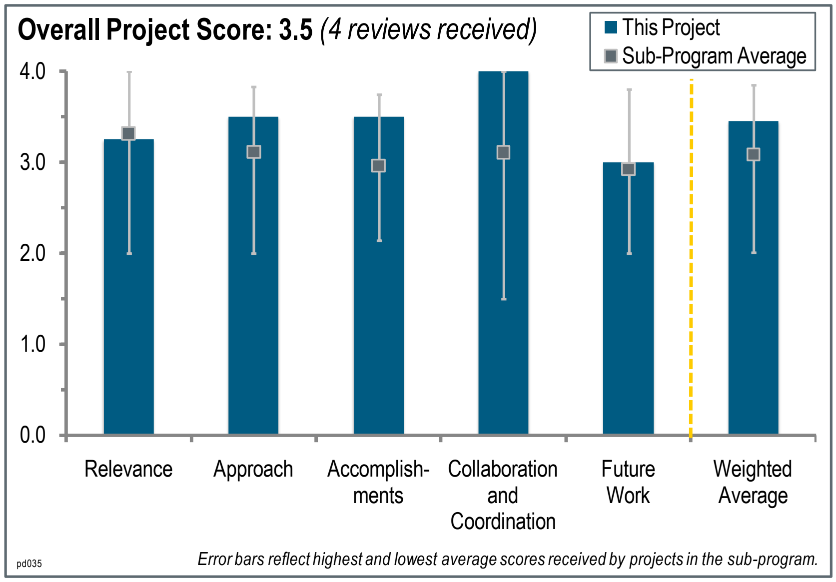
Recommendations for additions/deletions to project scope:

- Researchers should see the above recommendations for guidance on interactions with additional collaborators.
- The reviewer would be interested to see the PI work on the anode as well, but believes he has plenty to do with the hydrogen electrode.

Project # PD-035: 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) achieves 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 of stability under solar conditions; and (4) adapts to volume manufacturing techniques. The main focus of the work this past year has been to develop and optimize state-of-the-art materials that have been identified as promising for meeting the U.S. Department of Energy's (DOE) near-term efficiency and durability targets.

Question 1: Relevance to overall U.S. Department of Energy objectives

This project was rated **3.3** for its relevance to DOE objectives.

- This project has a very good statement of objectives that is unusually clear and contains specific metrics.
- The tasks undertaken by this project are consistent with the overall collaborative plan of the Photoelectrochemical (PEC) Working Group, and reflect specific facilities and capabilities essential to execute the effort.
- The National Renewable Energy Laboratory (NREL) project is quite expansive, and overall does a good job of pushing the technology forward to enable the DOE metrics for hydrogen production. Of particular relevance is the development of the PEC standards.
- Alignment with the Hydrogen Production sub-program is good, but could be better articulated within the broader scheme of the DOE Hydrogen and Fuel Cells Program. The temptation is to simply prove that this method is better than photovoltaic electrolysis.

Question 2: Approach to performing the work

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

- The project approach is outstanding, but there are insufficient resources to execute all of its critical elements. The decision to seek material-durability solutions for the best-performing PEC material is probably the right decision. However, the search for alternative materials suffers throughout the integrated PEC project, as researchers are seeking incremental improvements to existing materials that offer performances that will likely continue to be inadequate. As a consequence of this, a fallback material option has yet to be found. The use of theoretical teams to help understand performance issues of existing materials is a definite improvement over earlier "hit-or-miss" approaches, but progress could be accelerated by a small team of chemists and materials experts in much closer collaboration with the theoretical teams. Such an approach could both establish the general underlying materials characteristics enabling PEC performance and formulate a plan for how those characteristics could rapidly be discovered through modeling and simulation of different materials combinations. Articulation of such a general materials science effort might allow for the integration of current

PEC capabilities with much larger capabilities and efforts throughout the DOE's portfolio of sponsored research and development. These comments are meant to encourage the DOE to emulate the highly successful PEC Working Group approach through integration of and collaboration among similar resources and capabilities throughout the Program to accelerate progress in resolution of technology and knowledge barriers common to many essential research and development (R&D) efforts.
- This team is well integrated and divided the project tasks in a logical manner.
- The NREL group is a leader in tying together many of these PEC efforts. The combination of their individual effort along with guidance and support for the collaborators within the PEC Working Group is a viable approach. However, in some ways it seems that the effort could be more focused.
- A lot of work is proposed, and only a little bit of work has been done on a lot of things.

Question 3: Accomplishments and progress towards overall project and DOE goals

This project was rated **3.5** for its accomplishments and progress.

- Establishing benchmarking and characterization facilities for general PEC support is an outstanding accomplishment. Hopefully this achievement will discourage redundant, nonessential investments at other institutions. Typically it is always notable to report new performance records concerning the use of the ruthenium oxide (RuO2) counter electrode; however, such performance improvements could be irrelevant if adequate material durability is not achieved. One could question the priority of record performance investment over material durability investment. The reported improvement in durability of III-V materials through surface nitrogen incorporation was not quantified in the presentation, so it is impossible to determine if this approach is viable. The reported degradation in performance by bulk nitrogen in these materials was not quantified, nor was the degradation in performance due to surface nitrogen. In light of this, it is not possible to judge the viability of nitrogen for durability improvement in III-V materials. No obvious pathway has been shown for continuing the amorphous silicon (a-Si)/amorphous silicon carbide (aSiC) material R&D. Cheap fabrication methods will not supplant the need for greater than 10% solar-to-hydrogen (STH). A pathway needs to be articulated or development and characterization of this material should be terminated. The use of density functional theory (DFT) modeling to explain the performance degradation of copper aluminum telluride by oxygen contamination is an outstanding example of good scientific work by the theory and characterization teams. However, there are still too many binary candidates and innumerable ternary and quaternary candidates for serial testing or even serial theoretical evaluation. A new approach to winnowing the possible candidates to a set of promising candidates is required. One approach might be to assign this duty to a small team of chemical, materials, and theoretical experts with the task of developing an approach to reduce the number of candidate materials for a more detailed study.
- There are many facets to this project, and this reviewer organized comments into three distinct areas:
  1. NREL's champion material remains the gallium indium phosphide ($GaInP_2$)/gallium arsenic (GaAs) tandem, with the effort focused on eliminating the corrosion issue. Collaborating with the Ogitsu and Heske groups to help identify the mechanisms for corrosion is a solid approach. Within the framework of the collaboration, knowledge is being gained regarding the mechanisms by which the material corrodes.
  2. Oxide materials/DFT modeling: Although there appears to be quality modeling to identify new potential materials as well as the capability to develop new material classes, there does not appear to be a closing of the loop where models are married to the experimental results of synthesized materials.
  3. The PEC standards group is an important initiative to help focus resources and benefit future go/no-go decisions. This is a key accomplishment for the PEC group and it is long overdue.
- NREL has a sizeable capability and investment in GaAs/GaInP2 and seems reluctant to let go of it. It may be time to stop experimenting with water and move on to something else. The various surface treatments will not improve durability that much. If the researchers are going to stay with this approach, they should look to encapsulation in the same way that other groups are putting indium tin oxide on a-Si. Making a better dark anode is a legitimate strategy; however, it is unclear whether the researchers actually measured 16.3% or think they can reach it. The DFT calculations are interesting, but with all the copper-indium-gallium-diselenide-like components and proportions possible, there could be an incalculable amount of combination. This reviewer asked if there is some way to formulate general trends and head in that direction. NREL is properly exercising its position in the PEC community to do the standards task.

- This project demonstrated 16.3% STH conversion efficiency on GaInP2, but durability is still an issue. Ion bombardment nitridation led to reductions in corrosion rates. Why this works is not clear. New materials were identified that demonstrated 1.6% STH with a potential growth to 3%–5%. This does not meet targets, but is a promising system for production using low-cost, high-volume methods.

Question 4: Collaboration and coordination with other institutions

This project was rated **4.0** for its collaboration and coordination.

- The NREL group does a very good job of interacting and collaborating with members of the PEC Working Group. There appears to be ongoing collaborations across all areas of technologies with every member of the PEC Working Group, including synthesis, characterizations, and modeling.
- This is a well coordinated and integrated team.
- There is ample mention of the group's collaboration with many organizations. It is clear that it is really helping some of the other groups.
- This project reflects exceptional collaboration among the members of the Photoelectrochemical (PEC) Working Group. The PEC Working Group is open to all participants in the DOE Hydrogen and Fuel Cells Program who undertake R&D in the technology areas essential to the successful examination of cost-effective hydrogen production through inorganic PEC water splitting. The PEC Working Group is a model for collaborative effort that should be emulated throughout the Program.

Question 5: Proposed future work

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

- This project has lots of work to keep the researchers busy if the funding holds up.
- The proposed future work tends to be a bit scattershot. There is a list of various efforts that will provide incremental continuation for the advancement of the technology. However, as stated in the summary slide, this project is "not going to meet DOE technical targets with slight modifications of the usual (oxide) suspects."
- The planned work is appropriate, but insufficient effort is devoted to the methodology to be used in identifying a small set of promising materials for detailed investigation.

Project strengths:

- The NREL effort does a good job of tying together the many varied efforts in PEC. The establishment of standards is an important step in creating a viable technology.
- This project is an ambitious, well constructed program focused on finding a fundamentally new material system for PEC.
- This is a collaborative effort. Its use of the various skills and facilities throughout the PEC Working Group is outstanding and provides an exemplary performance for DOE. The project planning within the available resources, communication of the challenges and achievements within the group, and technical skills and dedication of the Working Group researchers have been outstanding.
- The researchers are reasonably exercising their leadership role in PEC hydrogen production. The reviewer cannot imagine a PEC program without them.

Project weaknesses:

- It would be helpful to see a clear delineation between the efforts championed by NREL and those in support of other collaborators. For example, a principal advancement of the GaInP2/GaAs effort was attributed to RuO2. This reviewer wondered if the improved electrode for the oxygen evolution reaction was a result of an NREL effort, from the electrolyzer community, or simply an off-the-shelf component that had not been used before. The reviewer would also question whether there is a viable path forward for the III/V semiconductor material class. These materials are quite expensive and are difficult to process defect-free. It is understood that a viable material needs to be fabricated first before costs are a concern. However, the reviewer does not think there is a viable way to produce the large areas required for a cost compatible with DOE's objectives.

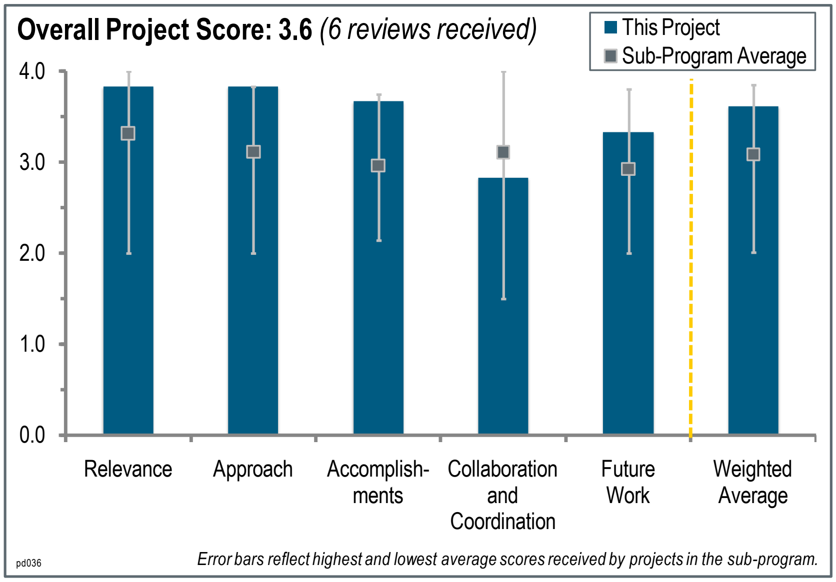
- This project could further justify its calculations by making and testing some of the new materials that appear to have promise.
- The magnitude of this project exceeds the available resources for timely progress. The persistent lack of a capable PEC material should encourage the dedication of some efforts by the project and by DOE to discovering a new approach to identify candidate materials for rapid screening and investigation.

Recommendations for additions/deletions to project scope:

- The conversion efficiency of all of these systems is limited by their bandgap. Consequently, a maximum theoretical efficiency calculation is possible. This value should be stated for all materials under consideration because it explains why the titanium dioxide (anatase) system can never attain the performance of a gallium system.
- This project should add resources for the establishment of a small group of chemical, materials, and theoretical experts to explore a better way to identify promising candidates for screening and study.

Project # PD-036: 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 used in 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 U.S. Department of Energy objectives

This project was rated **3.8** for its relevance to U.S. Department of Energy (DOE) objectives.

- Low light saturation of photosynthesis is one of the major barriers limiting hydrogen photoproduction yields in algal cultures. This project is trying to overcome this barrier and increase the sunlight utilization efficiency in mass algal cultures. Therefore, it is highly relevant to overall DOE Hydrogen and Fuel Cells Program objectives.
- This project is relevant to the Hydrogen Production sub-program element and provides an excellent tool for developing microorganisms with optimized and sustainable photobiological hydrogen production. While understanding the genetic determinants behind antenna size in Chlamydomonas could be directed toward fundamental research, the principal investigator (PI) has done an excellent job of focusing the project on application and not on increasing basic knowledge of antenna structure and function.
- This project has made good progress toward the declared goal of reducing chlorophyll antenna size in the biophotolytic alga Chlamydomonas. This goal arises from one strategy for overcoming the problem that biophotolytic hydrogen production saturates at lower light intensity in this alga than photosynthesis itself. The results also demonstrate that there are multiple genes of partially overlapping function that can be inactivated to achieve the stated objective. This latter finding is not surprising, but is significant in that an algal strain bearing multiple mutations is likely to have greater genetic stability in a practical application where strains with better growth (larger antenna) are likely to be under strong positive selection.
- This project is relevant for the Program, and directly addresses the objectives and barriers for the Program laid out in the multi-year research and development plans. This project is addressing and helping to overcome the critical barriers of photobiological hydrogen production.
- Improving the efficiency of photosynthetic hydrogen producing algae is very relevant to the Program's photosynthetic biological production pathway.
- The PI has been a leading proponent of reducing the antenna size of the photosynthetic apparatus in algae with the goal of increasing the efficiency of photon capture. This work is broadly relevant to any envisioned process using algae to produce energy-rich compounds of any sort.

Question 2: Approach to performing the work

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

- The research team used very efficient molecular and biophysical approaches to generating and screening for the mutations associated with low chlorophyll antenna size. As a result, the project demonstrated outstanding step-by-step progress and finally resulted in the truncated antenna mutant (Tla3) with approximately 150 chlorophyll molecules for both PSII and PSI. It is important that the antenna size in the tla3 strain is close to the theoretical size limit of 132 chlorophyll molecules (37 chlorophyll molecules for PSII and 95 for PSI), and that this mutant was obtained significantly earlier than originally planned in the project. However, the research team used the arginine-dependent strain for generating these mutants, which makes their physiological comparison with the parental strain almost impossible, especially under high light conditions and in the absence of arginine.
- This project is clearly focused and targeted. Experimental methods are appropriate for identifying Tla genes, regulating antenna size, and assaying the effects of truncated antenna size.
- The approach uses the advantage of established methods of genetic modification and screening in Chlamydomonas and combines it with the PI’s technical strength in measuring chlorophyll/reaction-center ratios.
- The PI has been using relatively straightforward mutant generation, screening, and characterization processes that, to date, have yielded encouraging, if not impressive findings. The use of the word “straightforward” is not meant to trivialize the cleverness of the PI's approaches, especially in characterizing the mutants he has generated.
- The reasonable and logical approach of this project has been validated by the positive results and publication record over the years. This project was worth the investment.
- This project adopted the Program targets and met them ahead of schedule.

Question 3: Accomplishments and progress towards overall project and DOE goals

This project was rated **3.7** for its accomplishments and progress.

- This project has not only met and exceeded its milestones, it has produced and will continue to produce several peer reviewed publications that will share this work with others in the field and encourage more work in this area.
- This project very successfully exceeded the Program target for 2015, eight years early.
- This project has made outstanding progress due, no doubt, to the hard work of the PI and his students and team members. More importantly, the PI has been guided by a sound hypothesis that informs his choices, making the probability of success much greater. As evidence of the progress made by the PI, several companies have adopted his technology.
- The PI has made excellent progress identifying and characterizing the three genes involved in regulating chlorophyll antenna size. The presented data suggests that excellent progress has also been made in reaching the targets for chlorophyll antenna size. Experiments in the model system suggest that this approach could serve as an effective mechanism to enhance the efficiency of solar energy capture and utilization, leading to possible increases in photobiological hydrogen production as well as biomass.
- This project resulted in the identification of the three different genes (Tla1, Tla2, and Tla3) responsible for the regulation of the chlorophyll antenna size. Two of these genes (Tla1 and Tla2) were fully characterized. As a result, the project sheds some light on the regulatory mechanisms that determine the chlorophyll antenna size in photosynthetic organisms. The project resulted in several peer reviewed publications and one patent. The Tla1 mutant was also made available to the industry and the research community.
- This project made good progress toward the stated goal. However, the goal is based upon a treatment rather than a remedy for the barrier arising from low light saturation of algal hydrogen production. In that sense, it offers a work-around rather than actually overcoming the barrier. For some reason, the number of candidate mutant strains analyzed to date is very modest (approximately 20,000 strains over 7–8 years) in comparison to the capability of the fluorescence screening method employed (more than 500 strains in a single 10-second image). Much larger insertional mutant libraries are available at the University of California, Berkeley (UCB) and at the Carnegie Department of Global Ecology at Stanford University, and could have been screened very quickly.

Question 4: Collaboration and coordination with other institutions

This project was rated **2.8** for its collaboration and coordination.

- Although some collaboration activities were presented on the slides, the overall collaborative efforts were not sufficient for this project. However, some improvements in collaboration were demonstrated this year.
- Judging from industrial interest, this project appears to be outstanding. However, there is not enough information to judge other areas.
- The resulting strains from this project are having an increased uptake by the research and industrial communities. This significantly increases the likelihood that the results of this project will translate into a useful advancement for the field. The PI did not speak about the level of coordination and feedback that is occurring between his group and the other projects that are leveraging the results (strains) of this project. No collaborative work for the actual project itself was noted other than the PI's ability to leverage capabilities at UCB.
- Collaboration during research was not apparent and seemed to be unnecessary. The dissemination of results through peer reviewed publications and a DOE webinar as well as the broad sharing of a mutant strain with industry, academia, and government laboratories is outstanding.
- As this is a sole-source effort, there are no specific collaborators. Although, the mutant strains developed by the PI are apparently being used by researchers in other university, industry, and government laboratories. The National Renewable Energy Laboratory (NREL) also seems to be using the Tla1 gene as a tool for increasing hydrogen production.
- It is a significant weakness of the project that the PI does not acknowledge or explicitly utilize researchers with substantial expertise in Chlamydomonas genetics and photosynthesis physiology that are available to him close at hand at UCB and at the Carnegie at Stanford; some of whom are listed as collaborators in the early parts of this work. Several laboratories, including those close at hand, have imaging systems that are capable of much more rapid mutant screening. These extensive resources could help to keep the project abreast of best practices in the genetic work. If these resources are in fact being used, they should be acknowledged as collaborators.

Question 5: Proposed future work

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

- The PI continues to be guided by a sound fundamental hypothesis that leads him to make wise experimental choices. Some of this work now appears to be moving beyond research and into the early stage of development. This reviewer wants to know how the PI's interest will evolve, although it almost does not matter because this reviewer is confident the PI will excel at the next steps based on past performance.
- The project is "wrapping up" with the Tla2 mutant. The technology appears to be ready for application and is applicable to many areas in addition to hydrogen production.
- The PI basically proposes to continue work on the Tla3 gene, which is pretty far along already and is a simple extension of the previous work.
- This project is close to completion. The PI stated he will continue work on resolving the function of the Tla3 gene, which is the appropriate next step. Other follow-on steps (for someone, possibly not the PI) should involve translating this information into industrially relevant strains and assessing performance and durability in the "field." The PI noted this is happening in the commercial space. These findings should also be applied to the question of whether hydrogen production is the immediate next step. This was mentioned by the PI and is being done in collaboration with NREL.
- The future work builds on the PI's past research and will complete and publish studies of Tla2 as well as initiate characterization and use of Tla3 in the experimental system. The proposed studies are thus quite narrowly focused. It is not clear if the PI will extend the studies to other algae potentially more suitable for industrial application.
- The Tla3 gene was cloned but has not yet been characterized. Therefore, the suggestion to complete the biochemical analyses and process elucidation for the Tla3 gene is quite reasonable. However, the project is approaching the end of its funding period and it is not very clear if the research team can do this in such a short period of time.

Project strengths:

- The final concept that the mass algal cultures with the truncated chlorophyll antenna size are more productive under sunlight conditions than the wild-type strains has been proved. The mutants were successfully generated and their cultures demonstrated a high photosynthetic productivity under high light conditions.
- This project is well focused, has made excellent progress, and has gained the research community's interest (including industry) in using the gene for other projects.
- The PI's expertise in the measurement of chlorophyll/reaction-center ratios is a strength, as is the effective use of insertional mutant libraries.
- The PI is guided by a sound hypothesis, which is very critical. The PI also appears to be a good experimentalist and can see the bigger picture.

Project weaknesses:

- There are no major weaknesses in the research plan. Overall, the project may be too focused.
- The project does not directly address the hurdles that are likely to arise in the use of small antenna mutants in practical applications. If the strains are to be grown photo-autotrophically during use, as claimed by the PI in his presentation, then there will certainly be a strong selection for the overgrowth of strains with restored antenna size. If the strains are grown on acetate medium to reduce the selection for restored antenna size (it will not be eliminated), then the cells have a substantial energy input that is proportional to cell size, rather than just chlorophyll antenna size. That energy input must be taken into account when working out the energy balance of the proposed hydrogen production system. While the progress is significant now, it has been slower to develop than it could have been.
- The research team did not demonstrate that these mutants can produce hydrogen more efficiently under high light conditions. Although the research from the NREL team proved the concept, it was done under low light intensities.
- The PI's scheme to grow algae in plastic tubes to produce mixtures of hydrogen and oxygen is problematic at best. The reviewer is not sure whether this is to be taken seriously or was merely a complex way of showing a device that performs a simple task in an indirect, convoluted way.

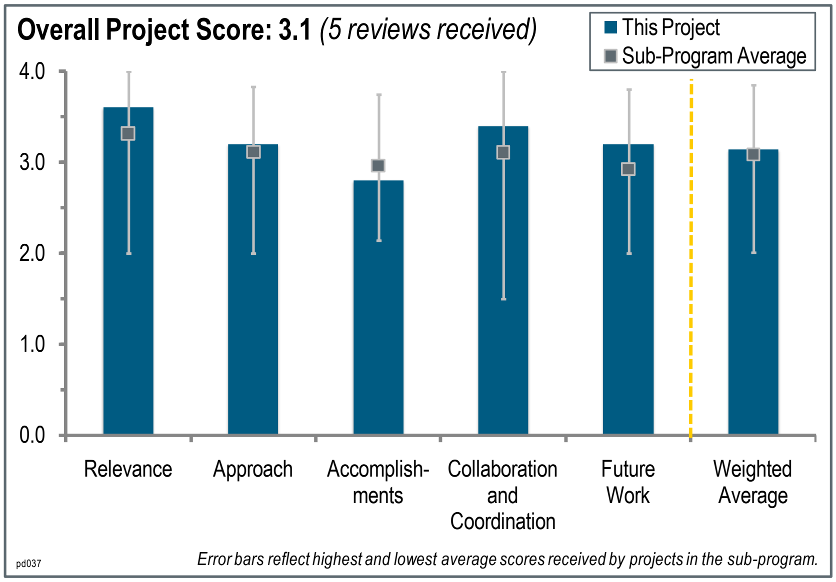
Recommendations for additions/deletions to project scope:

- This project is solid basic research with clear applications moving toward industrial application. This is a good fit for the Program.
- The project is almost completed, and therefore it is hard to make any additional recommendations. However, the project will definitely benefit if the Tla3 mutant is fully characterized.
- The PI may want to consider translating the research on Tla1, Tla2, and Tla3 into other commercial algal strains.

Project # PD-037: Biological Systems for Hydrogen Photoproduction

Maria Ghirardi; National Renewable Energy Laboratory

Brief Summary of Project:



The overall objective of the project is to develop photobiological and integrated photobiological/ fermentative systems for large-scale hydrogen production. Task objectives are to: (1) address the oxygen gas (oxygen) sensitivity of hydrogenases, which prevents continuity of hydrogen photoproduction under aerobic, high solar-to-hydrogen conditions; (2) utilize a limited solar-to-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 U.S. Department of Energy objectives

This project was rated **3.6** for its relevance to U.S. Department of Energy (DOE) objectives.

- This project has provided advancements in several of the biological areas that are of most significant interest to DOE. This includes the development and understanding of oxygen resistance in hydrogenases, the development of a ferredoxin, hydrogenase hybrid enzymes, the optimization of chlamydomonas cultures, and thin films for hydrogen production, as well as optimization of fermentation coupled with anaerobic phototrophic hydrogen production.
- This project is relevant to the DOE Hydrogen and Fuel Cells Program and directly addresses the objectives and barriers of the Program laid out in the DOE Office of Energy Efficiency and Renewable Energy, Fuel Cell Technologies Program's *Multi-Year Research, Development and Demonstration Plan* (MYRDDP).
- The relevance of this project to DOE is high, as renewable hydrogen is an objective worth pursuing.
- In principle, biophotolysis, the production of hydrogen from water and solar energy that is driven by the photosynthetic apparatus, can be more efficient in solar-to-hydrogen energy conversion than any process that involves photosynthetic carbon dioxide reduction as an intermediate energy store. The primary barriers are: (1) inhibition of the hydrogenase enzyme that catalyzes hydrogen production by oxygen, which is a necessary co-product of the process; and (2) saturation of biophotolysis at a lower light intensity than photosynthesis. This project addresses the first barrier by attempting to engineer an oxygen-tolerant hydrogenase and, as an alternative, working to optimize a system for temporally separating hydrogen and oxygen production. The project also attempts to address the second barrier by engineering a conditionally uncoupled photosynthetic apparatus. Furthermore, the project attempts to develop an immobilized cell film system for producing hydrogen, but the relevance of this effort is not explained. The project includes a third objective of using biomass fermentation that gives up the energy conversion efficiency advantages of primary hydrogen production through biophotolysis. The relevance of this objective is poorly defined.
- This project is pursuing three long-term, high-potential technologies that are well aligned with the MYRDDPs biological production of hydrogen pathway: (1) oxygen-tolerant hydrogenase, (2) sulfur-deprived hydrogen production, and (3) integrated fermentative and photosynthetic hydrogen production.

Question 2: Approach to performing the work

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

- The research outlined by Dr. Ghirardi is very focused on several projects that involve collaborators at the National Renewable Energy Laboratory (NREL) and other institutions. The approaches that have been outlined in the presentation are highly appropriate. Genetic manipulation of algal cultures will likely increase hydrogen production, and the principal investigators (PIs) are taking the right approaches. If these systems are not used in the short term for large-scale optimization, the manipulations will be useful in the future in helping to understand what can and what cannot be useful.
- The overall approach is logical and potentially innovative. Though it is a regular peril of research, some tasks have not yielded the expected results, for instance, task one mutagenesis has not yielded a sufficiently high oxygen-tolerant catalyst and the heterologous expression of Ca1 had background expression that made interpretation challenging. However, the PI noted this and has a strategy for moving forward that will focus more on positive results from other parts of the project if additional attempts fail. It would be beneficial to have had references for the cost projections presented.
- The investigators employ differences in structure between an extremely oxygen-sensitive hydrogenase and one that is less sensitive (though not sufficiently stable) to test methods for engineering oxygen resistance on the product (hydrogen) side of the active site. In parallel, they have engineered a link between the enzyme and ferredoxin, which could address oxygen sensitivity from the substrate (electron) side of the active site. The project proposes to overcome light inhibition of biophotolysis by relieving constraints arising from the buildup of a proton gradient across the photosynthetic membranes. The plan properly recognizes the need for an inducible promoter, but does not seem to appreciate the fact that most known adenosine triphosphate (ATP) syntheses mutants in the target alga are known to remain coupled. No rationale is given for the approach of using an alginate film, so the reviewer is unable to tell what problem it is supposed to solve. It appears that the cells in many cases are grown on acetate medium. The rational for doing so (and its costs) are not mentioned. This reviewer wants to know if the energy content of the hydrogen produced exceeds that of the acetate consumed. This is a necessary determination for a process that is supposed to be a primary method for solar energy conversion and storage.
- This project addresses multiple biological pathway barriers by developing multiple technologies through the application of sound scientific principles. This project, while strong in certain respects, suffers from trying to accomplish too many peripherally related objectives. The task of designing and constructing a truly oxygen-tolerant hydrogenase alone is a complex project; intermingling such an objective with another geared toward treating potato waste seems like a stretch. This reviewer is not convinced of the merit of using random mutagenesis to generate more stable hydrogenases. This reviewer questions why this effort should be continued when it has been so singularly unsuccessful, and what the PI will try that gives her a basis to believe she will succeed where so many others have failed. Rehydrogenase-ferredoxin fusions are worth pursuing. The ATP syntheses data is not very convincing. The reviewer also wants to know why potatoes were chosen—potatoes are inherently starch, so it is questionable if they are an appropriate choice of feedstock.

Question 3: Accomplishments and progress towards overall project and DOE goals

This project was rated **2.8** for its accomplishments and progress.

- Significant progress has been made during the past year toward the overall goals of this project.
- Overall, demonstrated progress has been made in this project; most of the project milestones have been met on time and with encouraging results. Those that were not met on time were due to understandable circumstances, such as funding cuts or delays. Though understanding this is exploratory research in an applied program, it would have been good to have a more thorough explanation of what the state of the technology and technical benchmarks were at the beginning and throughout this project to help the reviewer quantify improvements and put the results in a better context.
- The project has explored the impacts of several modifications of the hydrogenase enzyme on the product side. These have not been as effective at relieving oxygen sensitivity as hoped. A hydrogenase-ferredoxin fusion has been constructed and reported to divert 70% of photosynthetic electron flow to hydrogenase; however, the method for determining this value is not disclosed and hence cannot be judged. This fusion has not yet been

tested for oxygen sensitivity. Studies on alginate-immobilized cells clearly confirm the predictable negative effect of diffusion limitations on hydrogen production and hence reinforce the likelihood that this is an unproductive approach. These findings will enable the reordering of priorities for future work. Similarly, a number of problems were encountered in the attempt to provide a biomass-based source of acetate for growing the photosynthetic algae. The results encourage caution when relying on this process. If this is the actual goal of the integrated fermentation-biophotolysis system, an approach that utilizes biophotolytic hydrogen to support autotrophic acetogenesis might prove a more productive and stable route. It would also lay bare the problem of energy balance in the system, since it will only work if the algae produce more hydrogen than is necessary for producing the acetate that they need for growth. The figures in the presentation lack axis labels, and data is presented and the relevance of it is not clearly discussed.

- Of the seven subtasks with milestones that have passed, two milestones were carried over from fiscal year (FY) 2010, including 3.3.6 and 3.3.8 (3.3.8 was due to issues obtaining equipment funding), and one FY 2011 subtask (3.3.3) has passed its milestone. One FY 2011 subtask (3.3.5) has a future milestone as its progress. Good progress has been made on (1) optimizing the sulfur-deprivation platform culture conditions and (2) assembling and initially testing the integrated reactor system; development of an oxygen-tolerant hydrogenase has been slower.
- This reviewer would rate this project’s progress somewhere between two and three. However, considering the funding that has been provided to the investigator, this reviewer gives it a two. There has not been anywhere near the productivity on this project that the reviewer would have expected, given the level of investment.

Question 4: Collaboration and coordination with other institutions

This project was rated **3.4** for its collaboration and coordination.

- This project involves several collaborations and all appear to be successful.
- This project has several collaborations that are clearly active, but their relevance to the key objectives is sometimes difficult to discern.
- This project involves several collaborators who appear to be working synergistically on this problem. This project is also nicely leveraging other research funds through programs such as the DOE Office of Science to achieve project milestones.
- The collaboration among NREL, two funded partners, and two unfunded partners is commendable.
- Though the reviewer gave this project a score of two in terms of collaboration, in reality he would give it a two and a-half. The reviewer is not convinced that all these collaborations are necessary, as the project, by trying to accomplish so much at so many levels, ends up using inappropriate collaborators because of the objectives selected. For example, this reviewer wonders if the potatoes were chosen because they are of interest to the project's Russian collaborators. If yes, that is fine. However, the reviewer also wants to know if, in terms of the project's collaborators, the potatoes were included not for merit but because there was a need or desire to have Russian collaborators.

Question 5: Proposed future work

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

- The proposed work appears to be on target.
- It is good that the PI has set a defined target date for concluding the work on engineering oxygen resistance of hydrogenase. Further study of the ferredoxin-linked hydrogenase should be a very high priority. Since the data for further pursuit of this work on either alginate-embedded cells or fermentation co-processing is not promising, they do not belong in strong coupling with this project.
- The results from tasks two and three are very promising (high hydrogen yields). This project should continue beyond this year to complete the scale-up and longer-term studies that are part of these tasks.
- The future work, for the most part, is an extension of the existing effort. This project is mitigating the risk involved with difficulties of hydrogenase engineering by considering alternative paths to acquiring oxygen tolerant organisms. No explicit milestones exist past FY 2011 because continued funding by DOE is uncertain. The inclusion of quantitative or some other tangible measures of progress, especially for task three, would be helpful.

- The reviewer gave this a score of three, but would have given it a two and a-half. The reviewer suggests limiting the random mutagenesis objective and concentrating on other aspects of the project that are worth continuing.

Project strengths:

- This is a solid collaborative project from an excellent PI at NREL. The researchers have been making solid progress and are achieving their goals.
- The ferredoxin-linked hydrogenase is an important step forward that should be pursued vigorously. The concept of conditional uncoupling of ATP synthesis is a good one, though not original with these investigators.
- This project has good investigators.

Project weaknesses:

- The only potential weakness of this work is that it has such a broad scope. It may be possible to narrow the focus somewhat; however, the PIs are already deeply invested in all aspects of the project. This reviewer would not recommend any changes.
- The rationale for several of the objectives is missing.
- Productivity for this project is not impressive, and the amount of work done for the amount of money spent is lower than expected considering the quality of the personnel.

Recommendations for additions/deletions to project scope:

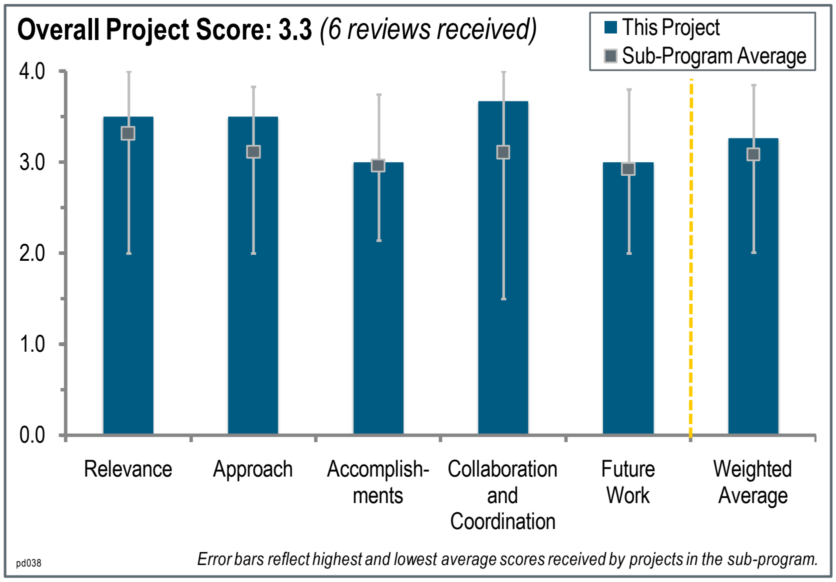
- The work on alginate-embedded cells has shown it to be a dead end, and it should not be continued. The work on attempting to incorporate potato waste into the process is counterproductive and should be dropped.
- Using random mutagenesis to generate oxygen-stable hydrogenase is unlikely to be successful.

Project # PD-038: Fermentation and Electrohydrogenic Approaches to Hydrogen Production

Pin-Ching Maness; National Renewable Energy Laboratory

Brief Summary of Project:

The overall objective of project is to develop direct fermentation and electrohydrogenic technologies to convert renewable, lignocellulosic biomass resources to hydrogen. Task goals are to: (1) address feedstock cost and improve the performance of bioreactors for hydrogen via fermentation of lignocelluloses; (2) improve hydrogen molar yield (mol hydrogen/mol hexose) via fermentation; and (3) improve hydrogen molar yield (mol hydrogen/mol hexose) by integrating dark fermentation with a microbial electrolysis cell (MEC) reactor to convert waste biomass to additional hydrogen.



Question 1: Relevance to overall U.S. Department of Energy objectives

This project was rated **3.5** for its relevance to U.S. Department of Energy (DOE) objectives.

- This project is relevant to the DOE Hydrogen and Fuel Cells Program and directly addresses the objectives and barriers of the Program as they are laid out in the DOE Office of Energy Efficiency and Renewable Energy (EERE) Fuel Cell Technologies Program's *Multi-Year Research, Development and Demonstration Plan* (MYRDDP).
- This project is well aligned with the MYRDDP's fermentative pathway objectives of improving hydrogen yields through genetic and electrochemical means and reducing feedstock costs by co-culturing and optimizing the fermentation of cheaper, less-processed feedstocks.
- Generating hydrogen from lignocellulosic biomass, if it can be done in an economically competitive way, is clearly a relevant objective for DOE.
- This project involves a two-step fermentation/microbial fuel cell to convert lignocellulosic biomass to hydrogen. This is a good, innovative idea and progress is being made. This type of system could be very useful, and other researchers are also developing the primary step for biomass conversion. The reviewer is unfamiliar with other work on developing a clostridium system for hydrogen production.
- This research aims to generate microorganisms for efficient, sustainable hydrogen production. The project also includes the development of a technology, MEC, for increased hydrogen production and more efficient use of lignocellulosic biomass as an energy source. It is still unclear how cost-effective this approach will be for lignocellulosic biomass, but this project should provide some important insights into this question.
- The goal of this project is to develop efficient methods for converting energy (originally solar) stored in the chemical bonds of lignocellulosic biomass to hydrogen. One element of the project involves coupling electrical energy with the biomass conversion to increase the absolute yield of hydrogen. This approach involves adding energy, but it is difficult to determine from the data presented whether this combination represents a net energy gain. To find out, the system that produces the electricity must be included in calculating the energy and material balance of the combined system. One way to measure would be to determine if, when the hydrogen produced from the fermentation is used to run a fuel cell to power the bio-electrolysis reaction, the net hydrogen yield increases or decreases. Another way to measure would be to determine if natural gas consumed by an electric

generator would provide enough electric power to generate more hydrogen by this method than the same amount of natural gas subjected to conventional steam reforming.

Question 2: Approach to performing the work

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

- The general approach here is excellent and the principal investigators (PIs) have made significant progress. The researchers are doing the right thing in working on developing a genetic system for Clostridium. This reviewer would suggest that the PIs speak with other DOE scientists who may also be working on this. The recruitment of Dr. Logan was very productive.
- The research plan is well designed and the goals of the project are well integrated. The project is clearly challenging, and the PI has done a good job assessing the research progress and modifying the experimental approach as needed.
- The approach of working with a consortium of organisms that are managed through a fed-batch system that retains the majority of organisms and substrate in the fermentor as the medium is renewed is good. It does, however, move away from the DOE's objective of integrating the entire lignocellulose conversion metabolism into a single organism. The approach of adding MEC processing to the waste medium is probably good, but it could be better integrated into the overall process design.
- The results from task one, in which corn stover is used, are promising and this reviewer would encourage more of the bioreactor optimization work to be done with this feedstock in the future as this, or similar feedstocks, is what will actually be used in scaled-up bioreactors. The overall approach is logical and sound.
- The fundamental approaches of the PI and collaborators are solid and based on a mix of strong basic research as well as applied science and engineering. Moving from more defined substrates (e.g., Avicel), to corn stover, to other more complex materials is helpful in defining fermentation parameters and getting a firm handle on required residence times.
- The multipronged approach of co-culture and feed optimization, genetic modification, and the electrochemical means to improve hydrogen yields and production rates as well as utilize cheaper substrate substantially enhances the likelihood of improving substrate utilization and reducing costs.

Question 3: Accomplishments and progress towards overall project and DOE goals

This project was rated **3.0** for its accomplishments and progress.

- The PIs have made some significant accomplishments and have achieved many of the goals of the project. There have been some problems, but several have been overcome. There are still two issues that could create long-term roadblocks for the project, and these need to be dealt with using a rational approach.
    1. The development of the genetic tools for Clostridium thermocellum is an issue. The PIs should consider searching for other researchers with similar goals and working together on this problem. Developing a new genetic system is never trivial and could take years. Some progress has been made, but there appears to be much left to accomplish.
    2. The issue with the production of methane in the MEC also needs to be addressed. As a long-term solution, moving the electrodes will most likely not work. The PIs should consider using something more specific for methanogens. There may be some Archaea-specific antibiotics. Some compounds such as chloroform are fairly specific for methanogens as well as BESA.
- Steady progress has been made, experimental drawbacks have been identified relatively quickly, and alternative or modified approaches have been incorporated into the project. There are still barriers that will need to be overcome, such as the genetic engineering aspect. The plasmid instability is presumed to be a problem, but it was unclear if other options will also be explored. The reviewer wonders if there is possibly some low-level expression from the plasmid that could be affecting the stability of the strain. The reviewer asks if genetic engineering is the only approach, or if possibly finding the appropriate consortium of microbes would be similarly effective.
- Good progress is being made toward the defined milestones in both tasks.
- This project's 53% increase in average hydrogen product due to an improved feeding regimen and better acclimated culture, 64% improvement in hydrogen yield due to co-culturing, and reduction in competing

methane production is commendable. However, the time period in which these improvements were achieved was not obvious in the presentation. Also not obvious was the amount of improvement 0.8 cubic meters of hydrogen per day represented in task three.
- The data clearly showed that the fed-batch reactor system does not scale well with increased substrate feed rates. This is an important observation because it raises a new barrier between achieving practical use. It is disappointing that the investigators plan to continue the scale-up rather than focusing on determining the cause of this problem. The data also clearly shows that the culture ceases hydrogen production before the physical substrate is consumed. Either there is an inhibitory substance that accumulates (the usual case in this type of digestion) or only a specific and limiting portion of the substrate can be consumed. It is important to know the difference. The experiments involving the co-inoculation of carbon-thermocellum with an unspecified consortium look promising, but unfortunately they lack the necessary control comparison with the consortium alone. Understanding the nature of the microbial community will be essential if the gains shown are to prove stable over the long run. It will be important to know if the community is integrated through syntrophic interactions or other stabilizing sources. If not, a long-term culture could be treated as an enrichment culture and pure organisms isolated to determine which is responsible for the improved performance. On the downside, it is perfectly possible that the improved performance will not be sustained over an extended period. Determining this will be important as well. Apparently a transformation system for carbon-thermocellum is now working; however, it is not as flexible as thought and an improvement using a standard gene replacement strategy is planned. This system is being used to inactivate the formate synthesis pathway to see if reducing power can be directed toward hydrogen production. Of course, if the organism has (or could be engineered to have) an active formate dehydrogenase (that would produce hydrogen and carbon dioxide [CO_2] from formate with a negative delta-G), this experiment could be self-defeating. It is unknown if the hypophosphite inhibitor used in preliminary reconstruction experiments is sufficiently specific to exclude this possibility. Results have been obtained showing that an MEC can use the reduced carbon compounds in the supernatant from the fed-batch culture to support hydrogen generation at anode potentials of –0.2 volts. The claim is made that this boosts total hydrogen production to the range of 10 hydrogen per hexose. Unfortunately, the basis for this calculation was not presented. This reviewer wants to know if that hexose is consumed and, if so, how that is determined. Oddly, adjustments of the anode potential that increase hydrogen production lead to decreases in CO_2 production. The reviewer asks what the oxidized product of the reaction is. It is not obvious if the investigators have developed a careful energy and carbon balance for the process.
- Incremental progress across most of the objectives is obvious, but the big question is whether this incremental progress will be sustained and lead to a commercially viable process. That is an important question in this project, and certainly the experimental work is worth continuing.

Question 4: Collaboration and coordination with other institutions

This project was rated **3.7** for its collaboration and coordination.

- This project has extremely strong collaborative work. This group of PIs was assembled by Dr. Maness and they are developing each area successfully.
- This project has excellent collaborators, especially on the applied science and engineering side. They bring the right mix of skills to this project, which benefits the PI.
- The collaboration among the various tasks appears to be very good. The tasks, for the most part, are independent (except for providing effluent from task one to task three), so little coordination effort is required.
- This project has good collaboration with other researchers at the National Renewable Energy Laboratory (NREL) and similarly excellent use of the resources at NREL. The collaboration with Dr. Logan at Pennsylvania State University (PSU) brings important expertise and resources to the MEC aspect of the project. The development of genetic tools for carbon-thermocellum also brings a good international collaborator to the project.
- The collaboration with PSU has clearly proven fruitful. However, it will be necessary to generate an integrated overall energy and material balance including the fermentation process, the MEC process, and the electric power generation system to optimize performance and decide if the electrochemical system is as valuable as it initially seems. Given the possibility that there is an inhibitory substance that accumulates in the fermentation culture, it may prove valuable to directly integrate MEC processing of the culture fluid into the fermentation step of the process. Doing so will require running both processes at the same location.
- Several collaborators are involved in this project and the PIs are leveraging efforts and funds from other entities.

Question 5: Proposed future work

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

- The proposed research is logical and builds on the previous research results. The PI is aware of the barriers and has included targeted research to address specific problem areas, such as improving the proprietary plasmid. Foundational studies are underway for the genetic engineering of metabolic pathways and this may be more complicated than discussed. This reviewer asks how the modifications will affect the overall physiology of the microbe, and about the stability of the engineered traits and pathways. Although the initial focus is on deleting the pyruvate to formate pathway, these questions will undoubtedly be addressed by the proposed experiments.
- The future work proposed for this project follows the logical next steps. It would be good to continue to leverage the DOE EERE Biomass Program efforts in this research area and use realistic feedstocks whenever possible.
- The project's tasks are continuing along their current paths. Task two (genetic manipulation) has experienced a setback, but not one sufficient enough to recommend consideration of an alternative approach at this time.
- In general, the proposed approaches are appropriate. The reviewer is somewhat skeptical of the proposed important role of pyruvate formate lyase in diverting electrons from hydrogen, given the fact that formate does not seem to be an important fermentation product. This reviewer suggests that, for pathway modification, the PIs should focus on logically important hydrogen diverting steps. This is likely to yield the best information regarding the role of those processes in hydrogen metabolism.
- While progress has been made in different aspects of the project, it is disappointing that an overall status assessment has not been established to better integrate the disparate elements of the work and address the changing landscape of known barriers.
- This project is likely to lead to further incremental progress. The reviewer does not see anything in the future plans that is likely to lead to a breakthrough.

Project strengths:

- This project has an excellent and interesting collaborative effort.
- This project has a good combination of objectives that are not necessarily dependent on each other. It will be great if the goals of all three objectives are met, but the project will still provide important technologies and tools if only one or two of the objectives are successful.
- This project has a solid PI who is well versed in science and in command of her subject and solid collaborators. This reviewer asks if the problem is intractable. The reviewer also asks how methane generation will be avoided or minimized, and if that is even desirable. If the goal is to produce hydrogen, then that is a problem. If producing methane is also valuable, then it is not. Such are the trade-offs when working with consortia.
- It is important to investigate the microbial catalysis of hydrogen production from lignocellulosic waste streams. This project is building strength in genetic analysis of one of the potential catalytic organisms. The researchers' experience in MEC development is a strength that could be better used.

Project weaknesses:

- This project has no major weaknesses. The genetic engineering aspect to improve hydrogen molar yield may be more complicated than presented. Anytime metabolism is retargeted, the physiology, growth, and stability of the organism can be significantly affected. The proposed experiments are important for developing an "optimal" strain for hydrogen production, but future research will also need to consider long-term viability and stability of the strain.
- The PIs need to focus their efforts on the potential roadblocks.
- The project is weak in the integration of its various objectives. It also lacks an external reference for performance. It is recommended that the researchers use, for instance, hydrogen production through the steam-reforming of lignocellulosic biomass as a point of comparison. This reviewer asks if best practices with their system have potential advantages through some metric (such as process productivity, process stability, capital requirements, and energy efficiency) relative to best practice steam reforming.

- The economic viability of this project is a concern.

Recommendations for additions/deletions to project scope:

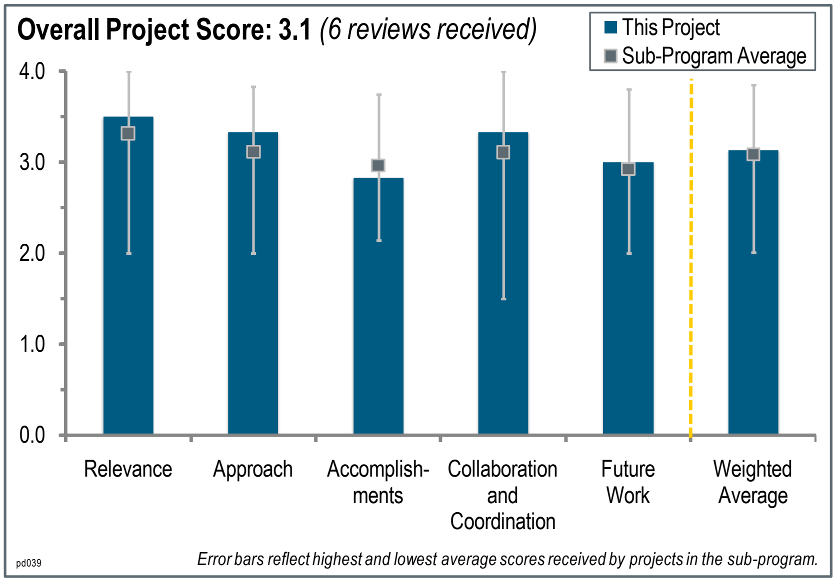
- While acknowledging that a previous reviewer suggested determining the nature of the microbial consortium, this reviewer does not see that as a priority. It could be good to know how diverse and which microbial strains make up the optimum consortium. However, if the goal is to develop an optimal strain, then such a consortium may not be needed. Perhaps a different consortium may be more effective with the new strain than with the existing strain(s).
- The investigators should identify the mechanism responsible for the problem with scaling the fed-batch reaction to higher feed rates. The investigators should conduct full-system energy and material balances for their process as a guide for developing improvements.
- This project is worth continuing and the PI should set go/no-go decision points.

Project # PD-039: Hydrogen from Water in a Novel Recombinant Oxygen-Tolerant Cyanobacterial System

Phil Weyman; J Craig Venter Institute

Brief Summary of Project:

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



Question 1: Relevance to overall U.S. Department of Energy objectives

This project was rated **3.5** for its relevance to U.S. Department of Energy (DOE) objectives.

- This project addresses the challenge of optimizing hydrogen production in a cyanobacterium. As cyanobacteria are potentially useful and versatile organisms for biofuel production, this is a highly relevant system.
- The identification and optimization of oxygen-tolerant hydrogenases is an important component in attempting continuous hydrogen production during oxygenic photosynthesis. Thus, the project is clearly relevant to DOE's objectives and may lead to new microbial or cyanobacterial strains with enhanced hydrogen production.
- This project's objectives align well with goals of the DOE Hydrogen and Fuel Cells Program. In the presentation, though a table was presented that defined 2009, 2011, and 2018 targets and statuses, this was not detailed enough to judge the actual progress this project has made in improving hydrogen production in the presence of oxygen.
- The development of an oxygen-tolerant, hydrogen-producing photosynthetic organism is an important path to biological hydrogen production, which this project supports.
- The goal of biophotolytic hydrogen production is to create the most efficient solar-to-hydrogen conversion path catalyzed solely by living organisms. In the past, the use of cyanobacterial hosts for this process has been limited by the activity of nitrogenase for hydrogen synthesis and by the oxygen sensitivity of hydrogenase. While not directly assessed yet, it is likely that this system will also encounter the barrier of low light saturation in comparison with photosynthesis, which has been recognized in similar green algal systems.
- Oxygen-tolerant hydrogenases are a holy grail that many researchers are seeking to discover and/or engineer. However, this may not actually exist due to a fundamental incompatibility and the metal centers at the active sites of hydrogenases. It may well be that too many principal investigators (PIs) are trying to achieve something that is impossible. Having said that, the discovery and engineering of oxygen-tolerant hydrogenases is very relevant to the Program's mission.

Question 2: Approach to performing the work

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

- The research plans are logical and well thought out. The systematic approach by both the J. Craig Venter Institute (JCVI) and the National Renewable Energy Laboratory (NREL) groups is appropriate to engineer the various genetic components for enzyme production and function in new host strains. Both groups appear to be

addressing various steps in a systematic manner and have some alternative approaches in mind if needed. As noted by the researchers, the lack of some tools and fundamental knowledge regarding hydrogenase structure and function in some of the organisms in the study, such as the Casa Bonita strain (CBS), will make some aspects of the overall project difficult. It is not entirely evident why CBS was chosen over other strains; perhaps this reviewer missed this in the presentation.

- The approach is to optimize the expression of a less oxygen-sensitive hydrogenase in the cyanobacteria, thereby allowing the hydrogenase to function longer during oxygenic photosynthesis and produce more hydrogen. The general approaches have been used by both of the collaborators using different oxygen-tolerant hydrogenases in different model hosts. The NREL group is focused on optimizing expression and assembly, and the JCVI group is focused on expression and the addition and manipulation of ferredoxin. The general ideas are good and the development of expression systems is critical but not really exciting. Once the legwork is done to optimize expression, it would be worth doing some enzyme characterization. The approach to modify the redox potential of the ferredoxin is very exciting and has yielded some significant results. This type of approach will likely be useful for other systems.
- This project proposes to engineer an oxygen-tolerant hydrogenase into cyanobacteria with two candidate structural and maturation gene complexes from different organisms being tested in parallel at NREL and JCVI. Because of the use of relatively lower turnover NiFe hydrogenase (in comparison with Fe-Fe hydrogenase) in both cases, expression of adequate levels of hydrogenase activity in vivo is a challenge that is being met by promoter engineering.
- Researchers are taking reasonable steps to try to develop expression systems for novel and known oxygen-tolerant hydrogenases. Though this reviewer recognizes this is a basic project and the milestones are setup around expression of the hydrogenases, it would have been good to get a better idea of how this project is progressing in terms of hydrogen production time.
- Continuous hydrogen production by photosynthetic organisms is a longer-term development path. Developing multiple systems is a commendable risk-reduction strategy.
- The PI stated that the approach was based on the annotation of metagenome data referenced to the sequence of a known "oxygen-tolerant" enzyme. Oxygen tolerance is relative and the reviewer would not in any way consider what is currently described as "oxygen -tolerant" as actually possessing oxygen tolerance. This reviewer questions the fundamental approach when there is no ecological reason why an unknown hydrogenase from an unknown organism living in the ocean would have any more oxygen-tolerance than any other hydrogenase. The PI also claimed thermal stability in the same enzyme and, again, this reviewer questions the claim of thermal stability because it is not compared to anything. No data was presented and this reviewer doubts that the hydrogenase being characterized would be more thermo-stable than an enzyme isolated from thermophilic organisms. This project is based on a less-than-sound foundation.

Question 3: Accomplishments and progress towards overall project and DOE goals

This project was rated **2.8** for its accomplishments and progress.

- This project has made good progress with a difficult system. The lack of some tools and basic knowledge (as noted by the researchers) is making aspects of the project challenging and slow going. Nevertheless, the researchers are making steady progress toward their objectives.
- Both partners seem on track to complete the project milestones for both tasks in a timely manner. Though much additional work will be required to achieve long-term DOE goals, the projects are following a logical path.
- In both cases, the hydrogenase has been heterologously expressed. The JCVI group has done two very elegant experiments. One is the cloning of a large fragment containing the hydrogenase and assembly proteins from a metagenomic library. The other is the manipulation of the redox potential of the ferredoxin to increase hydrogen production activity. These are both exciting experiments and major breakthroughs in developing hydrogenase systems. The NREL group should focus on understanding the hydrogenase function in the heterologous host.
- The technical progress toward transgenic expression of both hydrogenases in cyanobacteria has been reasonably good. Progress toward identifying the necessary maturation genes in Rubrivivax CBS has also been good; however, progress toward gaining oxygen tolerance is modest. The "environmental" hydrogenase under study at JCVI shows 20% activity after two hours in 1% oxygen. This is to be compared with the hyperbaric oxygen (33% or more) that is expected to be encountered within cyanobacteria if the system functions as desired. This project has made some good progress, but there is still a long way to go.

- Four of the five milestones are complete and the incomplete milestone is 80% complete at four months past the milestone. One of the three remaining milestones is 50% complete with one month remaining in the timeline, while the other two are 50%–95% complete with about four months remaining. The fiscal year (FY) 2011 goal of producing one cyanobacterial recombinant evolving hydrogen through an oxygen-tolerant NiFe-hydrogenase appears to be at risk. Recent progress has been understandably modest. Achieving the 2013 target of 30 days of continuous hydrogen production might be a challenge, but at this time it does not appear to hinder the achievement of the 2018 target of three months of continuous hydrogen production.
- The progress has been moderate, which is not unexpected due to the shaky foundation on which the project rests.

Question 4: Collaboration and coordination with other institutions

This project was rated **3.3** for its collaboration and coordination.

- The collaboration between the two main groups seems good and has effective data sharing.
- This project has tight collaboration between NREL and JCVI, entities that both have strong expertise in areas relevant for this project. JCVI has particular expertise in genomic mining and is a valuable asset for seeking and developing novel hydrogenases in nature. Additionally, this project leverages funds and efforts at other entities that will enhance the work.
- NREL and JCVI appear to be collaborating on three of the five tasks in the first milestone, as well as maintaining collaborations with researchers at three universities.
- The PI is collaborating well with the investigators at NREL. It appears that the NREL partner is driving the basic science aspects of the project with the PI's institute providing access to metagenome data and some molecular biology. In this reviewer’s opinion, making an oxygen-tolerant hydrogenase is a chemistry problem and is unlikely to be solved using sequence data and molecular biology.
- The collaborators are both strong scientists. The choice of host organisms was likely made so that at least one group would be successful. Because both groups are successful, they each are working on their own cyanobacterium. A more successful collaboration would occur if both groups studied the same systems but different aspects or enzymes. The PIs should not change now with one year left in the project, but should consider adopting a single host if the project is renewed.
- The presentations gave the impression that the two institutions are working in somewhat parallel paths. However, it appears the two institutions are sharing information and have complementary strengths (JCVI on the genomics side and NREL on the biochemical and physiological side). The integration between the two institutions could be better illustrated, but perhaps it will become more evident as the strain development phase matures.

Question 5: Proposed future work

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

- The planned research is logical and will build on previous progress. There is still much work to be done for the engineered organisms to become viable production strains. The researchers are aware of barriers, although some experiments depend on serendipity. For instance, in cases where there seems to be redundant functions, it is not clear how the researchers will identify the next gene to express. An intrinsic issue for any metabolic engineering or pathway design is the effect of the modifications on the organism's physiology. For example, it is unclear how the changes affect the growth and survival compared to the wild type strain. The researchers are clearly aware of these issues, but they were not addressed in the presentation materials. Similarly, there will likely be numerous challenges in engineering a multi-subunit, functional enzyme with the proper structure and regulation. Again, the PIs are well aware of these issues.
- The proposed next steps are logical, but the key tests on the viability of this approach lie beyond the scope of what is proposed.
- The proposed work is well laid out and will be successful. The focus over the next year at NREL is to fully understand and optimize the assembly proteins. The focus at JCVI is to continue working on ferredoxin and increase expression of hydrogenase. The PIs are experienced in this work.
- The future work proposed for this project follows the logical next steps, although they are somewhat incremental and reduce the potential for a giant leap in productivity. The reviewer hopes JCVI is also continuing to search for

novel, high-oxygen-tolerant hydrogenases. This is a capability relatively few research laboratories have and is complementary with all other enzyme engineering methods and expression systems for known hydrogenases.
- The project's proposed future work continues the current work. The project's presentation described no milestones past FY 2011 due to the uncertainty of continued DOE support. Despite this uncertainty, it would be helpful if proposed future work provided quantitative or some other tangible measures of expected performances by the systems being developed.
- The reviewer finds it difficult to muster enthusiasm for this project. It is not that the PI lacks skills in his chosen discipline, it is that the discipline itself is ill-suited to accomplish the goals of the project. There is no attempt to understand why the hydrogenases are oxygen sensitive. If the cause is not known (this is a chemistry problem), it is not clear how can a cure be found.

Project strengths:

- The innovative work done at JCVI is a strength.
- This project is generally well planned with logical approaches, and the two research groups have complementary expertise.
- This project has good genetic engineering expertise and tools.
- The development of multiple systems is a good approach.

Project weaknesses:

- The expression issues in both hosts need to be overcome. A larger effort on a single expression system could produce more results.
- There is lack of clear integration between the two research groups. As acknowledged by the PIs, the researchers lack some of the needed tools to work with some of the organisms (although the tools are being developed).
- There is a seemingly incomplete appreciation of the biochemical and physiologic barriers that lie ahead.
- The wrong set of tools (high-technology tools) applied to a challenging problem will not yield positive results no matter how many terabytes of data get searched. The reviewer even finds the “query” put into the database problematic.

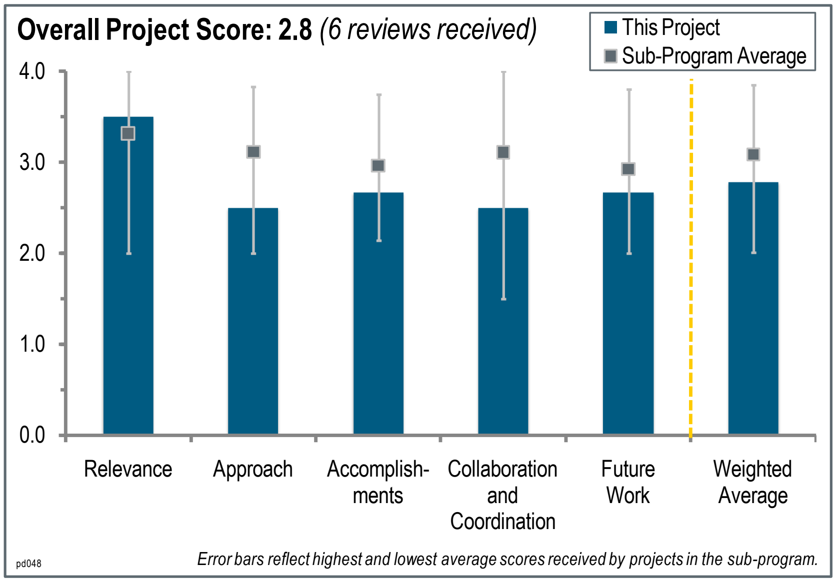
Recommendations for additions/deletions to project scope:

- The approach (homology) used to identify novel environmental hydrogenases could be missing some truly novel hydrogenases. This could be difficult, but if the goal is to identify unique oxygen-tolerant enzymes, it may require some “brute force” experiments based on activity, not simply homology.
- If the PI wants to find new thermo-stable hydrogenases, he should search metagenome data from hot springs. The PI should not be searching metagenomic data from seawater organisms. This is fundamental microbial ecology. There is no basis to believe this project will succeed. However, it will it generate publishable data, and therein lies the problem.

Project # PD-048: Electrochemical Hydrogen Compressor

Ludwig Lipp; FuelCell Energy, Inc.

Brief Summary of Project:



The objectives of this project are to: (1) develop designs and materials to increase electrochemical hydrogen compressor (EHC) pressure capability from 2,000 to 6,000 pounds per square inch (psi); (2) improve cell performance to reduce power consumption; (3) reduce the EHC cell cost by increasing current operating density; and (4) study thermal- and water-management options to increase system reliability and life. Use of an EHC will: (1) increase reliability and availability over current mechanical compressors; (2) ensure that there is no possibility of lubricant contamination (no moving parts); (3) increase compression efficiency to 95%; and (4) potentially reduce the cost of hydrogen delivery to less than $1/gasoline gallon equivalent.

Question 1: Relevance to overall U.S. Department of Energy objectives

This project was rated **3.5** for its relevance to U.S. Department of Energy (DOE) objectives.

- Electrochemical compression is a very promising approach to addressing the DOE Hydrogen and Fuel Cells Program targets and challenges for hydrogen compression based its inherent low or no contamination and high efficiency, while simultaneously addressing reliability (no moving parts) and cost.
- Compression is critical for hydrogen delivery, especially for hydrogen refueling stations. The objective of this project is to develop a new compression technology that will increase energy efficiency, improve reliability, eliminate contamination, and reduce cost. All of these goals are in line with the objectives of the Hydrogen Production and Delivery sub-program.
- It is good to have a cost-effective compressor at the stations with no moving parts, as it will reduce capital and operation and maintenance (O&M) costs.
- This project's current concepts show the potential to reach DOE targets.
- This project has a highly capable team with the appropriate expertise and functions to complete this work. The technology has strong theoretical benefits, particularly with respect to efficiency, size, and complexity. The technology is also relevant to a variety of industrial applications and diverse hydrogen fuel sources (e.g., biogas and natural gas).
- The overall goal to increase reliability and efficiency while decreasing the cost of current mechanical compressors is an appropriate goal that aligns with Program objectives.

Question 2: Approach to performing the work

This project was rated **2.5** for its approach.

- This is a good approach to cover fuel cell electric vehicle (FCEV) fueling functionality through up-scaling; however, there are uncertainties and issues with this. FCEV fueling capability is essential for the success of the product.

- Electrochemical compression appears to be a good way to increase compression efficiency and reduce O&M costs. Costs and durability will continue to be a challenge, much like fuel cells.
- This approach builds on Fuel Cell Energy, Inc.'s (FCE's) prior fuel cell; electrolyzer; and hydrogen production component and systems development, demonstration, and deployment experience. The cell cascade approach seems promising; however, the approach presented was fairly generic and did not have sufficient detail to assess its likelihood of success.
- The approach, based on the use of an electrochemical compressor, is broadly defined as improving the technology for higher pressure and higher capacity, but lacks details. The project milestones presented in the table should be better described to facilitate the evaluation of the current status of the technology.
- The general objectives were clearly stated, although the specific approach remains a bit unclear. The detailed technical barriers for the technology were not identified. Comparisons to current, truly-competitive five-stage (or more) mechanical compressor technologies should be made, particularly with respect to cost and durability.
- The description of the approach was rather general and specifics regarding the concept along with the design improvements would have been helpful. It was unclear if the project had a clear cost assessment to compare to a mechanical compressor.

Question 3: Accomplishments and progress towards overall project and DOE goals

This project was rated **2.7** for its accomplishments and progress.

- The project is still in the beginning phase and the accomplishments to date are good. The main progress is in the development of a two-stage compression concept validated at the 2,000/6,000 psi level. The capital cost is reduced by 50%, but there is no mention of the key parameters that enabled this improvement.
- This project reported some very good accomplishments and the current status is better than the target. This reviewer wants to know if the degradation mechanisms are understood.
- The project showed progress on slide 16, but the details of the improvements were not provided or known during the time of the presentation. The accomplishment has not shown the potential to provide better efficiency than a three-stage compressor. The project comparison should actually be evaluating the investigators' progress against a five-stage compressor.
- The primary accomplishment during this performance period was demonstrating a two-stage approach. Most of the other technical targets that have been met are carryovers from the prior program. The real tests are to scale the cell-active area and achieve the target hydrogen flux in a multistage system, as proposed.
- The summary of the technology status of phase two goals highlighted progress, although comparisons to other important targets, such as cost and robustness, were absent. A demonstration of technical progress was exemplified by continuous performance improvements toward the 12,000 psi target. Again, a comparison to a current, five-stage mechanical compressor technology is more appropriate. It is not clear what the concept-to-concept differences are, and which are responsible for the performance gains. The reviewer asks what the underlying material, design, and property differences are between the concepts.

Question 4: Collaboration and coordination with other institutions

This project was rated **2.5** for its collaboration and coordination.

- The principal investigators state that a primary function of the subcontractor Sustainable Innovations is to examine EHC cost, but no cost information or studies were apparent. This cost information is a vital part of comparing this technology to competitive mechanical compressor technology.
- The collaboration with Sustainable Innovations provides expertise in cell design and fabrication. No other collaboration or coordination was mentioned.
- The collaboration between FCE and Sustainable Innovations is noted, but their specific contribution shown on the slide is too general and could be better described. As the project plans scale-up, an end user could be added as a partner.
- Only one industry partner is involved. The reviewer asks why that is the case. There is no collaboration with other infrastructure providers.

Question 5: Proposed future work

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

- The proposed work is acceptable. It is focused on high-pressure capability, durability and cycling, and scale-up. The team should conduct a cost estimation to better position this technology with others.
- The future work seems logical based on the current status, but should include a cost analysis.
- The proposed future work builds on prior work. The value of baseline stack durability testing, if the team is planning to incorporate additional improvements, is questionable, as some improvements could have significant impact. This project would benefit from some specific interim technical metrics for planned future work because it is clearly focused on the next year of the project, which has approximately 26 months remaining.
- This reviewer wonders if it is right to test durability on the 2,000–3,000 psi level, and what the effects are (e.g., cost and degradation) of up-scaling.
- The presenters should provide further details regarding their improvement ideas and methods to validate their next design iterations. The project should include an assessment of cost.

Project strengths:

- The strength of the project is the ability to use a compression technology that does not need moving components. The team members are well qualified to drive the work even if an additional partner, which uses the technology, would provide added value.
- This project has made proven technical progress with most performance targets achieved.
- The project is clearly showing progress from the initial design concepts.

Project weaknesses:

- A lack of insight into the approaches to achieve improvements and meet targets limits the lessons learned from this project, whether successful or not.
- There is no mention of the issues that could occur in the project due to the scale-up. There is no clear goal of the cost that could be reached.
- This project is missing some key industry collaborations—see above.
- The researchers need to assess the costs and generally benchmark performance, cost, and durability attributes for EHC against current mechanical compressor technology.
- The project needs to provide further details regarding the past and future design improvements. The project needs to be able to predict the potential of providing a compressor technology that is better than a mechanical type in both efficiency and capital cost when compared on the same capacity and pressurization basis.

Recommendations for additions/deletions to project scope:

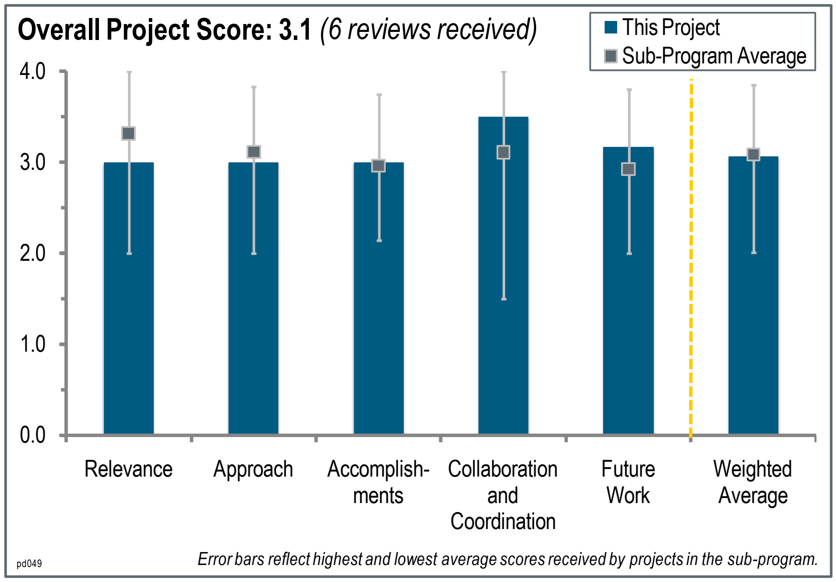
- The EHC is potentially a breakthrough technology, so it is important to continue this project with some improvements. In this scale-up phase, the team should provide a detailed analysis of the various steps of the project and how they are linked, improve the milestones with well defined tasks, and identify the key barriers that could slow down the project and propose solutions, if any. The team also must include an economic analysis of the expected costs of the system at full-scale deployment for comparison with conventional and other emerging compression technologies.
- This project should get infrastructure providers (i.e., gas or energy companies) on board. A focus on one application may help.

Project # PD-049: Integrity of Steel Welds in High-Pressure Hydrogen Environment

Wei Zhang; Oak Ridge National Laboratory

Brief Summary of Project:

The overall objective of this project is to improve resistance to hydrogen embrittlement in steel welds and reduce welding related construction costs. Project objectives over the past year include: (1) validating the fracture toughness testing methodology for pipeline steel welds in high-pressure hydrogen environments; and (2) demonstrating the effectiveness of friction-stir welding for improving resistance of pipeline steel welds to hydrogen embrittlement.



Question 1: Relevance to overall U.S. Department of Energy objectives

This project was rated **3.0** for its relevance to U.S. Department of Energy (DOE) objectives.

- Information on the impact of high-pressure and hydrogen embrittlement on fracture toughness is critical to the design of pipeline systems to transport hydrogen in a safe, cost-effective manner.
- Assuming the first generation of hydrogen fuel pipelines will look a lot like the existing hydrogen pipelines used today, reducing costs with improved joining technologies and improving weld reliability are extremely relevant.
- This project will be relevant if hydrogen pipelines develop on a large scale. However, the presentation should make a better case for why this is important. This reviewer wonders if steel pipelines are incompatible with hydrogen, and, if so, why that is the case. The reviewer also asks if this project addresses the key issues with steel pipelines.
- This project appears to be approaching 90% complete. Welding of steels is considered the weak link in the construction of fuel cell systems because little is understood or known about how hydrogen affects the long-term integrity of the weld.
- The DOE Hydrogen and Fuel Cells Program pipeline barrier is the high capital cost and hydrogen embrittlement of pipelines. Hydrogen embrittlement of steel is not completely understood. The current joining technology for steel pipes is a major part of the labor costs and impacts the steel microstructure in a manner that can exacerbate hydrogen embrittlement issues. This project supports improved weld, but has contributed little to reducing labor costs.
- This project will study weld susceptibility to hydrogen embrittlement in pipelines steels and is a necessary project to ensure the safe hydrogen transport in metal pipelines.

Question 2: Approach to performing the work

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

- This project has a good technical approach with a contained device for testing the different materials in hydrogen.
- The high-pressure spiral notch torsion test technique is unique; however, it remains to be validated and accepted by the broader community. The application of the data the investigators generate and who will use it was not discussed. It was unclear who will use this information. It was also not obvious why the principal investigators

(PIs) used 4340 steel. This reviewer asks if this is a common pipeline steel. The reviewer also wants to know how it differs from common pipeline steels such as X-52 and X-80, and whether they are the same. If not, the reviewer wants to know why the researchers used 4340 instead of an X-series steel. The size of the "simulated weld zone" material is questioned. It is unclear if there a reason the PIs did not extract material from actual pipeline weld for these studies.
- The critical barriers identified are in line with the objectives of the Program.
- While the approach is consistent with the main goals and objectives, it seems that the investigators occasionally spend too much time on interesting, but not extremely important, issues. For example, the spiral notch torsion test (SNTT) is an interesting way to identify the most susceptible microstructure in a weld zone and to compare the relative resistance of the weakest part of weld and heat affected zone microstructures created by different thermal histories (joining technologies). However, fracture resistance does not usually scale well with sample size, shape, etc. As a result, no matter how much finite element modeling one does of the SNTT geometry to accurately determine the absolute fracture toughness in hydrogen, additional testing will be required with samples and geometries more closely resembling the actual loading conditions.
- This project involves a wide range of stakeholders, including industry, equipment manufacturers, and national laboratories. Friction stir technology is attractive and promises better quality weld, and this project has a reasonable approach for pursuing it.
- This project's approach seems sound, but it needs assurances that a multiple notch test is adequate to predict weld durability under all pipeline joining scenarios.

Question 3: Accomplishments and progress towards overall project and DOE goals

This project was rated **3.0** for its accomplishments and progress.

- Good progress has been made on the development of the SNTT technique since the inception of this project. Data obtained on 4340 steel demonstrates how hydrogen lowers fracture toughness.
- The investigators have done excellent work, made significant progress, and developed important testing methods that will improve joining technologies. However, it is unclear from the presentation whether the two goals of reduced cost and improved reliability are still well within reach.
- The accomplishments seem steady and directed toward goals. Finite element analysis was mentioned, but it was not explained how the analysis results were used to benefit the project. The reviewer did not understand the details of graphs on slides 13 and 16. The meaning of these trends is unclear.
- This project's accomplishments seem adequate, although the friction stir welding joints should have been tested earlier.
- Hydrogen pipelines employed in existing technologies have operated satisfactorily for decades. This project's approach lacks a strong justification and target. This reviewer wants to know what performance is satisfactory and what the existing technologies' levels of performance are. The reviewer also asks, if existing technology performance is unsatisfactory, how much better friction stir is. The reviewer wonders if it is satisfactory and if its costs and benefits justify adoption, and what the tradeoffs are between the weld quality and cost.

Question 4: Collaboration and coordination with other institutions

This project was rated **3.5** for its collaboration and coordination.

- This project has good collaboration with many important institutions.
- The interaction with friction stir processing firms (Megastir and ESAB) is excellent and has led to the development of a federal test procedure process for solid-state welding. The discussions on the interactions with other partners were limited.
- This project has a strong collaboration with the fuel cell programs, as well as other cross modal programs with other federal agencies.
- This project has excellent coordination and collaborations with other DOE laboratories, outside laboratories, and standards developing organizations.
- The partners' roles are well defined, but interaction and coordination is not apparent in the presentation.
- This project has a big list of collaborators, but few joint projects were mentioned in presentation.

Question 5: Proposed future work

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

- This project has good final plans and is near completion.
- The proposal to investigate pipeline steels such as X-65 is welcomed.
- Logical next steps are proposed for the program.
- This project's future work needs to consider cyclic pressure and concentration of hydrogen.
- This project will install a hydrogen embrittlement test apparatus and acquire a baseline arc weld to collect performance data and make a comparison of friction stir with arc weld. No milestones were mentioned in the presentation.

Project strengths:

- This project seems to have developed a thorough capability for testing the materials when immersed in hydrogen.
- This project provides needed information on the impact of hydrogen on fracture toughness for weld metal in pipeline steels.
- The tasks identified in the project are organized and correctly weighed to address the gaps and challenges.
- The goals and objectives are important and the path to these goals makes sense from both a scientific and economic perspective. The investigators have developed testing methodologies and an apparatus that promises to deliver high-quality data on the properties of different weld microstructures and thermal histories.
- This project focuses on the valid and necessary objective of using steel pipelines for hydrogen transport.

Project weaknesses:

- This reviewer asks why this project is using surrogate "welds" instead of testing heat-treated materials that may theoretically behave like a welded material. The researchers should test the real thing. Even though there would be variability in the results, that information would be valuable.
- Data on 4340 steel may be of questionable use unless it is similar to pipeline X-series steel.
- Looking at the effects of hydrogen pressure is not as critical as looking at the cycling of pressure and consternation of the hydrogen.
- This is a complex, multifaceted problem that is requiring a great deal of ground work. However, now that the ground work is done, hopefully the researchers will sharpen their focus on the main objectives.
- This project could use clearer explanations of some of the graphs and a better understanding of how finite element analysis was used to benefit the project.

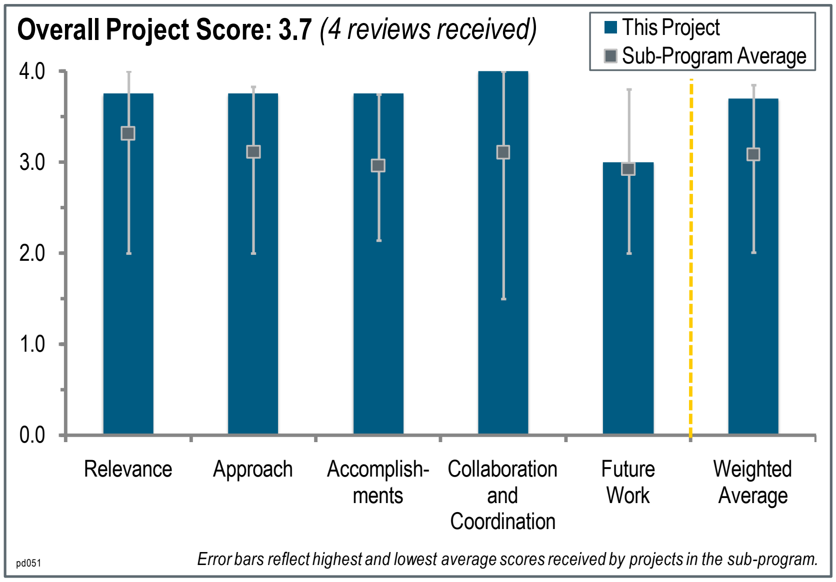
Recommendations for additions/deletions to project scope:

- This project is almost over, but the researchers should try to test a real weld and compare the results with those of the heat-treated materials.
- The reviewer encourages the continuation of the work on X-65 steel as well as an indication of how the data will be used to select alloys and joining techniques for the safe transport of hydrogen.
- Once the project has completed the evaluation of 4340 steels, additional work needs to be focused on current pipeline steels and fuel cell components under consideration by other groups working on fuel cell technologies.
- These investigators have taken on a wide range of complex issues and have done a good job of addressing them all. This reviewer does not think any additions or deletions to the project would be appropriate, but does think that the investigators need to sharpen their focus on the main goals and the relevant materials and welding technologies.

Project # PD-051: Characterization of Materials for Photoelectrochemical Hydrogen Production

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 U.S. Department of Energy (DOE) Photoelectrochemical (PEC) Working Group to determine status-quo, find unexpected findings, propose modifications to partners, and monitor the impact of implemented modifications. 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 bandgaps, energy-level alignment, chemical stability, and the impact of alloying and doping.

Question 1: Relevance to overall U.S. Department of Energy objectives

This project was rated **3.8** for its relevance to DOE objectives.

- The efforts by the Heske group to characterize and aid in the development of new materials is extremely relevant to meeting the metrics of the Hydrogen Production sub-program.
- A consistent, well-calibrated evaluation of PEC is critical to the investigation of the PEC materials.
- This project brings unique and world-class materials characterization capabilities to the PEC Working Group. While some of the characterization capabilities are available at different institutions, others are available nowhere else in the world. This project brings consolidated access to expertise and materials characterization technologies in a "one-stop-shop" experience and supports all members of the PEC Working Group. This project's membership in the PEC Working Group permits resource allocation without redundant, institutional investment in common capabilities.
- It is hard to show program alignment on a project this sophisticated and tightly focused. The alignment is as good as the PEC program as a whole.

Question 2: Approach to performing the work

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

- The ability to characterize materials, and more importantly the interface between the semiconductor and electrolyte, is extremely important in aiding the materials community to turn the right knobs to create new viable materials. It is very important for the materials community to rely on the tool chest more to better understand how changing certain parameters affects band edge positions and how strong the knob really is.
- The approach is to create a tool chest of evaluation techniques and equipment that can be used to assess a wide spectrum of potential PEC materials and samples.

- This project is applying vacuum X-ray, photoelectron, and nano-imaging methods to semiconductor systems. This work raises important questions as to validity of applying uniform bandgap from surface to bulk. This project is well-integrated with other efforts.
- This project participates in the overall planning and scheduling activities of the PEC Working Group and executes mutually agreed work and schedules for the PEC Working Group participants.

Question 3: Accomplishments and progress towards overall project and DOE goals

This project was rated **3.8** for its accomplishments and progress.

- This project has made excellent progress in analyzing and interpreting the samples supplied by the PEC Working Group.
- Based on the tasks and budget, the characterizations completed were done well. AFM analysis of the gallium indium phosphide surface is particularly interesting. The corrosion looks like localized cathodic or anodic reactions, which implies non-uniform sites (composition) at the surface. The AFM in the transition region is accounting for what looks like a direct current component to the slope and appears to have build-up and erosion. This type of data provides important feedback to the synthesis and corrosion modeling group.
- The progress of this project is somewhat controlled by the samples provided by other group members. It appears to be providing useful information that others might have difficulty obtaining themselves.
- Characterization results from this project have consistently identified differences among samples previously thought to be identical and provided explanations for unexpected performance. The procedures for sample preparation, handling, and shipping have evolved to allow the observation of materials changes accompanying changing operational environments such as photoactivity, charge transport, and electrolyte exposure. In collaboration with theoretical groups participating in the PEC Working Group, as well as other institutions, this project has achieved a first-of-its-kind code validation through the comparison of calculated valence band spectra with X-ray emission spectroscopy mappings. Another outstanding accomplishment for this project was the development and water-testing of an in-situ cell permitting characterization of interface states in contact with liquids. The replacement of water with electrolytes can help enormously in explaining the mechanisms and possible remediation of stagnant corrosion processes of photoactive PEC materials. Additional cell development would permit characterization under simulated photoactive conditions and observations of surface states accompanying PEC performance. Data collection under these conditions has never before been possible and it is impossible to predict what understanding could accrue due to this development. Iron oxide characterization may possibly explain why this material violates the expectation that it should perform better than most other PEC materials. Whereas the observed bandgap is favorable, the bare interface band edges barely straddle water redox levels. When the electrolyte is introduced, effects on the effective bandgap and movement of band edges need to be measured to correlate the PEC-functional conditions of iron oxide with the necessary conditions. The introduction of photoactivity and charge exchange processes could further modify material states sufficiently to explain why iron oxide does not come up to performance expectations.

Question 4: Collaboration and coordination with other institutions

This project was rated **4.0** for its collaboration and coordination.

- The team appears to work in very tight coordination with the PEC Working Group.
- The team is trying very hard to make its instrumental capabilities relevant and helpful to the other Working Group members.
- This project collaborates exceptionally well with the PEC Working Group and participates in both national and international collaborations with other groups with similar technical objectives.
- By definition, the efforts of this project require collaborations. In some respects, a negative would be that the researchers are entirely dependent on the collaborators to provide materials for testing.

Question 5: Proposed future work

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

- Developing the SALSA technique for semiconductor electrodes looks very interesting. However, this project still has to wait on other group members to provide samples to study.
- The reviewer is interested in the continued development of the in situ spectroscopy and validation as an experimental technique. This is a key part of characterization and better understanding the various PEC material classes. The reviewer would like to see a continued partnership with the Ogitsu group to complete the loop between the characterization and modeling of PEC materials.
- The proposed future work should emphasize the need for investment in cells and the equipment necessary to undertake in situ characterization of PEC materials under active operational environments.

Project strengths:

- These characterizations are highly precise and offer tremendous insight into the chemical environment at the semiconductor surface.
- This effort is a very good match with and complementary to the PEC Working Group.
- This project has great capabilities in surface analysis when applied to PEC problems, getting data that is clearly insightful and useful.
- The outstanding technical skills of the project personnel is a strength, along with other PEC Working Group projects' access to international capabilities and world-class materials characterization capabilities.

Project weaknesses:

- While not strictly a weakness, the project is dependent on PEC materials being supplied to them, and does not directly control the research direction or investigation.
- This may be beyond the purview of the Heske group, but it would be good to see a bit of a technological pull in asking for future materials. As experts in characterizing the band edge positions at the interface, there must be some insight, ideas, or personal interest regarding modifications to the current material classes or seeking other materials of interest for future testing and evaluation. It is also not clear to what degree these efforts have aided the materials community in turning knobs to improve the PEC response. This reviewer wants to know if there is follow-up after the characterizations to see how this information can be applied and utilized to make a better PEC material.
- The principal investigator may have to wait on other groups to provide samples worth examining.
- The inadequate availability of infrastructure support to ensure continuing development and availability of the unique capabilities of this project is a weakness.

Recommendations for additions/deletions to project scope:

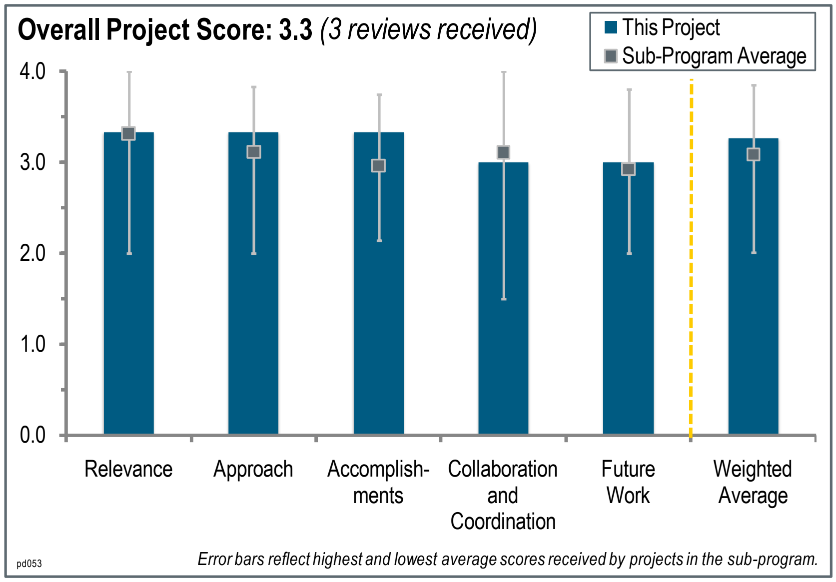
- If the University of Nevada, Las Vegas group was allowed to make its own samples, it could chart its course better and perhaps garner a higher reviewer score. However, real collaboration involves a division of labor, where each group contributes what it is good at in a complementary manner. This project is doing a good job with the funding received and should continue in the present mode of operation where the researchers are concentrating on getting XPS-related insights on what is happening to other groups' samples.
- In situ cell development and accompanying equipment investment is necessary to permit full operational PEC characterization capability.

Project # PD-053: Photoelectrochemical Hydrogen Production

Arun Madan; MVSystems/Hawaii Natural Energy Institute

Brief Summary of Project:

The overall objective of this project is to develop a monolithic hybrid photoelectrochemical (PEC) device powered by MVSystems' low-cost amorphous-silicon (a-Si)-based tandem solar cell. Three material classes are covered in this project: amorphous silicon carbide (a-SiC), tungsten oxide (WO_3), and I-III-VI2 (copper chalcopyrite-based). Project objectives are to achieve a solar-to-hydrogen efficiency of 5% and a durability of 200 hours, to increase to 500 hours by the end of phase II.



Question 1: Relevance to overall U.S. Department of Energy objectives

This project was rated **3.3** for its relevance to U.S. Department of Energy (DOE) objectives.

- This project is highly relevant to supporting the Hydrogen Production sub-program. The focus on prototyping viable devices is especially encouraging.
- The goals and relevance of this project are clearly laid out. However, the stated goals for this project are much less than what is needed in a finished system. This project should also include a long-term durability goal.
- The researchers are aware of relevant DOE Hydrogen and Fuel Cells Program targets.

Question 2: Approach to performing the work

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

- This project is trying to make an efficient, durable PEC cell out of multijunction a-Si. It has three distinct approaches to accomplishing this objective and seems to be well focused.
- This project is a collaboration between several groups and targets three primary materials for PEC hydrogen. Two of the materials, copper indium gallium diselenide (CIGS) and a-Si, have a historical basis in the photovoltaic (PV) community, and there is a good understanding of the issues regarding fabrication and performance of the materials. The concept of multijunction represents a viable approach to achieving the performance required for DOE milestones. However, the complexities with fabrication and integration into a system might make it difficult to achieve the targeted price per kilogram of hydrogen.
- This project breaks the investigation down into three materials systems, which are each examined and addressed individually.

Question 3: Accomplishments and progress towards overall project and DOE goals

This project was rated **3.3** for its accomplishments and progress.

- Three materials were presented, each having its own accomplishments:
    - Amorphous silicon carbide (a-SiC): Based on last year's results, only modest success has been made with pushing this technology forward to a viable state. The researchers have identified a primary issue with

carrier mobility across the a-SiC/electrolyte interface. However, the more the top surface of this device becomes catalyzed, the more it starts to look like an integrated PV-electrolysis system.
    - Tungsten trioxide (WO3): This as a useful system to validate concepts for multijunction devices and to aid the development of modeling techniques, and to this end, WO3 is still an important material. Unfortunately, there is no obvious path toward viably improving the bandgap. What enables WO3 to work as well as it does are its favorable transport properties for carriers, which are unusual for metal oxide semiconductors. It has to be recognized that deviation from the pure material effectively compromises the good transport. Although copper tungstate (CuWO4) may indeed show an appropriate bandgap, there is nothing to suggest that the transport properties will be any better than any other oxide.
    - Copper indium gallium diselenide (CIGS): This is an interesting material class because the PEC community can leverage the knowledge gained through its developments within the PV community. The base material has many of the attributes necessary for effective PEC hydrogen, with the primary issue being a bandgap that is too low. Good progress has been made on moving this material forward. A drawback is that the current progress is toward a PV-PEC hybrid, and how that would compare in cost and performance to a PV-electrolyzer is unknown.
- This project achieved high efficiency (4.3%) with a copper gallium diselenide (CGSe) material system. However, the durability and lifetime investigation seems to be limited to testing durability rather than assessing mechanisms for degradation. The projections of three configurations for the CGSe system (current, intermediate, and ultimate) are a very useful and an illustrative layout of device development.
- The proprietary catalyst layer enables performance enhancement by improving kinetics at the electrode/electrolyte interface with a sputtered metal catalyst. The noble metal nanoparticles look expensive, but there are encouraging results with CuWO4.

Question 4: Collaboration and coordination with other institutions

This project was rated **3.0** for its collaboration and coordination.

- This project does a very good job of interacting with other members of the PEC Working Group to fabricate the three classes of materials and facilitate characterization.
- This is a well integrated team.
- The researchers have a narrow focus and a proprietary interest to protect, and there does not appear to be much collaborative activity.

Question 5: Proposed future work

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

- Concrete proposals have been put forth to circumvent the identified issues with the three materials classes. The proposed solutions are narrowly targeted and should clearly determine if these materials are viable candidates for cost-effective PEC hydrogen.
- The areas of investigation for each material system are clearly defined and reasonable.
- There is adequate progress on each task to warrant the projects continuation. It looks like it will be the CIGS that gets the researchers past the Program objectives.

Project strengths:

- The reviewer is pleased with how the project leverages state-of-the-art practices from solar cell fabrication to enable viable PEC devices. It is important to move the overall PEC program to development of prototype systems, even if efficiencies are quite low. This will be instrumental in validating the DOE economic models.
- This project already has a fairly good PV cell to build upon. A good vacuum apparatus gives the researchers the capability of trying modifications with little difficulty.

Project weaknesses:

- Each of the champion materials has issues and, in spite of efforts to resolve each material's "Achilles heel," only modest progress has been made in moving the performance toward DOE's stated goals.
- The fabrication apparatus does not appear to be a continuous roll. This reviewer wanted to know if this method is going to be capable of scale-up, especially the monolithic integration. Coupling PV cells to augment performance of the PEC cell could be programmatically dangerous and critics might argue that the logic points toward PV-electrolysis.

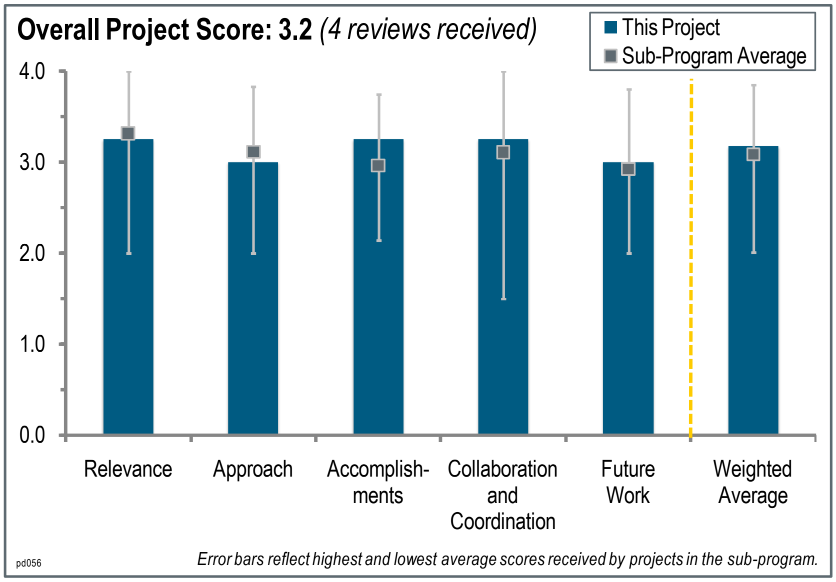
Recommendations for additions/deletions to project scope:

- The role for this project should be narrowed to compliment the strengths of this group. The focus should be on taking the three materials to the next step and attempting to fabricate fully working electrodes that can be integrated into a small-scale system.
- This reviewer would like to see a statement of the upper-bound solar-to-hydrogen of each system. This would gauge the potential of each material system.

Project # PD-056: 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 the critical technologies required for the 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 photoelectrochemical (PEC) cells: (1) an immersion-type PEC cell in which the photo-electrode is immersed in the electrolyte; and (2) a substrate-type PEC cell in which the photoelectrode is not in direct contact with the electrolyte. During the recent go/no-go review in December 2010, it was decided that the immersion-type PEC work will proceed into the second phase and the substrate-type PEC work would come to an end. It was also determined that the transparent, conductive, and corrosion resistant work will proceed and the photoactive semiconductor work will be halted.

Question 1: Relevance to overall U.S. Department of Energy objectives

This project was rated **3.3** for its relevance to U.S. Department of Energy (DOE) objectives.

- As outlined in the Hydrogen Production sub-program overview in the plenary session, PEC hydrogen production seems to be a large component of the funded research. As such, this project is an appropriate fit. In addition, the research clearly supports the research and development goals and objectives. By leveraging efficient, low-temperature, scalable/processable, and stable light absorbers made from well understood materials (i.e., silicon), the project is geared toward rapid prototype production and scale-up.
- This project is focused on meeting DOE Hydrogen and Fuel Cells Program objectives with multiple materials and configurations.
- The project is a straightforward effort to produce low-cost hydrogen using renewable energy. However, it has to compete with a number of other approaches to renewable hydrogen that are currently less expensive.
- If the technology can be demonstrated at the costs claimed, this approach could be very competitive. However, more analysis (or at least reporting) is needed of the critical issues that need to be addressed, where the efficiency losses are, what kinds of land use would be required to reach the needed loads, and why this approach is better than a straight photovoltaic (PV) cell based on the same amorphous silicon (a-Si) technology and an electrolyzer.

Question 2: Approach to performing the work

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

- The increased organization in comparison to last year's renewal is duly noted. The barriers that have been addressed are clearly explained.
- This project made good use of the go/no-go decision process. However, the slides did not always seem to be in agreement with the down-selection decisions.

- The chemistry and materials science work seems fairly well designed. Again, a better and more thorough cost analysis is warranted now that the team has shown some technical feasibility and has a better idea of the efficiencies and construction that will be needed. This is especially important for the balance of plant in terms of separating and storing the product gases, which currently represents a significant portion of hydrogen generation costs and did not seem to be considered here.
- The researchers appear to be taking a PV cell that already works well on its own and attaching exterior layers that will protect it from the electrolyte, conduct electrons, and be catalytic toward water-splitting. That involves putting an anode catalyst on indium tin oxide that is active and optically transparent, as well as can be deposited via a continuous process, and then putting high-surface-area nickel onto the steel substrate.

Question 3: Accomplishments and progress towards overall project and DOE goals

This project was rated **3.3** for its accomplishments and progress.

- Significant progress has been made since last year, and the team is more focused on a single pathway and showing some practical demonstration level.
- Work is progressing according to schedule.
- The immersion-type PEC cell seems to be a rather promising technology and has met all targets that have been assessed ahead of schedule. Although not directly stated, successful transparent, conducting, and corrosion resistant (TCCR) materials could be integrated with other effective PV technologies due to the low-temperature synthesis and generality of the TCCR materials, possibly enabling other PEC hydrogen projects to reach their DOE goals. The reviewer did not rate this project as a four because there are still some undetermined targets to assess (e.g., efficiency and cost) that may be major impediments to the successes of these materials and architecture.
- The effort seems to be mostly focused on developing cobalt oxide (Co3O4) as an anode catalyst. Improvements on transparency while maintaining activity were noted, although the fact that some faded after several hundred hours was noted as well. Low voltage drops across the Co3O4 layer was an achievement, but it is uncertain whether that measurement should be made under load instead of open circuit. A lot of effort was expended on the nickel cathode as well, with reasonable success. The multideposition/leaching process appeared to be pretty tedious; there must be a better way to put down porous nickel in an energy efficient manner.

Question 4: Collaboration and coordination with other institutions

This project was rated **3.3** for its collaboration and coordination.

- Introducing the additional collaboration with Sun Catalytix is a great step toward realizing the group's goals. The previous partnerships with the a-Si triple junction company (Xunlight) and John Turner (National Renewable Energy Laboratory [NREL]) resulted in a well-rounded scientific team.
- This project has a good set of collaborators well known in the PEC field.
- The collaboration between the University of Toledo and Xunlight appears to be close, but it is not at all clear what NREL is contributing to this work. It is also not really clear what the relevance of the Sun Catalytix catalyst is if the team already has a process for making rolled goods.
- Each entity appears to have specific objectives and contributions, although it is not clear what the difference is between Xunlight and Midwest Optoelectronics, LLC. The contribution from Sun Catalytix is a bit mysterious (a nice photo with lots of fizzing, but no data of any kind), and it is not listed in the title as a collaborator. Nevertheless, the amount of area on the poster describing its effort effectively makes it a collaborator.

Question 5: Proposed future work

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

- The increased focus in this year's renewal over last year's is clear. The go/no-go decisions were appropriately made. However, there was no mention of any subsequent decision points, which would be nice to incorporate. It

would also be advisable to present alternative strategies in case the current best cobalt-based, immersion-type systems do not meet target efficiencies or costs.
- The project is coming to an end soon, and future work should be mostly focused on an end analysis of where this technology has reached and how the costs compare.
- The project's direction toward scaling up is obvious, but the researchers may not be ready. While they had plenty of data on depositing Co3O4, there was very little on the performance of the cell itself. The 4-inch (in) by 4-in. cell appeared to be complete, but the table has "not applicable" for the immersion cell in 2010, and "to be determined" for 2011. This reviewer asked how the researchers could have run a cell for 606 hours and not made an efficiency measurement. It appears to be another year of small-cell testing.
- This project is moving forward with down-selected compositions and configurations.

Project strengths:

- This project is a much-needed research endeavor. Use of proven a-Si technologies for large photovoltage PEC devices is a solid research plan. The identification of thin films of TCCR material using a modular testing approach is essential to this proposed work.
- The roll-to-roll processing is an important advancement that enables the reduction of edge effects for better data and also demonstrates a pathway for end manufacturing.
- This project is attempting to build a PEC cell around an efficient PV cell that can be mostly made through a continuous process.

Project weaknesses:

- The device efficiency and cost for the immersion-type PEC cells is still yet to be determined. The 5% solar-to-hydrogen efficiency for the substrate-type PEC device is not promising, as those systems do not suffer from the same optical complications and photocorrosion stability issues as the immersion-type cells.
- As with many of the PEC projects, there is so little focus on balance of plant that it is difficult to understand where this technology is really going to fall in terms of efficiency and cost versus existing, more-established technologies.
- Whether the researchers are really ready to scale things up is unsure. There is a lack of performance data. The presenters indicate that two tasks were dropped last year, yet much of their effort was dedicated to them. The researchers did good work, but it was confusing trying to correlate their accomplishments with those tasks that were being continued over those that had supposedly been dropped.

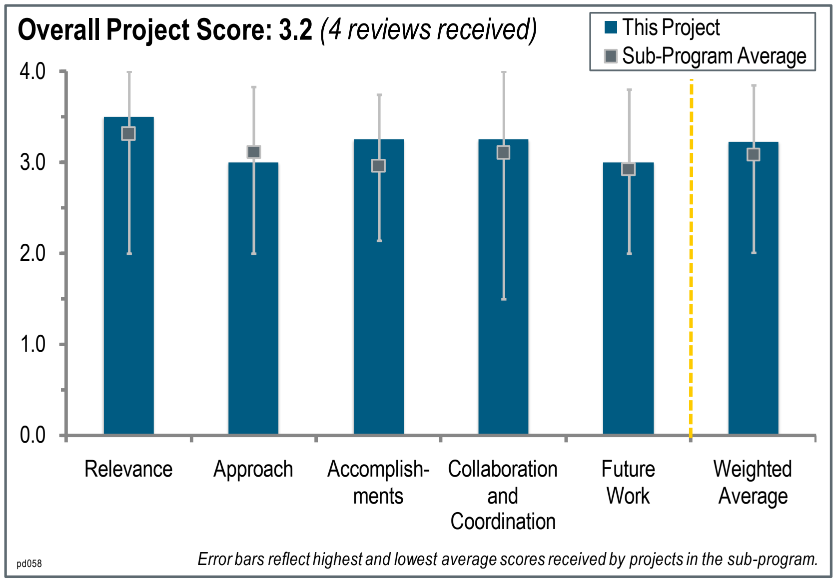
Recommendations for additions/deletions to project scope:

- The voltage drop across the TCCR/PV-cell layer stack should also be assessed near the maximum power point of the current-voltage curve, operational current density, or proposed target current density (e.g., 10 milliamps/square centimeter). There is contact resistance and interfacial fields between the materials that will be present under open-circuit conditions, but the iR potential drop is current dependent and would have a large impact on the overall operational device performance. The durability and stability metric needs to be better defined as "a certain percentage of initial activity remaining after a given time period." The spinel Co3O4 seems rather unstable (approximately 50% loss by 481 hours), and this reviewer would argue that the 2012 target of approximately 700 hours stability is far from being achieved. Although large electrodes are ideal and proposed, there could be large complications from solution iR potential drop for more efficient systems. Proposing a smaller-sized prototype may be in order. The absorption of spinel Co3O4 resulting in 65%–75% temperature from 250–500 nanometers will significantly hinder the performance of the largest bandgap amorphous silicon (a-Si) cell. It may be wise to explore additional TCCR materials or, as stated by the researchers in their presentation, focus on the fabrication of very thin layers. An alternative would be to reinvestigate the bandgap sizes of the a-Si, triple-junction PV so that even with shading of the top a-Si cell, maximum photoelectrical properties can be achieved.

Project # PD-058: Characterization and Optimization of Photoelectrode Surfaces for Solar-to-Chemical Fuel Conversion

Tadashi Ogitsu; Lawrence Livermore National Laboratory/National Renewable Energy Laboratory

Brief Summary of Project:



The objectives of the project are to: (1) develop a theoretical tool chest for modeling photoelectrochemical (PEC) systems; (2) compile a publications database of research on relevant photoelectrode materials; (3) uncover the key mechanisms of surface corrosion of semiconductor photoelectrodes; (4) understand the dynamics of water dissociation and hydrogen evolution at the water-photoelectrode interface; (5) evaluate electronic properties of the surface and water-electrode interface; (6) elucidate the relationship between corrosion and catalysis; (7) provide simulated X-ray spectra to the University of Nevada, Las Vegas for interpretation of experimental results; and (8) share research insights with the PEC Working Group members.

Question 1: Relevance to overall U.S. Department of Energy objectives

This project was rated **3.5** for its relevance to U.S. Department of Energy (DOE) objectives.

- This work may provide the key understanding in choosing the appropriate materials to research for PEC hydrogen, and therefore is extremely relevant to DOE objectives.
- This project is doing important background work to understand basic corrosion mechanisms, but it is at such a seemingly basic and fundamental level as not to have direct application to PEC systems. The material set may not be appropriate to achieve relevance.
- The techniques in this project provide the only way to understand the energetics of interactions between electrolytes and solid-state interfaces. Such an understanding appears to be critical to understanding and predicting the consequences of photoactive and charge exchange processes that are essential to PEC.
- This project is aware of DOE objectives with regard to photoelectrochemistry.

Question 2: Approach to performing the work

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

- The molecular dynamic simulation is an important tool in developing the PEC materials. The validation of simulations for the simple system indium phosphorus and gallium phosphide is an important first step. It is true that the binary solution is easier to calculate, but it is important for the simulations to model the material that is under testing in the laboratory so correlations can be drawn.
- The reviewer likes the broader view of what they are trying to accomplish (slide 4).
- This project is applying the available skills and resources to its assigned objectives with vigor and dedication. The downside is the turn-around time for quantifying states and dynamics for identified materials and electrolytes. Some effort should be applied to identifying underlying common themes of

performance and establishing rapid incorporation of such themes in a detailed study of concepts. A specific study should be undertaken to quantify information quality in terms of simulation scale and computational methodology in an effort to reduce turn-around time.
- The selection of examined materials does not match very well with PEC materials under investigation elsewhere.

Question 3: Accomplishments and progress towards overall project and DOE goals

This project was rated **3.3** for its accomplishments and progress.

- Based on the budget and tasking, this project did a great job. Models were successfully created for the III-V semiconductor system and three corrosion scenarios were identified. It is important, now that these results are compared to the experimental results from the National Renewable Energy Laboratory's (NREL) efforts in III-V systems and to Heske's characterizations, to close the loop and provide direction for future efforts.
- The relationship of possible hydrogen release mechanisms to localized energy states is an outstanding accomplishment. The proposed corrosion mechanism is outstanding, but needs to be accompanied by identified and quantified remediation measures. In collaboration with the PEC Characterization Project, as well as with other theoretical groups, this project has achieved a first-of-its-kind code validation through comparison of calculated valence band spectra with X-ray emission spectroscopy mappings.
- This project has made significant progress, but needs to have a practical application and not just add to theoretical understanding.
- This reviewer realizes the researchers only have so much manpower and computer time, but they seem stuck on III-V semiconductors. Verifying the X-ray spectra is encouraging and a literature search was mentioned. This reviewer wanted to know if there is any experimental data to verify what the researchers have predicted so far.

Question 4: Collaboration and coordination with other institutions

This project was rated **3.3** for its collaboration and coordination.

- The basis for this project is collaborative in nature and does a very good job leveraging the talents of NREL and the Heske group.
- This project reflects highly specialized and relatively unique skills, but has integrated exceptionally well within the PEC Working Group. Members of this project and the distributed skill sets among Working Group participants are all working effectively to establish common grounds for communications within a widely disparate set of technical backgrounds.
- Until this project can expand its effort to look at other systems, collaboration will be limited to only those groups studying III-V semiconductors.

Question 5: Proposed future work

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

- This reviewer likes the future work (applied bias, surface nitrogen atoms, and gallium and indium together) and hopes it will not take too long to achieve it.
- The proposed future work integrates well with the PEC Working Group plans and priorities, but resources, as well as the complexity and difficulty of the work, will inhibit timely progress. Milestones six, seven, and eight are very important to the III-V tasks scheduled by other Working Group participants, but will lag behind the schedule others need to meet.
- The future work appears to focus on attempting to find a specific solution to the III-V corrosion problem. The limited resources might be better served studying some of the other materials systems in the Working Group, such as amorphous silicon carbide, copper indium gallium diselenide, or molybdenum disulfide (MoS_2) to better understand the issues regarding these materials.
- The principal investigator understands that future work needs to focus on strengthening the feedback cycle with experimental collaborators to provide specific suggestions for device improvement.

Project strengths:

- These types of simulations can really elucidate the issues that take place at the semiconductor electrolyte surface.
- This project has a powerful predictive capability that has been verified at least by X-ray spectra.
- The project members have exceptional skills and dedication and access to super-computer capabilities.

Project weaknesses:

- There needs to be a better effort in correlating the models with actual experimental data derived from working systems.
- This is elegant work, but this reviewer cannot see the logic of how modeling hydrolytic oxidation of gallium indium phosphide in complete detail makes for a better PEC cell. It would be good to see the "theoretical tool chest" used to fix some other systems. The pay-off from this work will be apparent when someone can propose a surface treatment to prevent surface oxidation or enable hydrogen or oxygen evolution, and this project will accurately predict whether it is going to work. That day seems to be rather far off.
- Turn-around time for simulations must be shortened if this capability is to remain useful to the PEC project objectives. Whereas the knowledge accruing to successful simulation of PEC system behavior will be useful and valuable, it will be so to the PEC project only if the product becomes available in time for interpretation and application to existing PEC project objectives.

Recommendations for additions/deletions to project scope:

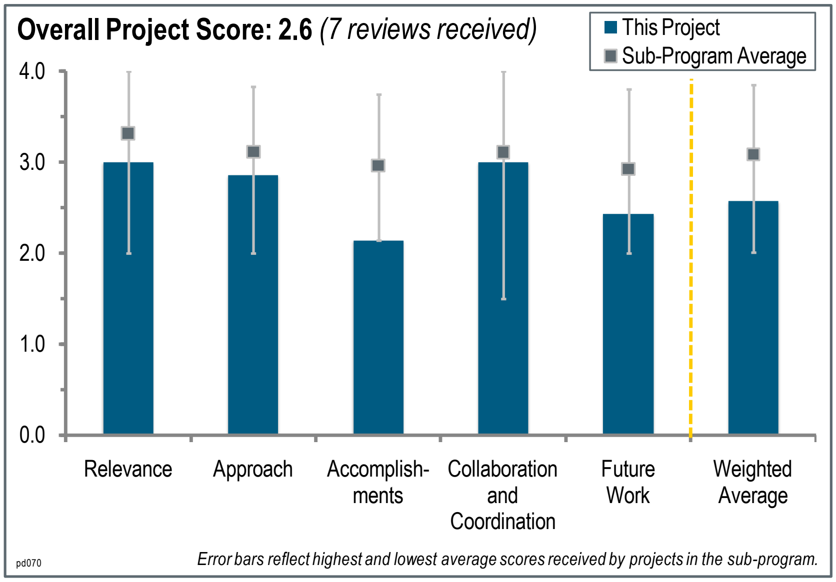
- This reviewer thinks that these models could first be applied to only the dynamics of the catalytic hydrogen evolution reaction (HER); for example, Jaramillo has experimental results on the HER performance of MoS2. As the models are refined, the dynamics for a photo-catalyst could then be explored and validated.
- This project should consider the selection of materials under investigation and strengthen feedback with developers so that knowledge gained on the project becomes actionable.
- This team should comprise an element of a small group of chemicals, materials, and theoretical experts convened to seek a methodology to select PEC materials candidates and winnow to a few promising materials for detailed investigation.

Project # PD-070: One Step Biomass Gas Reforming-Shift Separation Membrane Reactor

Michael Roberts; Gas Technology Institute

Brief Summary of Project:

The long-term goal of this project is to determine the technical and economic feasibility of using the gasification membrane reactor to produce hydrogen from biomass. The short-term goal is to evaluate synthesized metallic and glass ceramic membranes to fabricate a module for testing with the bench-scale gasifier.



Question 1: Relevance to overall U.S. Department of Energy objectives

This project was rated **3.0** for its relevance to U.S. Department of Energy (DOE) objectives.

- This project appears to be viable and likely to lead to a commercial process whereby hydrogen of sufficient purity can be produced from biomass. As such, it meets DOE research and development objectives.
- This project supports the DOE Hydrogen and Fuel Cells Program goals of lower-cost hydrogen production.
- The project objectives are in line with DOE's goals.
- This seems like the most viable approach for the production of hydrogen from biomass and should be investigated and supported. The specific use of a membrane within the gasifier or after the first cyclone is challenging but interesting.
- Producing hydrogen from biomass with power cogeneration can increase efficiency and reduce carbon footprint.
- While reducing the overall cost of renewable hydrogen production from biomass is an appropriate goal consistent with DOE objectives, the project supports this goal only partially. It is more focused on membrane development with the assumption that it will make a major impact on cost. This assumption is doubtful and first needs to be validated.
- The relevance of this work is poor because it presents membranes as the preferred way of doing separations. It is unclear what is wrong with other approaches, such as pressure swing adsorption (PSA).

Question 2: Approach to performing the work

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

- The approach is a logical sequence of tasks and milestones.
- The project addresses efficiency improvements by way of potential simplification through the proposed "one-step" biomass reforming and water-gas shift (WGS) separation reactor.
- This project first needs to evaluate various perspective costs; technology readiness; and risks, such as how membranes fare versus other gas separation options.
- The potential increase in hydrogen production efficiency and cost reduction ascribed to the process appears reasonable, but Hydrogen Analysis (H2A) cost modeling could provide more convincing evidence. The advantages described on slide 10 of the project presentation might be quantified to provide additional support for continued work and should allow one to see which is the most critical avenue. The preliminary analysis did not provide the needed justification.

- The approach seems mostly to aim at the evaluation of different candidate membrane systems. It would be helpful to have a summary of the different membrane approaches and their potential positive and negative factors. The approach of using a membrane seems risky, but high risk can have high rewards. However, there does not seem to be much discussion of the potential issues other than dealing with sulfur. For example, tars could easily contaminate the membrane and not be easily removed by shock pulses. It seems like the really difficult work is being put off until the later stages.
- It is not clear if the current project has been affected by the funding delays; however, the lack of progress and moving the location of testing is all due to the one-year hiatus. The project does not appear to have sufficient funds to resolve many of the critical issues still outstanding. The project should be re-scoped to manage the lower funding levels.
- Overall hydrogen production cost reduction is the goal, and the approach of using a membrane integrated with the WGS reactor does not sufficiently address the end goal. The impact of cost saving through this is not expected to be significant. This, to a large extent, may be a programmatic issue and should be examined closely.

Question 3: Accomplishments and progress towards overall project and DOE goals

This project was rated **2.1** for its accomplishments and progress.

- The process model and tasks appear to be well designed and the fabrication of five palladium-based alloys is a plus. However, the progress on bench-scale modifications of the biomass gasifier (task three) is not clear.
- Relative to the 2010 presentation, significant progress has been made in membrane screening and economic analysis. However, a few of the presenter's slides convey minimal information, and better slides could have been selected (e.g., slides 17–19). Moreover, it is difficult to know how good the membrane performance is relative to what is required. The production of hydrogen at $1.50 per kilogram does not seem to be credible, although the reviewer admits to not being competent enough to look into the details of the analysis.
- This project needs to do the opportunity analysis first, then actual development work around membranes if feasible.
- The short-term goal defined on slide five of the presentation is an evaluation of synthesized metallic and glass ceramic membranes to fabricate a module for testing with a bench-scale gasifier. The technical accomplishments section did show hydrogen permeate for three membranes, but not enough information was provided to say whether the short-term goal was met. This project needs to expand on the preliminary economic analysis. It was noted that membrane testing was put on hold, so this aspect of the work was beyond the project's control. The data on slide 15 gives a permeability of 0.25, but the permeability of the metal membranes on slide 13 is on the order of 0.00000001. This reviewer missed this difference in the preliminary "look-over" and in the actual presentation, and did not ask a question about it during the review. The importance of electronic conductivity could not be appreciated because it was only supplied for the glass-ceramic membranes.
- While some progress has been made in membrane development and testing, the fundamental premise is questionable. There are several issues with the logistics of the program, which are discussed below.
    - The main problem is that the preliminary economic analysis presented in slide 21 shows that the net cost of hydrogen using the membrane approach is slightly higher than that with PSA. If so, this reviewer wants to know he motivation for doing this work.
    - Test results with different types of membranes are presented, but it is not clear if the type of membrane is down-selected, and what that is. This reviewer wants to know which membrane is used in the economic calculations.
    - Based on the configuration shown, if the membrane is placed after the first cyclone, the impact of particle impingement on the membrane surface at the high temperature needs to be addressed.
- This project needs more progress in membrane development.
- There has not been a great deal of progress on developing new membranes for hydrogen purification that come close to the goal of 250 standard cubic feet per hour per square foot of flux. Also, there is no specific temperature used for testing, and the results are shown in both Fahrenheit and Celsius. More modeling work has been accomplished than experimental, but this may be due to the funding issues.

Question 4: Collaboration and coordination with other institutions

This project was rated **3.0** for its collaboration and coordination.

- This project's collaborations are excellent.
- The collaborations complement Gas Technology Institute's experience well.
- There seems to be some good collaboration in terms of membrane development and module design.
- The work to date reflects good coordination between partners, especially with membrane manufacturers.
- The collaborations are adequate.
- More details on partner accomplishments would have been more informative. The difference in units, source pressures, differential pressures, and general test conditions may be due to the different organizations conducting the work. No one organized the data for the presentation.
- This project needs to involve more industry partners.

Question 5: Proposed future work

This project was rated **2.4** for its proposed future work.

- The proposed technical work is excellent, but an economic analysis is the most critical.
- The future work supports the overall project scope, but could be more specific to the activities and milestones in the coming year.
- The proposed future work is fairly generic and primarily focuses on ongoing membrane development. Again, it is useful to know where the performance is relative to where it needs to be, and to understand which approach might have the most promise and why. Otherwise, the work seems pretty open-ended.
- The proposed work plan is reasonable with respect to experimental work, but the priority needs to be changed. It is recommended that the economic analysis be firmed up first to establish a basis for doing the membrane work. The go/no-go decision should be based on the economic incentive.
- If funding is to be an issue in the future, it would be better to re-scope the project based on what has already been learned. The projected work tasks may be important for the whole project objective, but the work should be specific to the lower funding amounts provided.
- This project needs to consider the effect of biomass feed variability on the selected membrane. Thermal shock; stress; and durability tests are critical, especially with the metal, glass, and ceramic membrane modules.

Project strengths:

- This project is an interesting concept and has good collaborations.
- The researchers' technical knowledge is good.
- This is a good team and a reasonable proposed work plan based on anticipated funding.
- The metal membrane manufacturing and module design is a strength of this project.
- This project has good understanding and capabilities with respect to membrane development.

Project weaknesses:

- It is not clear whether the key performance issues and tests are being done, or if they are being delayed (e.g., realistic feedstocks).
- The economic analysis with respect to this project and PSA was not convincing.
- The work scope of this project was reduced based on available funds, but no priorities appear to have been changed with its schedule.
- The relative location of the reactor membrane relative to the cyclone may result in membrane fouling. There are also not enough hydrogen-permeability tests.
- The program basis should be re-examined.

Recommendations for additions/deletions to project scope:

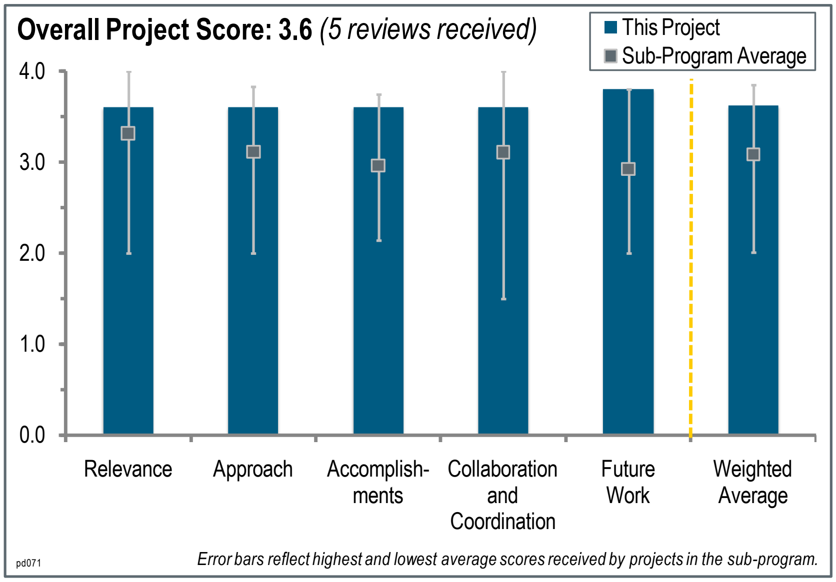
- This project should conduct longer-term tests to check for membrane stability and fouling.
- A quick membrane screening via hydrogen permeation tests is suggested.
- Follow the recommendations stated above.

Project # PD-071: High Performance, Low Cost Hydrogen Generation from Renewable Energy

Katherine Ayers; Proton Energy Systems

Brief Summary of Project:

The objectives of this project are to: (1) improve electrolyzer cell stack manufacturability, including consolidation of components, incorporation of alternative materials, and improvement of electrical efficiency; and (2) reduce the cost of electrode fabrication, including reduction in precious metal content and alternative catalyst application methods.



Question 1: Relevance to overall U.S. Department of Energy objectives

This project was rated **3.6** for its relevance to U.S. Department of Energy (DOE) objectives.

- Water electrolysis is a near-term pathway of the DOE Office of Energy Efficiency and Renewable Energy, Fuel Cell Technologies Program's Hydrogen Production Roadmap. The project, based on polymer electrolyte membrane electrolysis, aims to improve electrolyzer system efficiency and reduce capital cost by integrating it with renewable electricity. All of these goals are well aligned with the objectives of the DOE Hydrogen and Fuel Cells Program.
- Reducing the capital cost and improving performance of the electrolyzer is critical to the Program. This project clearly addresses both of those areas.
- This project is highly relevant to DOE's goals and objectives and addresses both component and system-level issues and barriers.
- This project is focused on hydrogen production costs, but neglects the goal of efficiency. In 2010, its efficiency was reported as 64%, while Giner Electrochemical Systems, LLC (GES) reported 75%. Proton Energy Systems did not address efficiency in 2011.
- It is not clear whether electrolysis can ever be more than a transitional technology, considering the costs of using electricity directly (as in battery electric vehicles) versus converting it to hydrogen and then back to electricity. Hydrogen costs are only as low as they are due to unrealistic assumptions about electricity costs (this is not a project issue, but a DOE issue).

Question 2: Approach to performing the work

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

- The approach to stack cost reduction is good. The tasks include catalyst optimization, new flow field design, and alternate materials for plates that could be easier to manufacture.
- This is a very focused and well planned approach. This project has made good use of the available resources through partnerships with volume manufacturers, academia, and national laboratories. Design for volume manufacturing is a key area of cost reduction.
- This project has a very sharp focus and has paid outstanding attention to cost reduction.
- This project is very well designed and focuses on the critical barriers.

- The team fully exploited the work started in 2010 to obtain significant advancements. The reduction in noble metals using a new application method was 55% in 2010. In 2011, it was 55% for the anode and greater than 90% for the cathode. This appears to be a significant advancement, but the absolute loading was not mentioned. It is not clear why efficiency was not discussed.

Question 3: Accomplishments and progress towards overall project and DOE goals

This project was rated **3.6** for its accomplishments and progress.

- The project has shown progress with significant catalyst loading reduction; improved flow field design, thanks to modeling; and encouraging results with composite bipolar plates tested up to 3,000 hours.
- This project has made excellent progress in reducing cell costs and made good use of modeling to improve plate design. The researchers have addressed a large number of design alternatives and down-selected on those that show the most potential, thus focusing the effort on areas that will have the largest impact on cost reduction. The reduction of catalyst loadings is very significant.
- This project has made excellent progress to date and has a clear path for continued progress.
- This project is rated very high; however, this is one of the highest-funded projects so the value per dollar amount is perhaps not as outstanding.
- Proton has an existing 0.6 square foot cell stack that produces about 1 kilogram per day per cell. Proton's focus on reducing costs for the stack components (e.g., new flow field design and the use of stamping versus machining) is very good and should be profitable as the existing system is retrofitted. It is difficult to gauge progress because most of the improvements are defined in terms of percentages, so it is not clear whether the improvements represent breakthroughs or incremental advances. The Hydrogen Analysis (H2A) results did not appear to be complete and the experimental details were minimal, which hindered this reviewer's understanding. The cell voltages were higher for the Proton electrolyzer than for the GES electrolyzer. Proton's voltages varied between 1.8 volts (V) and somewhat less than 2.0 V for what appeared to be similar conditions, while GES reported 1.72–1.75 V. The higher cell potential at Proton relates to the lower efficiency.

Question 4: Collaboration and coordination with other institutions

This project was rated **3.6** for its collaboration and coordination.

- The team has the appropriate partners to work on cell design and to investigate alternate materials in line with the adopted approach.
- There is good leverage of expertise from the industry, academia, and national laboratories to address specific technical challenges.
- The integration with Pennsylvania State University is an example of a really effective collaboration. The other collaborations are also productive and well coordinated.
- The collaboration with partners is well coordinated and properly integrated, but the number of participants is limited.
- This project has made excellent use of the experts at other institutions.

Question 5: Proposed future work

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

- The future work is clear. A key step is evaluating flow-field materials to demonstrate their stability under corrosive conditions and selecting the best one. The next steps will include prototype testing, scale-up, cost analysis, and implementation of the manufacturing process development.
- This project has a well-planned development path.
- This project’s future work is well planned and laid out.
- The plans are sharply focused on addressing the most critical barriers first.
- H2A analysis should have a high priority.

Project strengths:

- This project has a good approach to increase stack efficiency and reduce cost.
- This project has a well planned and executed development plan. The researchers have considered a large number of options and used modeling tools to select the most promising. There is good integration and leverage with volume manufacturers to make significant cost reductions.
- This company has excellent commercialization experience and is in a good position to assess the most critical issues for system cost reductions.

Project weaknesses:

- It is not clear if the materials testing conditions are representative of an electrolyzer operating under fluctuating power and there is no mention on the operating pressures.
- This project has limited partners.
- It appears that GES and Proton have complementary skill sets. This reviewer thinks that it would be helpful if they work together.

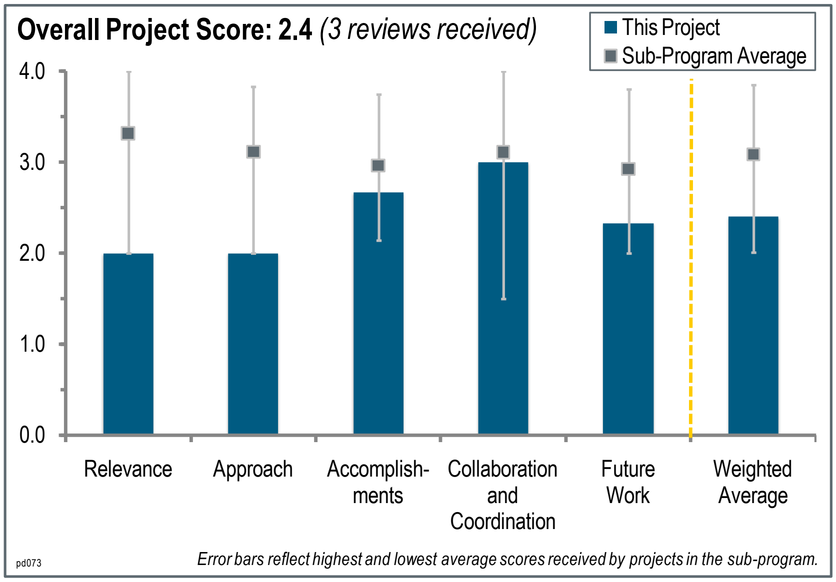
Recommendations for additions/deletions to project scope:

- Materials and coatings compatible with the corrosive environment should be selected, as this is key to meeting the project objectives. Long-term testing is necessary and the tests need to be performed in conditions representative of electrolyzer operation. The H2A cost analysis needs to include the compression.
- This project should continue down the current path with the overall objectives of increasing the electrolyzer to a multi-megawatt size.

Project # PD-073: Zeolite Membrane Reactor for Water-Gas-Shift Reaction for Hydrogen Production

Jerry Y.S. Lin; Arizona State University

Brief Summary of Project:



This project is a fundamental study of the development of chemically and thermally stable zeolite membrane reactors for the water-gas-shift (WGS) reaction in hydrogen production. Project objectives are to: (1) synthesize and characterize chemically and thermally stable silicalite membranes; (2) perform experimental and theoretical studies on gas permeation and separation properties of silicalite membranes; (3) synthesize tubular silicalite membranes under hydrothermal conditions and study gas separation properties; and (4) conduct experimental and modeling studies of the membrane reactor for the WGS reaction.

Question 1: Relevance to overall U.S. Department of Energy objectives

This project was rated **2.0** for its relevance to U.S. Department of Energy (DOE) objectives.

- The project objectives are in line with the DOE Hydrogen and Fuel Cells Program goals.
- This project supports some of the Program's objectives; however, the relevance of the work to overall hydrogen production and delivery is open to question.

Question 2: Approach to performing the work

This project was rated **2.0** for its approach.

- The chemical stability in the presence of hydrogen sulfide is a positive. However, this reviewer does not know if other technologies offer the same or better benefit. It would have been helpful if a comparison had been made to determine if this project meets DOE's research and development (R&D) objectives. For example, the WGS reaction is well understood and pressure swing adsorption (PSA) is a well-developed technology. Without some sort of cost analysis, it is not clear if this technology represents a breakthrough or is worth pursuing.
- The use of a zeolite-based membrane for WGS reactions is a reasonable approach, although it is still at a very basic stage of development.
- Reducing the cost of distributed hydrogen production from natural gas and renewable liquids is the main barrier. This reviewer asked about the impact the proposed work could potentially make on the cost, and what percent of the total cost of hydrogen production could be addressed with this approach.
- Long-term durability and manufacturability, mentioned in last year's review, were not addressed. Silicalite is available primarily as a powder and it is "friable," so its use in a flowing system is questionable. This project appears to be more academic in nature. The cost advantage as a driving force for continued R&D is not presented.

Question 3: Accomplishments and progress towards overall project and DOE goals

This project was rated **2.7** for its accomplishments and progress.

- The technical accomplishments were good, barriers were identified, and progress was made.
- Selectivity improvement results were impressive. Cost reduction was the only barrier identified, but cost and scale-up scenarios did not appear to have been considered.
- The fundamental work on membrane development is good, but more suited for DOE's Office of Basic Energy Sciences program. The main objective and barriers are not addressed. There is no mention of any economic analysis.

Question 4: Collaboration and coordination with other institutions

This project was rated **3.0** for its collaboration and coordination.

- The collaborations appeared to be excellent.
- The project could benefit from more industrial WGS catalyst collaboration in order to have a better grasp of hydrogen cost reduction and scale-up, or even catalyst membrane preparation and cost.
- Much of the collaboration is with other universities or research organizations (e.g., Sintef). Collaboration with the hydrogen production industry would be beneficial in addressing the cost goals.

Question 5: Proposed future work

This project was rated **2.3** for its proposed future work.

- All of the work focuses on fundamental membrane development; however, the justification for doing the work needs to be addressed first.
- The separation and stability work is important; however, the modified chemical vapor deposition synthesis of the proposed new tubular membrane could be a distraction in light of the fact that the project is in its last year. Focus on the obvious concluding step—optimize the WGS reaction or the ultimate scale-up and cost analysis.
- Cost analysis and comparative analysis with PSA should be a priority. Large-scale durability and manufacturability assessments are needed.

Project strengths:

- The researchers' technical knowledge is good.
- The membrane characterization and separation tests are strengths.
- This project has very strong capabilities with respect to material and membrane development.

Project weaknesses:

- The use of supports, such as yttria-stablized zirconia coated on an alumina support, indicates that the zeolite is not durable on a small scale. The need for subsequent modifications for hydrogen/carbon dioxide separation raises questions. This project does not appear to lead to a commercial process for cleaning up the gases in the WGS.
- The addition of system optimization work and a cost perspective would make this a stronger project.
- The project's good work and the end goal of cost reduction seem disconnected. The approach should first be to make a significant reduction in the overall cost of hydrogen production.

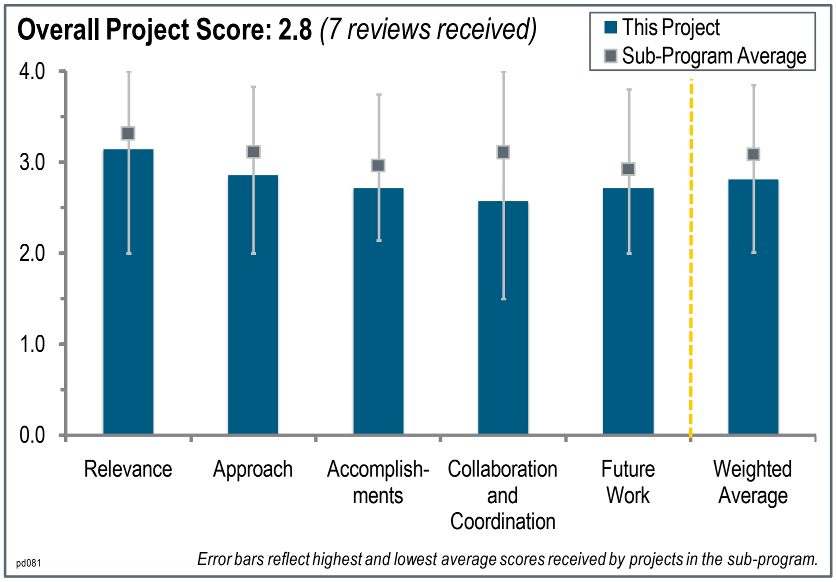
Recommendations for additions/deletions to project scope:

- This project should focus on wrapping-up efforts involving system optimization and rough cost estimates of existing WGS catalysts and zeolite systems, rather than exploring new materials.

Project # PD-081: Solar to Hydrogen Production with a Metal Oxide Based Thermochemical Cycle

Nathan Siegel; Sandia National Laboratories

Brief Summary of Project:



The overall objective of this project is to develop a particle-based thermochemical reactor for efficient solar hydrogen production. The successful development of this reactor will provide a solar interface for most two-step, non-volatile metal oxide cycles considered to be among the most efficient solar thermochemical processes. Targets are to: (1) reach $3 per gasoline gallon equivalent at the solar plant gate by 2017; and (2) achieve system-level solar-to-hydrogen production efficiency of approximately 20% (annual average) by maximizing efficiency and reducing costs. Accomplishments for fiscal year 2011 included: (1) identifying a reactor system concept capable of annual average solar-to-hydrogen production efficiency in excess of 20% (the reactor utilizes a particulate reactant to maximize kinetics and avoid issues with mechanical stress and failure); and (2) building a test platform suited to the characterization of rapid thermochemical processes.

Question 1: Relevance to overall U.S. Department of Energy objectives

This project was rated **3.1** for its relevance to U.S. Department of Energy (DOE) objectives.

- With what is currently known about economics, this technology will be hard-pressed to support Hydrogen and Fuel Cells Program objectives. The metal redox approaches appear to be the most attractive solar thermochemical hydrogen alternatives, but nonetheless face daunting obstacles that are discussed below. The economics of the project are much further from the target than believed because the target includes compression storage delivery. Also, the Hydrogen Analysis (H2A) model, while good for comparisons, ignores the total erected cost multiplier on capital, which is potentially a multiple of three on cost. This will dramatically increase the cost of implementation of these processes, which are essentially all capital.
- There is a strong relevance to achieving a solar or renewable conversion system with high conversion efficiency.
- The research effort aims to develop a particle-based thermochemical reactor for efficient solar hydrogen production. The successful development of this reactor will provide a solar interface for most two-step, non-volatile metal oxide cycles.
- In order for hydrogen to achieve its full potential as a basis for domestic and a low greenhouse gas (GHG) source of energy in the United States, solar energy should play a significant role in the production of hydrogen. A new cost-effective technology is needed for this to become possible.
- This project is one of the few down-selected options for splitting water by the use of high-temperature thermochemical cycles using concentrated sunlight as the only source of energy. The technology promises an outstanding 20% solar-to-hydrogen efficiency, versus 16% via electricity generation followed by electrolysis.
- The project objectives are in line with Program goals.

Question 2: Approach to performing the work

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

- The approach of developing a laser-heated flow cell is a critically needed step. There is a need to operate this system in a way that can replicate thousands of cycles to see how materials perform over long times.
- The reactor design causes concern. It seems that the oxygen and hydrogen gas can mix. In addition, the high-temperature operation will make it difficult for continuous operation. The high-temperature operation may have issues with materials for building a reactor that will have sufficient durability for a useful lifetime. The researchers correctly acknowledge the difficulty in moving large amounts of solids. They are spending a significant effort on modeling. The high vacuum conditions are possible, but it seems that at the high temperatures, they will have severe problems with sealing. The reviewer asks if there are any industrial processes that operate at this high temperature. Thermal cycling should add more problems.
- The project has a three-pronged approach of studying materials, developing reactor mechanical concept, and conducting system analysis. The reviewer gives the researchers high marks and credit for examining the mechanical aspects of the concept—aspects that are critical to the success of this high-temperature, moving apparatus system.
- The researchers are undertaking a three-pronged effort: (1) materials discovery and characterization aiming to evaluate the kinetic and thermodynamic performance of several reactant systems, starting with cerium oxide; (2) reactor development, including (a) testing high-temperature material compatibility, (b) using a packed bed solids conveyance, (c) incorporating advanced solar optics, and (d) building a prototype; and (3) systems analysis, including high-level performance models used to predict annual average performance.
- DOE has funded a significant amount of research over the past five years to examine the many potential routes to hydrogen production based on solar energy. The two-step metal reduction and water oxidation pathway being researched in this project was one of the most promising options. An examination of the potential solar-to-hydrogen efficiency was completed up-front to ensure it could be sufficiently high to potentially result in a cost-effective process. The project is currently focused on design and modeling of a reactor configuration and measurement of the kinetics of the cerium oxide (CeO_2) system. These are critical to the potential success of this approach. The reactor concept involves mechanical screw conveying of the CeO_2 powder. Solids handling is always problematic. Getting this approach to work at solar reaction temperatures and with very short reactor residence times will be extremely challenging. Having a system with moving parts at solar reaction temperatures is a high-risk proposition. The fact that the operation will be cycled from ambient to very high temperatures every day creates further challenges relative to seal integrities and other aspects of this moving-part reactor design. The reactor and process design rely on separating the evolved hydrogen and oxygen through the physical arrangement of the reactor. Getting good separation of these gases by this method will be very challenging. The concept requires beam-down solar optics. This requires very advanced solar optics and has a higher capital cost than other arrangements that could be used on different solar-based hydrogen concepts. The entire process operates only when the sun is shining. Previous solar-based hydrogen production research has shown that this results in the need for all of the equipment to be oversized by a factor of about three, and leads to high capital costs. It is imperative that a rough estimate for the potential hydrogen cost be done before this project proceeds much further.
- The project is well thought through, from the conceptual design of the high-temperature reactor to the laboratory evaluation of the active oxide material. As an only two-step cyclic system, it represents the simplest possible chemistry for water splitting. However, this is offset by the very high operating temperatures, which are very demanding in materials of construction and challenging in reactor design. The researchers should consider options for a continuous operation and using the oxide also as a heat storage medium.
- Although the approaches for material development and system analysis are not new, the high-temperature solar reactor design approach looks novel and worth pursuing.

Question 3: Accomplishments and progress towards overall project and DOE goals

This project was rated **2.7** for its accomplishments and progress.

- The researchers get high marks for their detailed understanding of efficiency drivers, and for beginning to make rapid cycle measurements. However, a lot of work is also going into reactor design, and the reviewer voiced strong misgivings about the reactor approach and its probability of success. A moving solid system at these conditions would be unprecedented. An industrial process operated at 0.001 bar may be unprecedented. A mechanically rotating industrial process operating in a high-temperature and low-pressure environment may be unprecedented. Keeping hydrogen from "leaking" to low-pressure zones is very difficult. This reactor might well be impossible even before the temperature is applied. Regarding process, the reviewer thinks the research team is underestimating the cost of compressing oxygen up from 0.001 atmospheres, keeping in mind that the H2A model has known weakness in that it describes only direct cost, not the total erected cost, which is typically two- to three-times higher.
- The researchers spent a significant amount of effort on modeling the system. While the models seem to be very good, the materials expectations seem very aggressive. The researchers may have problems with finding materials that can meet their expectations. They are using a screw auger to move the materials. At the extremely high temperature and the high-temperature differential (perhaps as high as a 1,000°C differential), it may be difficult for the auger to work. The materials will be going through extreme temperature stresses and will be subjected to severe reactions. Material degradation seems to be very likely. The researchers should assume they have a powder, because even if they start with pellets, disks, or felts, they will have powders in their system.
- The description and enumeration of solar energy losses is quite useful. Materials discovery work is promising, but needs to be placed in context of a full ASPEN (modeling software, computer code for process analysis).
- The principal investigators (PIs) identified a reactor system concept capable of annual average solar-to-hydrogen production efficiency in excess of 20%. The reactor maximizes kinetics and avoids issues with mechanical stress or failure. The PIs also built a test platform suited to the characterization of rapid thermochemical processes (materials development).
- There appears to have been good progress made on this particular solar cycle effort:
  - A novel laser-heated reactor for kinetic studies is operational and producing excellent data.
  - A reactor design and performance model has been developed.
  - A packed bed conveyer has been designed.
  - Solar-to-hydrogen energy efficiencies have been estimated.
- Excellent progress has been made in an overall system efficiency analysis, the design of the high-temperature reactor, and an evaluation of the redox oxide material properties in a laboratory-scale apparatus. It seems that in order to achieve the 4–20 liters per minute hydrogen for a 20-100 gram flow of CeO_2 production target, the oxide/steam system would have to function at approximately the peak hydrogen capacity rates that were seen in the laboratory experiments. There is some concern as to whether it will be possible to maintain this peak rate at the oxide flow conditions in the prototype reactor.
- It appears that the project's scope and objectives over the years have not been consistent, resulting in no obvious accomplishment from early years of the project. Nevertheless, the accomplishments of the current (2010?) objectives are impressive, especially the results on the high-temperature solar reactor design concept.

Question 4: Collaboration and coordination with other institutions

This project was rated **2.6** for its collaboration and coordination.

- It is less clear in this talk of how critical the partner interactions are, but the collaborations seem to be well in place.
- Bringing in Jenike and Johanson, Inc. (Jenike and Johanson) to do the solids material movement was a good choice. They are highly qualified for work in this area. Working with University of Colorado, Boulder and leveraging their experience is good.
- The researchers are working with Al Weimer's group at the University of Colorado, Boulder. Students are working at Sandia National Laboratories in California in the area of materials discovery and characterization. Jenike and Johanson is working on the development of particle conveyor concepts.
- The only collaboration discussed is with the University of Colorado, Boulder.

- The researchers stated that they are collaborating with Al Weimer's group, with apparently some differences of opinion, which is a positive thing, according to the reviewer. They provided design and engineering input on the solid flow reactor. There appears to be collaboration on the discovery and development of an improved oxide material, i.e., “doped” CeO_2, but its scope and level of effort were not conveyed during the presentation.
- The project needs to add more collaborators beyond the University of Colorado, Boulder. Unfortunately, the two institutions or research groups have been working on this area for so many years that, if they do not seek new ideas, they risk working in a bubble. Potential partners could be solar tower developers and outside metal-metal oxide materials scientists.

Question 5: Proposed future work

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

- The plans described in the talk are not highly detailed. With a realistic cost basis, this technology would be unlikely to overcome the cost barrier. Attention to reactor and materials is appropriate. The reviewer would have liked to have seen more explicit attention paid to highly cyclic evaluations and some of the reactor issues discussed above and in the question-and-answer session.
- The future work plans do not address the materials handling aspect of the project. The researchers need to verify that their design would not allow the hydrogen and oxygen to mix, which is not included in the future work plans. An H2A analysis that clearly differentiates between the heliostat costs and the rest of the system costs should be done.
- Testing a prototype reactor is a good step, but the reviewer would like to have a better feeling that the basic and critical operations from each part of the system are demonstrated before the project is pulled together. Perhaps that is the researcher’s plan, but it was not conveyed clearly in the presentation.
- The future work plan is excellent. It includes completing the kinetic studies, building a test prototype reactor to operate on-sun, and completing the full system design to be able to develop a solid estimate for the cost of hydrogen from this process. The proposed on-sun prototype reactor performance and hydrogen cost estimate are critical criteria for the continuation of this project.
- Further material development is proposed, but with little consideration of just what this would entail. Clearly a higher reversible capacity oxide operating at lower temperatures would be desirable, which would entail a complementary project. With the project now 80% complete in terms of funding, the reviewer asks if there will be sufficient resources for actually building and adequately evaluating the prototype on-sun reactor.
- There does not appear to be a solid pathway or even the right resources to accomplish all three proposed tasks. It requires a diverse skill set to (1) identify a practical two-step metal oxide material; (2) build and test a prototype reactor; and (3) perform detailed central-receiver-based reactor design (perhaps a beam-down concept). This reviewer recommends the project team focus on the second set of identified skills and perhaps the third set, but they should collaborate with someone else for the first skill set.

Project strengths:

- The solid redox systems are probably the best hope for solar thermochemical hydrogen.
- The researchers have the infrastructure to test the device on-sun. They have a great deal of experience in this area.
- The project is a novel system with potential for high solar-to-hydrogen conversion efficiency.
- The project demonstrates an integrated approach.
- In order for hydrogen to achieve its full potential as a basis for domestically sourced, low GHG and other emissions energy in the United States, solar energy should play a significant role in the production of hydrogen. New cost-effective technology is needed for this to become possible. DOE has funded a significant amount of research over the past five years to examine the many potential routes to hydrogen production based on solar energy. The two-step metal reduction and water oxidation pathway being researched in this project was one of the more promising options. There appears to have been good progress made on this particular solar cycle effort. The future work plan is excellent. It includes completing the kinetic studies, building a test prototype reactor to operate on-sun, and completing the full system design to be able to develop a solid estimate for the cost of hydrogen from this process. The proposed on-sun prototype reactor performance and hydrogen cost estimate are critical criteria for the continuation of this project.

- The project demonstrates the inherent simplicity of the chemistry (only a two-cycle system). There is also the potential (with considerably further work) of new and improved oxide materials. There are seemingly realistic high thermal and solar efficiencies.
- The project has a novel and interesting reactor design.

Project weaknesses:

- The project economics are very challenging. Materials were not evaluated under multi-cycle conditions, and the researchers have yet to show a promising reactor design.
- The reactors are operating at extremely high temperatures and will have issues with materials compatibility, materials durability, and seals. They have moving parts to move the physical materials at extremely high temperatures and move the materials over a large temperature and pressure range. The high temperature of operation will not allow continuous operation with existing or projected thermal storage technologies. They may have problems with hydrogen and oxygen mixing because the gases are not in separate chambers.
- This is a complex system with extremely high temperatures and high-temperature moving parts. Separation of hydrogen and oxygen through the column has not been demonstrated or described to the reviewer's satisfaction. This system operates on vacuum, necessitating high-capacity vacuum pumps, which are costly and energy intensive.
- It would be helpful to see a Gantt chart—a timetable with milestones for the various tasks undertaken—and to measure progress against this timetable. Without it, there is no indication or ability to assess how effective these efforts are and how long this project would last. The PI stated that there were frequent program-demanded redirections and, therefore, discontinuities in the work effort. This may be the case; however, it would still be useful to have a picture of the totality of the work undertaken and the milestones reached or abandoned in the course of the seven-year, $3.5 million expenditure.
- The reactor concept involves a mechanical screw conveying of the CeO_2 powder. Solids handling is always problematic. Getting this approach to work at solar reaction temperatures and with very short reactor residence times will be extremely challenging. Having moving parts at solar reaction temperatures is a high-risk proposition. The fact that the operation will be cycled from ambient to very high temperatures every day creates further challenges relative to seal integrities and other aspects of this moving-part reactor design. The reactor and process design rely on separating the evolved hydrogen and oxygen through the physical arrangement of the reactor. Getting good separation of these gases by this method will be very challenging. The entire process operates only when the sun is shining. Previous solar-based hydrogen production research has shown that this results in the need for all of the equipment to be oversized by a factor of about three, leading to high capital costs. It is imperative that a rough estimate for the potential hydrogen cost be done before this project proceeds much further. The only collaboration discussed is with the University of Colorado, Boulder.
- The sought-after improved oxide materials would require a substantial complementary effort (essentially another project) by investigators having specific expertise in inorganic and solid state chemistry.
- The project team does not appear to have a full grasp of the huge hurdles in bringing this technology to commercialization. The combination of current concentrated solar power central receiver technology and a high-temperature electrolizer is much simpler and closer to the 20% solar-to-hydrogen efficiency than the project team realizes. This type of system already exists or is being demonstrated, requiring fewer steps, simpler operation, and no need to wait for a ideal material. The project has mechanical moving parts at 1,500°C. The project relies on the huge pressure drop (100 Pascal to 1 atmosphere over relatively open space) for hydrogen-oxygen separation, which is not trivial. The reviewer notes the project has complete reliance on future breakthrough metal oxide material cycle for commercialization of concept.

Recommendations for additions/deletions to project scope:

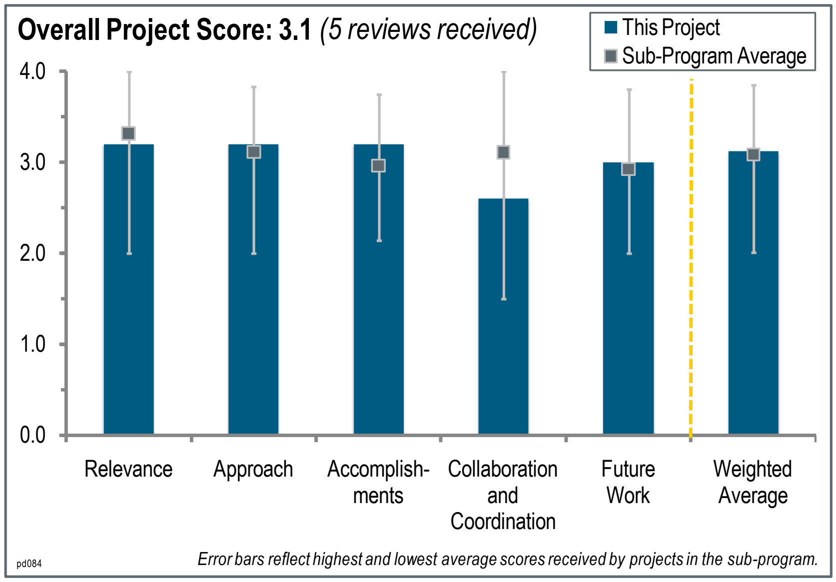
- The future work plans do not address the materials handling aspect of the research. The researchers need to verify that their design would not allow the hydrogen and oxygen to mix, which is not included in the future work plans. There should be an H2A analysis that clearly differentiates between the heliostat costs and the rest of the system costs. In models, the researchers should predict the heat-up time for the system. This may turn out to be important because the device is not in use continuously. It will probably be highly insulated so the temperature should not decrease too much, but it will have to be reheated. This heat-up time needs to be subtracted from the useful time on stream for hydrogen production. The researchers need to do cycling tests with

their materials. The tests need to examine both temperature and pressure effects jointly to determine if the pellets, felts, etc., are stable or if they break down.
- The researchers need to conduct full system ASPEN analysis and component tests prior to reactor demonstration. A demonstration of how the gases will be separated is needed. They need to further explore how the vacuum system will be maintained and how the pumps scale in size and cost.
- At least a rough estimate for the potential cost of hydrogen from this process should be completed before this project proceeds much further.
- The researchers need to consider ways in which hydrogen production could be extended beyond sunlight hours using some form of thermal storage—perhaps by somehow storing the very hot oxide.
- The project requires a diverse skill set to: (1) identify a practical two-step metal oxide material, (2) build and test a prototype reacto, and (3) perform detailed central receiver based reactor design, with perhaps a beam-down concept. The reviewer recommends the project team focus on the second skill set identified above for now and perhaps the third, but it should collaborate with someone else for the first identified skill set.

Project # PD-084: Advanced Hydrogen Transport Membranes for Coal Gasification

Joseph Schwartz; Praxair

Brief Summary of Project:



The overall objective of this project is to develop advanced energy technologies to facilitate the use of coal or coal biomass and to demonstrate the separation of hydrogen from coal or coal-biomass derived syngas. Phase one goals are to: (1) demonstrate hydrogen transport membrane (HTM) performance integrated with a coal gasifier to produce at least 2 pounds (lb) per day of hydrogen; (2) develop a contaminant management strategy; (3) develop an HTM manufacturing process; and (4) develop an improved process for integrating HTM into coal gasification. All goals are based on scaling-up HTM technology and integrating it with gasification to produce power and hydrogen while reducing carbon dioxide (CO_2) emissions.

Question 1: Relevance to overall U.S. Department of Energy objectives

This project was rated **3.2** for its relevance to U.S. Department of Energy (DOE) objectives.

- The project goals are good; however, the project is vulnerable to the cost of palladium. It is unclear whether utility-scale membrane separation will ever be commercially viable.
- The project addresses barriers related to long-term stability and flux targets for hydrogen transport membranes based on palladium alloys. Therefore, it is relevant to overall DOE objectives.
- This project clearly meets the DOE Hydrogen from Coal research program's objective of developing a cost-effective, high-performance membrane process integrated within a coal gasification cycle to produce hydrogen for energy and CO2 for capture and sequestration.
- This project supports the DOE Hydrogen and Fuel Cells Program's objectives by developing new membranes for hydrogen production.

Question 2: Approach to performing the work

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

- Just as in the fuel cell arena, where there has been a high degree of focus on reducing platinum content through reduced loading and non-platinum-group-metal catalysts, similar work should take place in membrane technologies to reduce palladium content. While the thermal cycling testing is good, the reviewer said it seems incomplete. The reviewer would like to see a membrane thermally cycled to failure in order to determine its ultimate reliability. Thermal cycles will be a fact of life in an industrial application.
- The project approach is good for developing and testing membranes that address the barriers of membrane flux, cost, and selectivity. MembraGuard seems to be working; however, there are many unknowns about it. MembraGuard is a dense layer and it not only blocks the fouling species reaching the palladium-alloy membrane, but also transports hydrogen. It may be worth investigating the hydrogen flux of MembraGuard.
- The project is focused specifically on technical barriers to commercialization, such as a focus on developing a membrane that is durable and resistant to syngas contaminants; a second focus on early scale-studies to reduce

the manufacturing cost of the membrane in order to achieve a commercially viable product; and a third focus on studying process integration options, which is important to improve the economics of the overall application. The plan to test the membrane in a slipstream from a real coal gasifier is a project strength.

- The approach to this work was considered to be good because the project appears to be focused on the development of a hydrogen transport membrane that can be tested, evaluated, and scaled. The principal investigator showed a well thought out technical approach for the development, testing, and scale-up of the membranes.

Question 3: Accomplishments and progress towards overall project and DOE goals

This project was rated **3.2** for its accomplishments and progress.

- The project appears to be on a trajectory to meet 2015 DOE flux targets. The results of MembraGuard are significant. The reviewer would like to see how many hours flux will remain stable, as it was only tested to 20 hours.
- MembraGuard significantly improved resistance to high sulfur at approximately the 200 parts per million level. Flux decreased within 15 hours of testing in a mixed gas stream. This is of great concern. Considering that this project started in October 2010, progress made so far is very reasonable. A large membrane (2 feet long) has been produced.
- This project has made excellent progress toward the objectives by focusing on the key barriers. The researchers have achieved reasonable flux with ternary palladium-alloy membranes in simulated syngas testing in the laboratory. Very important thermal cycling studies demonstrated flux stability. Production of 2-foot long membrane tubes using process techniques that are scalable was demonstrated. Studies on sulfur resistance were extensive and included both material development of the ternary alloys and demonstration of a potentially unique coating approach to sulfur poisoning inhibition (MembraGuard) through researchers' collaboration with T3 Scientific.
- The project was just started in early fiscal year 2011. However, there was a significant amount of data presented demonstrating that Praxair has made significant progress in a relatively short period of time. The consistency of test conditions among the data presented was not clear in the presentation and was questioned by the reviewers at the time. This would have been helpful to understand how the test conditions varied from test to test. While there was a lot of discussion about how palladium costs have increased recently, there was not any information provided regarding how that would affect the cost of the system. If the use of palladium is prohibitive, the researchers should provide some alternatives for its use.

Question 4: Collaboration and coordination with other institutions

This project was rated **2.6** for its collaboration and coordination.

- There is good collaboration with T3 Scientific and the Colorado School of Mines (CSM). The partners are providing solid value.
- Collaborations are with CSM in the areas of membrane development, testing, and modeling, and with T3 Scientific in coating palladium-alloy membrane with MembraGuard. General Electric (GE) plays an advisory role. Test conditions used at CSM differ from conditions used at Praxair, and it appears that there is not sound collaboration. Each partner seems to be working independently without coordination.
- It is not clear if there is a close understanding by the prime researcher regarding the approach and results of CSM.
- The project has an excellent academic and industrial-led team working work on all technical aspects of the project, including membrane development, testing, and contaminant issues. The addition of GE as gasification process advisor is likewise valuable to meeting the project objectives.
- Collaborations with CSM, T3Scientific, and GE (only in an advisory role) seem to be going well. Representatives from T3 Scientific were at the meeting; however there were questions as to how the MembraGuard materials affected the performance of the overall membrane. There seemed to be some confusion regarding what MembraGuard was doing.

Question 5: Proposed future work

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

- The future work is generally oriented in the right direction, yet it lacks well defined goals. The reviewer would like to see firm goals set for impurity resistance, thermal cycling life, flux degradation, and palladium content reduction.
- This project appears to be effectively planning its future work in a logical manner by incorporating appropriate steps in identifying, producing, and testing palladium-alloys with high flux in mixed gas streams with good sulfur tolerance. The proposed plan to test the membrane performance in gasification stream is good.
- Tests should be made with other contaminants in addition to sulfur, which could strongly impact flux and life expectancy, therefore impacting economics.
- The future plan for phase one is a logical extension of work to prove the membrane performance in an actual gasifier stream, and especially to demonstrate the performance of the MembraGuard coating under actual gasifier conditions. An ancillary objective is to continue to make progress in membrane flux performance by continuing to identify and test new alloy compositions.
- The team has made a lot of progress in a relatively short period of time with modest amounts of funding. The go/no-go decision will have to be made on performance as well as cost information. The cost information needs to be included; however, it was likely too early in the project to do that.

Project strengths:

- The project has achieved high flux under certain conditions.
- The approach focuses on developing a membrane that is resistant to contaminants. The test plan includes testing with sulfur and other contaminants as well as life and cycling tests. There is focus on reducing manufacturing costs and improving reliability.
- Praxair has considerable experience to draw upon for this work. Development from other programs should help move this project rapidly.
- The project clearly meets the overall DOE objectives. It is well designed and managed and led by a reputable industrial gas company capable of moving the technology forward into the subsequent phases once proof of concept in phase one has been unequivocally demonstrated. Considerable progress has already been made in the laboratory toward that end. Attention in phase one to cost issues in manufacturing the membrane is a major discriminator of the project, as was the considerable attention given to sulfur tolerance with the choice of a potentially innovative coating approach yet to be demonstrated in the future on real gasifier streams. Steering of the palladium-alloy membrane development toward ternary compositions along with focus on lowering the cost is also a strength of this project.

Project weaknesses:

- Tests need to be completed to the failure point. Too many of the tests ended prematurely or appeared to be tests that are substantially gentler than actual in-field conditions.
- There was no reporting of hydrogen purity and recovery. MembraGuard's composition is unknown. Therefore, the interaction between MembraGuard and palladium-alloy membrane is unknown. This could be a problem in real-world applications.
- It is not clear if there is any long-term testing scheduled in the near future. This will strongly impact economics and feasibility and should be conducted before the larger expense of scale-up occurs. It seems that the total focus is on sulfur contamination for all teams in this area, and they are not focusing on the many other contaminant possibilities that could become a shortfall of all programs.
- All work completed to date has been at the laboratory level and with simulated flue gas compositions so the first-time testing on a real gasifier stream, critical for project success, may reveal performance surprises once real gas testing is done later in phase one of the project. For example, attention to other contaminants in the gasifier stream, such as mercury and arsenic, has not yet been done, and these constituents may force reconsideration of the contaminant mitigation options chosen for the membrane.
- Constancy of test conditions needs to be clearly described in future presentations. While this is a membrane project, it appears that the contribution of the coating of the tubes is not well understood, and there does not

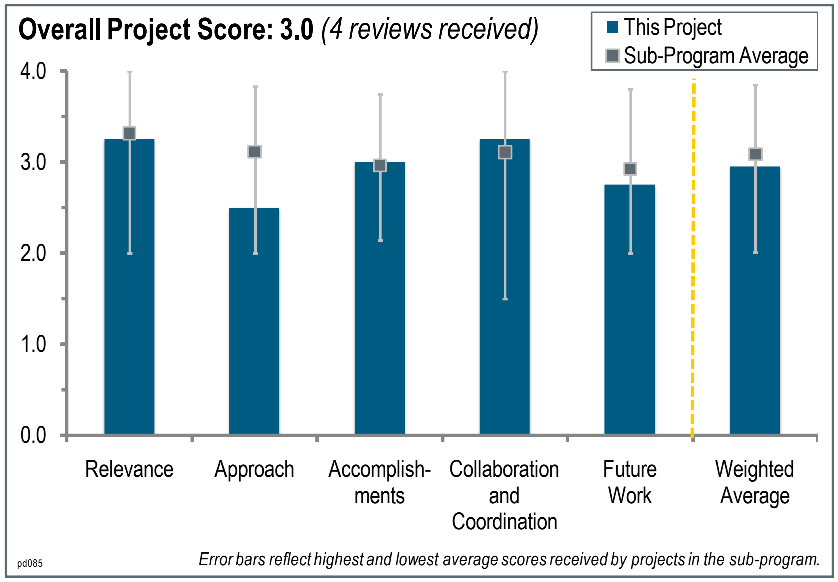
appear to be a good integration of the organization providing the coating with the membrane tube. There was discussion as to what happens at the surface and what happens as the hydrogen dissociates and is transported to the membrane through the coating. It seems that the entire membrane and coating is an important element of this work that should have some attention paid to it, as performance of the membrane “system” could actually be critical to the success of the project.

Recommendations for additions/deletions to project scope:

- It is recommended to continue to fund this project. The researchers should study the interaction between MembraGuard and the palladium-alloy membrane (inter-diffusion and intermediate phases formed at the interfaces). They should report hydrogen purity, recovery, and selectivity.
- The reviewer recommends considering adding other contaminant tests in addition to simply sulfur species.
- It is recommended to integrate small coupon testing in actual flue gas streams as part of further development work in phase one that is aimed at further optimizing membrane alloy compositions. As soon as possible, the researchers should verify the performance characteristics to define the limitations of the MembraGuard coating approach, as this may become a critical factor in contaminant control. They should definitely continue the strong focus on membrane manufacturing cost reduction.

Project # PD-085: Hour-by-Hour Cost Modeling of Optimized Central Wind-Based Water Electrolysis Production

Genevieve Saur; National Renewable Energy Laboratory



Brief Summary of Project:

The objectives of this analysis project (which represents a subset of the PD-031 project: Renewable Electrolysis Integrated System Development and Testing) are to: (1) analyze a variety of wind class sites to show a full range of hydrogen costs based on wind; (2) examine what components and factors have the biggest effect on system performance and efficiency; and (3) size components based upon hydrogen demand, wind farm size needed for that demand, and different operation scenarios.

Question 1: Relevance to overall U.S. Department of Energy objectives

This project was rated **3.3** for its relevance to U.S. Department of Energy (DOE) objectives.

- This project is performing highly valuable analysis on the renewable integration portion of hydrogen production. This is a key strength of the National Renewable Energy Laboratory (NREL) and represents good leveraging of its capabilities.
- Understanding the costs of hydrogen from renewable sources is important for the DOE Hydrogen and Fuel Cells Program in order for it to identify where research and development needs to be done to lower costs.
- Understanding the true interplay between wind and electrolysis is important in analyzing this potential hydrogen production pathway. Consequently, it is relevant to DOE's mission.
- The project does support overall long-term Program goals.

Question 2: Approach to performing the work

This project was rated **2.5** for its approach.

- This project has a well designed analysis of different wind classes, sensitivity, grid scenarios, etc.
- A large wind-based, centralized water electrolysis plant may provide a benchmark comparison to fossil-based hydrogen. However, this approach is unlikely to add value toward commercializing these systems without considering large and expensive hydrogen storage systems. Rather, a modest approach involving smaller and distributed electrolyzers with reasonable hydrogen compression and storage systems would be more valuable, as this would be the most likely scenario for early market entry.
- The assumption that hydrogen generation will be located at the renewable generation site is weak. Typical wind and solar central sites are located far from where the hydrogen is needed. For the cost analysis, the researchers assumed a Class-5 wind site with a 47% capacity factor. This is a very specialized wind site and not typical of the United States. The DOE Energy Information Administration numbers indicate that the average capacity factor is closer to 30%, which suggests that the wind cost should be much higher than what the researchers are proposing. It is not clear if the project is using electricity cost or price. Price would be a better number for this analysis. By colocating the production with the wind site, they are putting the production facilities at mostly

stranded locations. An analysis on the cost of locating the production facilities at the wind site versus locating the production facilities closer to where the hydrogen is needed should be done.
- The approach is not well defined. The researchers only state that they analyze hour-to-hour. The generation of hydrogen with wind is hampered by the hydrogen distribution costs, which are not included in the analysis. The scale of hydrogen production is not considered in the analysis; rather the size of the wind field is determined for a single set amount of hydrogen annual production.

Question 3: Accomplishments and progress towards overall project and DOE goals

This project was rated **3.0** for its accomplishments and progress.

- This project considered many different variables and aspects of the Hydrogen Analysis (H2A) model. For an analysis-only project, this category is difficult to rate because the work done does not directly make progress toward the barriers, but rather measures others' progress and shows what variables impact the cost of hydrogen. However, these analyses and comparisons by the laboratories are highly valuable in providing a neutral evaluation of the technology status.
- The hour-by-hour, cost-analysis model should be valuable for other wind- (or even solar-) to-hydrogen business evaluation scenarios.
- This project analyzed four scenarios. The scenarios chosen may not be optimal, but they cover the basic range of options. Overall, this project made a reasonable set of assumptions; however, a more meaningful analysis would be a simulation of what the industry would do. The reviewer is not convinced that any of the four cases cover that scenario. The electrolyzer runs almost constantly, which maybe should not be the case. The electrolyzer should not run if the sale price of hydrogen is less than the cost of the grid electricity used to make it.
- It is not clear why the hydrogen cost has not changed when the input electricity cost has increased, especially because electricity is the major cost contributor for hydrogen from electrolysis. The inclusion of more specific scenarios is good, and the use of time of day costing is very important.

Question 4: Collaboration and coordination with other institutions

This project was rated **3.3** for its collaboration and coordination.

- The key players, namely utilities, electrolyzer makers, and academia, are well represented.
- While several companies are listed as collaborators, most of the data is more general and from conglomerated sources such as the 2009 status report: “Genovese, J., et al “Current (2009) State of the Art Hydrogen Production Cost Estimate Using Water Electrolysis: Independent Review” 2009, NREL.”However, this is probably a better approach for this project rather than to risk bias from any of the manufacturers.
- This project has good connections with electrolyzer manufacturers and with Xcel Energy. It is not clear what the partners contributed to the project. One would think that Xcel energy would be able to provide them with better electricity cost numbers.

Question 5: Proposed future work

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

- The future work generally looks to be going in the right direction, but was a little vague on detail. The priority of the items listed is unclear. Solar will be an important comparison because there is so much going on in the photoelectrochemical area and solar technology has not come down in cost as much as wind.
- The presented work covers a basic analysis. The proposed future work is a good listing of topics worthy of investigation to understand interactions.
- This project suggests a shift from centralized to smaller distributed hydrogen systems; however, bulk hydrogen storage at this scale may not be feasible.

Project strengths:

- The project team has capabilities in modeling and access to relevant wind site data.
- The researchers have a good team that includes industry partners with expertise in fuel cells and grid electricity.
- The project's modified H2A “Wind2H2” Analysis model is valuable in this effort. The project team should consider sharing this model with other researchers, after appropriate technical review and vetting.

Project weaknesses:

- This project has no weaknesses.
- Given the cost of installing a hydrogen pipeline and the fact that the wind farm will already have a grid infrastructure in place, it seems a more likely scenario would be for the electricity to be generated by the wind towers and the hydrogen to be produced at a central or distributed location closer to where the hydrogen would be consumed, which limits the analysis. The partners’ contributions are not well identified and the roles and responsibilities are not clearly defined.
- This project only considered 50 tons per year of hydrogen generation.
- The project baseline assumption of centralized, 50,000 kilograms per day of hydrogen limits its practicality.

Recommendations for additions/deletions to project scope:

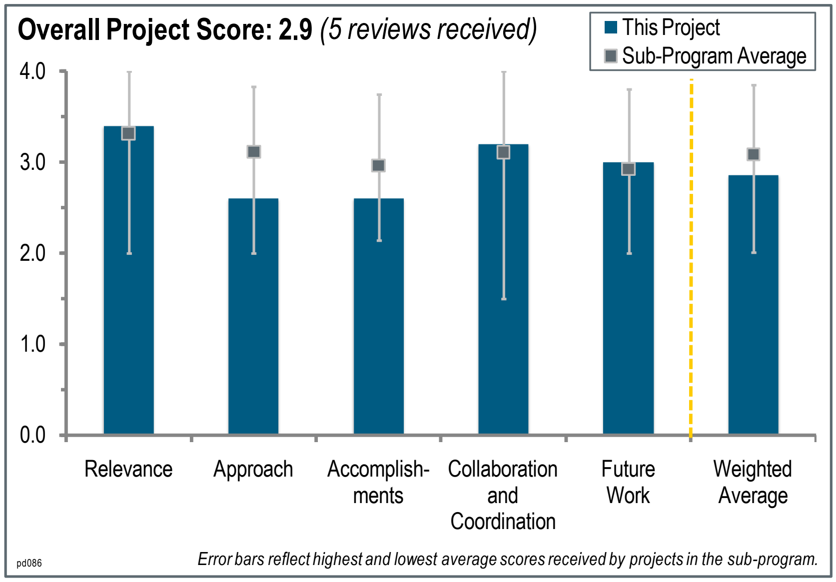
- The researchers should do an analysis looking at the cost and efficiency of locating the hydrogen production at the wind site or locating the hydrogen production closer to the city gate and using the electric infrastructure to transmit the electric power. The analysis should include the cost and inefficiencies of moving the hydrogen from the stranded locations to the city gate.
- This project should investigate whether there are some (perhaps niche) areas where wind produced hydrogen is economical from a marginal cost perspective. The wind-site generated hydrogen should be compared with the distributed electrolysis from wind electricity. These should be compared head-to-head, as the reviewer is convinced there is much difference. On-site hydrogen storage and delivery also need to be considered.
- The best bet for this technology's early market entry is a scenario of smaller and distributed hydrogen plant sizes. The project team should consider modifying the cost model accordingly.

Project # PD-086: Pilot Water Gas Shift – Membrane Device for Hydrogen from Coal

Thomas Barton; Western Research Institute

Brief Summary of Project:

The overall objective of this project is to demonstrate the separation of hydrogen from coal at the pre-engineering/pilot scale. The approach is to: (1) produce a water-gas shift (WGS) membrane device capable of 2 pounds (lb) per day of hydrogen production; (2) test the device under National Energy Technology Laboratory (NETL) protocol conditions and using coal-derived syngas; (3) demonstrate a modular fabrication suitable for larger scale; (4) scale the WGS membrane device to 100 lb/day of hydrogen; and (5) design a 4 ton/day hydrogen production unit.



Question 1: Relevance to overall U.S. Department of Energy objectives

This project was rated **3.4** for its relevance to U.S. Department of Energy (DOE) objectives.

- This project has a good balance between membrane development and reactor development that incorporates the membrane.
- This project is important to the Hydrogen from Coal research area, and it is clearly focused on DOE's technical objective of developing a cost-effective, high-performance membrane process integrated within a coal gasification cycle to produce hydrogen for energy and carbon dioxide for capture and sequestration.
- Extracting hydrogen from syngas will be critical to clean coal when carbon taxes are implemented.
- The goal of this project is to develop a device that will produce and separate 2 lb/day of hydrogen. This will include design, reactor fabrication, WGS catalyst development, membrane fabrication, and testing using a real coal gasification stream. Therefore, this project is relevant to the DOE Hydrogen and Fuel Cells Program. This team has been awarded additional non-DOE funding from the state of Wyoming to expand and transition the project toward phase two: 100 lb/day of hydrogen.
- This project supports the Program's objectives by developing new membranes for hydrogen production.

Question 2: Approach to performing the work

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

- This project's approach is good for the fabrication and testing of membranes under NETL test protocol conditions and in a coal gasification stream. It is surprising to hear that this membrane (palladium-copper thin disk supported by anodic aluminum oxide [AAO]) is immune from embrittlement by cycling between ambient and 400°C. A long-term stability study is very important before scaling-up this particular membrane.
- The intense focus on the manufacturability of the membrane and module is a good approach. Palladium-based nanoplugs offer a unique approach to the construction of the membrane active layer. The use of a structural WGS catalyst in a monolithic structure designed to direct flow may facilitate simultaneous hydrogen extraction and water-gas shift and improve the efficiency of both processes.
- The principal investigator (PI) is focused on conducting the WGS reaction in the vicinity of a hydrogen permeable membrane to drive the shift reaction toward completion. To be relevant for use in coal gasification,

tolerance to likely feed stream impurities must be considered; however, this point has been overlooked. Not only must the membrane be tolerant to sulfur and heavy metals, but the same can be said for the WGS catalyst; unless DOE guidance indicates that it is acceptable to assume these contaminants will be absent from the feed stream (the PI did not say this was the case). The reactor and membrane module design is risky; these circular geometries are inherently expensive and susceptible to non-uniform flow. The choice of using the Synkera composite membrane is risky, as this membrane has not been successfully scaled-up and is difficult to handle, brittle, and subject to fracture due to differential coefficient of thermal expansion.
- This is a very different approach to membrane design, which is beneficial to DOE for research and development risk reduction.
- The details of the approach were not well defined in the presentation materials, other than the uniqueness of the system design. While the details may be available, they were really not presented. The approach to this work was by far the most unique of all the approaches that were presented by other projects. The approach also has the most risk because the system does both the WGS and the hydrogen separation in a single unit. The concept is also quite complex from a manufacturing standpoint, and there are significant challenges in thermal cycling some of the dissimilar materials.

Question 3: Accomplishments and progress towards overall project and DOE goals

This project was rated **2.6** for its accomplishments and progress.

- Numerous laboratory tests using 1 inch AAO/palladium membranes were used to demonstrated target flux, selectivity, and reliability. The membrane fabrication approaches and equipment were scaled and a considerable amount of work was accomplished in novel fabrication approaches. The feasibility of depositing palladium-copper into the pores of the AAO membrane was established. Preliminary feasibility of structured catalyst approach for the WGS process was demonstrated in preliminary testing. No work was reported for sulfur contamination or membrane cost.
- There was a significant amount of work accomplished on this unique design in a fairly short amount of time. The Western Research Institute (WRI) team is working on several technical issues all at once. The actual system design, assembly, and manufacturability issues are being worked on while tests are being performed on small discs. The real proof of the concept will be when the prototypes get tested. There is a lot of work that needs to be done in order to compete with the other teams, which are using more conventional techniques.
- The researchers have demonstrated nearly 2 lb/day prior to the project start, which is very good. The researchers are just beginning to look at palladium-copper alloys, which is a concern because there is not much time left in the project to develop a cost-effective design.
- A 2 lb/day hydrogen device has been designed as a modular stainless steel pressure vessel containing both stacked hydrogen separation membranes and a structural WGS catalyst. The advantages of the membranes considered in this project include the resistance to cracking, presence of a joinable rim, and small amount of palladium-alloy required (low cost). The selectivity is low.
- The program is scheduled to span about 14 months and the target completion date is December 31, 2011. The data presented is extremely preliminary and the catalyst durability data is limited to 2 hours of testing. This reviewer asks why is it necessary to develop a WGS catalyst when so many are commercially available. No new membrane data from Synkera and the palladium-copper alloy membrane that is planned for this work has been made.

Question 4: Collaboration and coordination with other institutions

This project was rated **3.2** for its collaboration and coordination.

- This project has some good collaborators, but more materials expertise would be beneficial. The palladium-copper alloy being investigated will have an embrittlement problem if it is cycled between ambient and 400°C in an atmosphere containing hydrogen. Chart Energy and Chemicals (Chart) has considerable experience in engineering and fabricating large-scale devices. It is good to see a significant cost-share from the state of Wyoming.

- This project is represented by a good, multifaceted technical and commercial team. WRI conducts the WGS catalyst development and the testing of components, Chart is the engineering design and manufacturing partner that will commercialize the device, and Synkera Technologies is the composite membrane fabricator.
- For the type of system that is being considered, the team has a good set of collaborators with the appropriate expertise. Synkera is a great component for the team, and will provide significant help with some of the manufacturing and design issues that are likely to continue to occur.
- Chart Energy is in this project to develop a commercial product, which is impressive considering that the market is not likely to exist until there is a carbon tax.
- The collaborators (Chart Energy and Synkera) have good credentials, but performance has been limited. However, Synkera has lost the principal scientist (Dmitri Routkevitch) behind the membrane development work, thus its ability to be a strong contributor in the future is in question.

Question 5: Proposed future work

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

- The future plans are well defined on slides 19–22. The focus will be on additional catalyst development, large-scale membrane fabrication, high-pressure tests, and the design and construction of a 100 lb/day hydrogen device.
- Additional funding of $1.1 million from the Wyoming Clean Coal Technology Fund was announced to support this work. The development of a high-flux membrane that retains permeability under the operating conditions is key. The plan is to use a palladium-copper membrane made by Synkera. Overlaid on this is membrane scale-up. This is a lot for Synkera to do, and it has lost the primary scientist developing this membrane, making success difficult. The reviewer questions why the PI has the responsibility for catalyst development. He further questions what is deficient about commercially available WGS catalysts. In general, the future work plan neither identifies the potential technical flaws (low membrane selectivity, poor membrane durability, catalyst durability, reactor design that is expensive and subject to channeling, and mismatch in the coefficient of thermal expansion between the reactor and the membrane) nor presents an approach to correct the flaws.
- The future plans will continue to develop and scale-up the membrane to optimize performance and the WGS activity. The addition of $1 million in funding from the state of Wyoming will permit more extensive development work to be done in phase one, such as additional catalyst development, the development of larger-scale membranes, and higher-pressure testing and economic analyses. Syngas impurities and poison issues will be addressed using traps capable of regeneration. The membrane required for 2 lb/day testing will be fabricated and tested in the 35 lb per hour coal gasifier facility available at WRI.
- The funds from the state of Wyoming will help transition to phase two. Durability work is planned in the future, but should be done sooner rather than later.
- This project has more work to be done in order to get to the point where it can test a small-scale system. While this reviewer applauds the uniqueness of the researchers' work, it may be difficult to get to the point where they can really compete effectively for the next phase of work. The researchers understand what they are up against, and they will strive to have a working system that can compete with the other projects for the go/no-go decision. The project has received a modest amount of additional funding from the state of Wyoming, which may help them to accelerate the needed progress.

Project strengths:

- This project has good collaborative team work. The phase one effort is on schedule and there is significant cost-share by a non-DOE source. This project will be using actual gasifier feeds to test its membranes, thus being able to identify contaminant performance before proceeding to the 100 lb/day device.
- This program stands out as the only one to direct work at a combined reactor and separator. The team is qualified, but the Synkera team is weakened by the loss of Dr. Routkevitch.
- DOE's support is highly leveraged by funding from the Wyoming Clean Coal fund to permit more extensive membrane development for a smoother transition into phase two. Chart is a key collaborator who would become the commercialization entity for the membrane being developed by WRI in this project. WRI has its own coal gasifier facility to facilitate the required 2 lb/day tests.

- The membrane design is both a strength and weakness of this project. The membrane WGS modules that WRI has conceived are very unique and show a lot of promise. There are a number of significant technical issues that the team seems to understand need to be resolved. In particular, some of the manufacturing and thermal cycling challenges could prove to be difficult, but the PI seems to have a grasp of those issues. Hopefully, those issues will not impede progress toward testing the system.
- The doughnut membrane design is very unique.

Project weaknesses:

- This project lacks significant membrane materials expertise. The selectivity is low and embrittlement will be an issue if cycled between ambient and 400°C. There are no plans to look into alternate membrane materials and there are a lack of flux numbers in the presentation (one slide did have this, but the value is low).
- The proposed plan is very ambitious for the time and money awarded. The Synkera membrane is a risky choice and substantial further development is needed before this membrane selection can be viewed as technically viable. Modularization of the membrane will be very challenging due to inherent brittleness and a mismatched coefficient of thermal expansion (the membrane is based on microporous aluminum oxide sheets and the module is steel, which has very different degrees of thermal expansion). There are no plans to make the WGS catalyst and the membrane tolerant to sulfur and other feed stream contaminants from the coal gasifier. The module design is inherently expensive and subject to flow nonuniformity. The donut/cylindrical reactor design is very similar to the membrane module designs from Bend Research, ATI Wah Chang, Protonex, and LG Electronics, some of which are almost 20 years old.
- The membrane fabrication approach is complex and may be difficult to scale as well as too costly. No definitive plan for conducting the 2 lb/day testing was presented, and it appeared that considerable development work remains before the first test can be initiated. The approach of trapping contaminants may carry a large parasitic energy and cost burden that needs to be addressed.
- This project is unique, which makes it a target for weaknesses. It will be difficult to get this technology ready in time for the go/no-go decision that will be coming later during the down-select process. It is likely that they will be hard pressed to be in a position to be able to demonstrate their system against the other projects for the down-select. Some basic mechanical system issues need to be resolved before a system that is ready to be tested can be completed. The cost of this system may also prove to be a difficulty of this approach. While no cost numbers were provided, it is likely that this system will be more expensive than traditional membrane technologies in a WGS reactor.
- The doughnut membrane design is going to make manufacturing and scale-up a very challenging task.

Recommendations for additions/deletions to project scope:

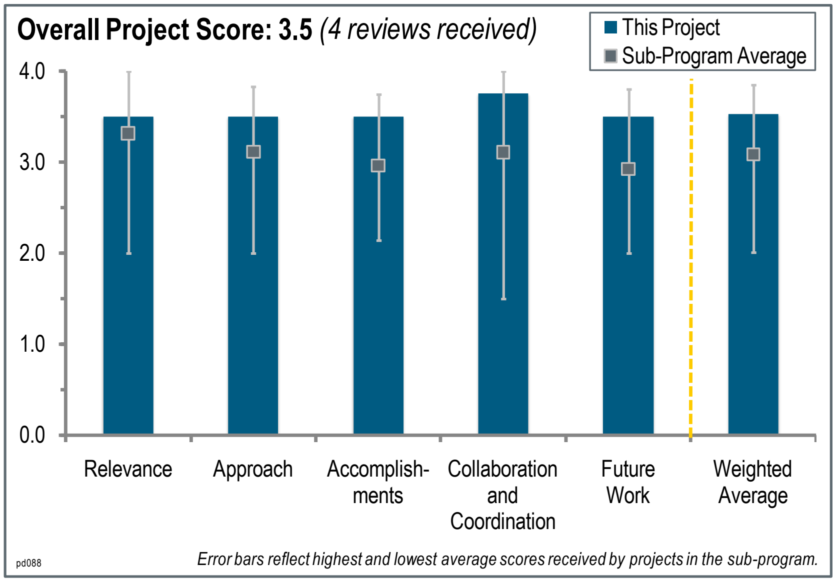
- This project should test the membrane's stability against trace contaminants before proceeding to test the 2 lb/day device. This project should also have a strong backup plan to develop stable membrane materials, and the flux and selectivity needs improvement.
- The project scope is too ambitious and should be scaled back to either catalyst design (composition and form factor) to achieving sulfur and heavy metal tolerance in an appropriate reactor design, or further development of the Synkera membrane. The reviewer believes the Synkera membrane will take more time than is presently scheduled to satisfactorily achieve scale-up and durability (to sulfur and heavy metals, plus coefficient of thermal expansion mismatch).
- The experimental verification of sulfur tolerance limits should be shown, as well as effects of other contaminants. The emphasis appears to be on extensive further membrane development, but phase one should be refocused to include activity directed to testing and verifying the membrane performance in real coal gasifier streams to establish a preliminary feasibility of the concept. Assessing membrane costs should be accelerated to verify the economic feasibility.
- The project needs to remain focused and work with a "sense of urgency" to be able to be in a position to make the go/no-go down-select decision.
- This project should initiate the durability testing as soon as possible.

Project # PD-088: Vessel Design and Fabrication Technology for Stationary High-Pressure Hydrogen Storage

Wei Zhang; Oak Ridge National Laboratory

Brief Summary of Project:

The overall project objective is to develop designs and fabrication technology for a cost-effective, high-pressure hydrogen storage system for stationary applications. Specific objectives during the current project year are to: (1) develop a conceptual engineering design of a bulk storage vessel for hydrogen capable of sustaining 5,000 pounds per square inch design pressure; and (2) demonstrate technical proof-of-feasibility for key design concepts and construction technologies.



Question 1: Relevance to overall U.S. Department of Energy objectives

This project was rated **3.5** for its relevance to U.S. Department of Energy (DOE) objectives.

- The barriers and gaps are identified and tie into the DOE Hydrogen and Fuel Cells Program goals and objectives needed to meet the intended stationary hydrogen storage. A 60% reduction in cost is required. The project's objectives are focused on meeting the American Society of Mechanical Engineers (ASME) codes and standards while also meeting the targets.
- There was an excellent presentation of the project's motivations, goals, and objectives. Large stationary storage tanks will be required, and understanding the hydrogen-modified properties of the construction materials and designing to account for these is an interesting challenge. Also, proof-of-concept and qualification testing of these tanks will be critical to the economic success of hydrogen as a fuel for vehicles.
- This project offers a potential low-cost technology for stationary hydrogen storage.
- Cost-effective storage is a key component of the program.

Question 2: Approach to performing the work

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

- It is good to see that the project is looking at three design considerations to establish the best and most economical approach. The investigators are addressing the critical barriers and taking a logical approach compared to other similar approaches currently being used in industry.
- Planning a full mock-up design, fabrication, and testing is a good approach, and condition monitoring is a good solution to remaining uncertainties. It is a great idea to evaluate this at the same time.
- This project has a good approach, using low-cost steel and low-cost concrete together to find a low-cost combined solution for hydrogen storage.
- The unique design approach, based on previous pressure vessel work combined with an innovative use of concrete, is a strength of the project.

Question 3: Accomplishments and progress towards overall project and DOE goals

This project was rated **3.5** for its accomplishments and progress.

- The progress looks very promising, and it seems that this work will be successful upon completion of the project.
- The presentation suggested that all critical barriers have been considered and will be addressed and eventually overcome. It may be early, but this project appears to have a good plan. The four-cylinder array looks viable, but the reviewer was curious as to why the researchers had not considered a close-packed hexagonal array.
- This project has not produced real results yet, and is still just beginning.

Question 4: Collaboration and coordination with other institutions

This project was rated **3.8** for its collaboration and coordination.

- This project has an excellent plan for collaboration with industry and universities. Also, the researchers discussed working with ASME pressure vessel codes and the relevant ASME committees during the presentation. This will be a vital part of making sure that any recommended designs that meet the DOE's economic and technical goals for stationary storage also meet current code requirements.
- There is good cooperation among the national laboratories and private industry to accomplish the goals of this project.
- This project's extensive collaboration is a strength.
- This project has an acknowledged working relationship with other industries and federal agencies along with industry partners.

Question 5: Proposed future work

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

- The project is just getting started and most of the work remains to be done. The principal investigator gave good indications regarding his plans for testing and qualification, which seems appropriate and comprehensive. He also referred to collaboration with other national laboratories, such as Sandia National Laboratories (SNL), that are experienced in this area.
- This project has a large and complex plan. The investigators need to make decisions and take action to stay on target.

Project strengths

- This project has an excellent approach and work scope.
- This project has an excellent plan for coordinated work between DOE, industry, and universities. This is a relevant problem to tackle and the researchers have proposed a reasonable approach to reducing stationary storage costs.
- Collaboration and innovative plans based on industry experience are strengths of this project.

Project weaknesses

- The researchers need to communicate project goals and objectives to the U.S. Department of Transportation Pipeline and Hazardous Materials Safety Administration, Hazardous Materials Safety Program Office. The qualification of vessels needs to include standards and system reliability over time for possible pressure cycling.
- This project has many complex issues with multiple laboratories that have different priorities collaborating. Keeping all parts working together toward the common goal will be challenging. The project has a large number of different paths it could take and decisions will need to be made early with all entities in essential agreement for the project to continue to progress smoothly.

Recommendations for additions/deletions to project scope

- The project team should clearly identify decision points on the path to the successful conclusion of the project and make sure all parties in the study are familiar with the decision points (reason for, and timing) and input expected from each team member for each decision. The researchers then need to make sure they have enough time to make their contributions and participate in the decision-making process.
- Close collaboration with SNL is recommended because it is doing so much tank qualification work now.